Proceedings of the International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS – 2024)

In commemoration of National Science Day

21 – 22 February, 2024

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Organised by

PG & Research Department of Physics
Sri Vidya Mandir Arts & Science College

(Affiliated to Periyar University, Salem)

(Recognized under Section 2(f) & 12(B) of the UGC Act, 1956)

(Accredited by NAAC with 'A' Grade [CGPA = 3.27])

Katteri – 636 902, Uthangarai, Krishnagiri, Tamil Nadu, India

In association with

Indian SpectroPhysics Association (ISPA), Chennai, India

Editor– In - Chief

Dr. R. Arivuselvi

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Katteri – 636 902, Uthangarai, Krishnagiri District, Tamil Nadu, India

PG & RESEARCH DEPARTMENT OF PHYSICS

Dr. R. ARIVUSELVI

Convenor, ICREAMS – 2024

Assistant Professor and Head

PREFACE

First and foremost I extend my heartfelt gratitude to all participants of the **International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS 2024)** held on February 21st and 22nd, 2024, at Sri Vidya Mandir Arts & Science College (Autonomous), Katteri, Uthangarai, Tamil Nadu, India. The conference serves as a global platform to share vital research findings, methodologies, and knowledge in the rapidly advancing field of modern materials. With about 118 submissions covering 29 relevant topics, we aim to make this an annual event and anticipate your enjoyment of the ICREAMS 2024 proceedings. Special thanks to all authors for their contributions, ensuring the success of ICREAMS 2024.

I express sincere appreciation to all conference presenters and acknowledge the unwavering support of **Thiru. V. Chandrasekaran**, Founder of Sri Vidya Mandir Group of Educational Institution, Uthangarai, and **Dr. S. Gunasekaran**, President of ISPA, for their valuable suggestions and ideas. My gratitude extends to our Principal, **Dr. N. Gunasekaran**, and Vice Principal, **Dr. D. Kavitha**, for their invaluable guidance and permission to host this conference. Lastly, I thank the faculty members and students of the PG and Research Department of Physics for their cooperation, ensuring the grand success of the conference.

R. ARIVUSELVI

Convenor, ICREAMS 2024

About the College

The visionary philanthropists of Sri Vidya Mandir Higher Educational Trust started Sri Vidya Mandir Arts & Science College in Uthangarai in the year 2000 with a noble aim of uplifting the Economically and Educationally Backward districts of Dharmapuri and Krishnagiri into the number one educational destination in Tamil Nadu. The college is surrounded by the culturally rich pilgrimage centers Hanuman Theertham (2 Km) and Theerthamalai (15 Km) associated with the famous epic, the Ramayana. The college is well – connected with nearby cities and is located in the Salem – Vellore state highways. Currently the college has attained the strength of more than 3500 students, 134 Faculty members, and 123 non – teaching staff members. Our College secured highest CGPA score in NAAC ('A' Grade, 3.27/4.00) among the Periyar University affiliated colleges in the first cycle and also recognized with the same till the year of 2025. Now our college has accomplished with the status of Autonomous from the academic year 2020 - 2021.

About the Department

The Department of Physics was started in the year 2000 in order to motivate the rural students to provide higher education in the field of Science. The Department offers UG, PG, M.Phil and Ph.D Programmes. 22 Gold medals and 131 other ranks were procured by our students from the Periyar University. The Department had successfully organized more than 35 State/ National/ International level Conferences/ Workshops/ Seminar/ Inspire Camps/ Webinars/ Special Lectures with the financial assistance of diverse leading funding agencies of Government of India, Government of Tamil Nadu and noteworthy contributions from the College Management. A recent unique accomplishment of the Department is that it has been sanctioned with the FIST (Funds for Infrastructure Development of Science and Technology) grant by the prime funding body of the Government of India, Department of Science and Technology.

About ISPA

Indian SpectroPhysics Association (ISPA) is a brain child of Veteran Professor and Scientist Dr. S. 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 84 ISPA Dr. S. 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. Annual and Life Team Membership forms can be availed from the website.

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- Magnetic Materials
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- Molecular dynamics
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Thiru. V. Chandrasekaran
Founder

MESSAGE

It is with great pleasure and anticipation that I extend a warm welcome to the **International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS 2024).** This conference represents a pivotal moment for the scientific community as we gather to delve into the latest research, innovations, and discoveries in the fields of materials science and spectroscopy.

ICREAMS 2024 provides a unique platform for scholars, researchers, and industry professionals to exchange ideas, foster collaboration, and shape the future of these rapidly evolving disciplines. As we embark on this journey of exploration and knowledge sharing, I extend my heartfelt gratitude to the organizing committee, distinguished speakers, sponsors, and attendees for their invaluable contributions towards making this conference a success. I encourage each of you to seize this opportunity to engage in meaningful discussions, forge new connections, and inspire one another towards greater heights of excellence.

I wish you all a stimulating and rewarding conference experience.

Thiru. V. Chandrasekaran
Chief – Patron, ICREAMS - 2024

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Dr. N. Gunasekaran
Principal

MESSAGE

It is with great pleasure that I extend a warm welcome to all of you to the **INTERNATIONAL CONFERENCE ON RESEARCH IN EMERGING ADVANCED MATERIALS AND SPECTROSCOPY (ICREAMS - 2024).** This conference serves as a platform for scholars, researchers, and students alike to converge, exchange ideas, and explore the latest advancements in the fields of materials science and spectroscopy. As we embark on this journey of knowledge dissemination and collaboration, I encourage each of you to actively engage in the discussions, presentations, and networking opportunities that this conference offers. Let us collectively strive to push the boundaries of scientific inquiry and innovation, with the ultimate goal of contributing to the betterment of society. I am confident that ICREAMS - 2024 will be a resounding success, thanks to the dedication and expertise of our organizing committee, presenters, and participants. May this conference inspire new discoveries, foster meaningful connections, and pave the way for future breakthroughs in the field.

I wish you all a fruitful and enriching experience at ICREAMS – 2024.

Dr. N. Gunasekaran

Patron, ICREAMS – 2024.

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Dr. D. Kavitha
Vice – Principal

MESSAGE

I am immensely glad that the Department of Physics is organizing the INTERNATIONAL CONFERENCE ON RESEARCH IN EMERGING ADVANCED MATERIALS AND SPECTROSCOPY (ICREAMS – 2024).The field of Science is evergreen and its applications keep increasing to quench the thirst of human comforts. In this ever changing field of technical education, technology is breaking through rapidly needing the scientist to update the knowledge and recent trends in innovations then and there. Hence there has been a need in today's competitive world to keep updated for the latest technologies in the emerging field of electronics.

The International Conference focuses on 3C's "Compute - Communicate - Control", which deals with the idea of recent advancements in many technologies. The International Conference targets on imparting the knowledge on high quality advancements in the field of Engineering, Science and Technology.. This Conference brings together leading researchers and students in the domain of interest nationwide to a common forum helping the delegates to present and share their experience and also to explore new avenues of thoughts. I know that the success of the conference depends ultimately on the many people who have worked with us in planning and organizing both the technical program and supporting social arrangements.

Recognition should go to the Local Organizing Committee members who have all worked extremely hard for the details of important aspects of the conference programs and social activities. This International Conference is a platform encouraging multiple disciplines of engineering and its applications leading to a large leap in research activities at our institute. It's my heartfelt gratitude to be a part of this institution and my best wishes for the conference and all the participants of the conference.

Dr. D. Kavitha

Dr. S. Gunasekaran, M.Sc.,Ph.D.,D.Sc.
TANSA Awardee
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Avadi, Chennai – 600 054. Tamil Nadu, India.
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Founder President, Indian Spectrophysics Association (ISPA)
Former Registrar, Periyar University, Salem
Former Head, Department of Physics, Pachaiyappa's College, Chennai.

E-mail: deanresearchspu@gmail.com

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

18.02.2024

Prof. S. Gunasekaran
Dean, Research & Development

PROLOGUE

I am honored to extend my heartfelt welcome to each one of you in this momentous occasion. We find ourselves at the threshold of the International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS 2024), an event that promises to be a hallmark in the realm of scientific inquiry.

ICREAMS 2024, meticulously orchestrated by the PG and Research Department of Physics at Sri Vidya Mandir Arts & Science College (Autonomous), Uthangarai, in collaboration with the Indian SpectroPhysics Association (ISPA), stands as a testament to the relentless pursuit of knowledge and innovation. It is a platform where the brightest minds converge, sharing their insights and discoveries to illuminate the path forward. ICREAMS 2024 recognizes the pivotal role spectroscopy plays in advancing our understanding of the world, and it seeks to push the boundaries of what is possible.

The Indian SpectroPhysics Association (ISPA) dedication to promoting excellence in spectroscopy and its unwavering support for scientific endeavors are truly commendable. Their partnership has been invaluable, and we are grateful for their commitment to the cause.

Over the course of two days, ICREAMS 2024 will serve as a crucible for ideas, a forum for discourse, and a launchpad for collaborations. It is here that researchers, scholars, and students will come together to explore the latest developments in spectroscopy, igniting new conversations and sparking innovative solutions to some of the world's most pressing challenges.

In my capacity as the President of the Indian SpectroPhysics Association (ISPA), I am deeply gratified to be part of this event. ICREAMS 2024 is a testament to our shared vision of advancing the frontiers of spectroscopy and nurturing the next generation of scientific trailblazers. As we embark on this intellectual odyssey, I extend my sincerest gratitude to all the participants, organizers, and sponsors who have made ICREAMS 2024 possible. Together, we shall illuminate the path toward a brighter, more enlightened future through the lens of spectroscopy.

My heartfelt felicitations extend to our esteemed Chief Patrons, including the erudite **Thiru V. Chandrasekaran, Founder, Sri Vidya Mandir Group of Institutions** and the illustrious Patron **Dr. N. Gunasekaran, Principal.** I must also extend my commendations to the Convenor, **Dr. R. Arivuselvi, Head, PG and Research Department of Physics** along with the entire organizing committee.

Welcome to ICREAMS 2024, where the fascinating world of spectroscopy awaits your exploration.

Dr. S. Gunasekaran
Founder President, ISPA

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Dr. M.N. PONNUSWAMY, Ph.D., D.Sc.,
Emeritus Professor

18-02-2024

MESSAGE

It gives me immense pleasure and delightfulness to wish Sri Vidya Mandir Arts & Science College, Uthangarai & Indian SpectroPhysics Association (ISPA). Sri Vidya Mandir Arts & Science College is a revered and dignified Institution with a significant foresight of its contribution to society and Academic. The college aims at make the students equal in first hand perseverance knowledge and make the knowledge to have an impact on Society. Likewise, the PG & Research Department of Physics, Sri Vidya Mandir Arts & Science College, Uthangarai which has a very distinguished, well-knitted and framed curriculum with the association of ISPA now has arranged an **International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS-2024)** between 21 and 22 February 2024 which covers all the aspects and Research areas of Spectroscopy and Materials Science, etc. I have no doubt that the conference will help the institutions as well as the students to create a platform for their research areas and new findings. I wish and hope for the Conference a grand success to serve for the betterment of the society.

On this occasion, I express my sincere wishes to the **Chief Patron Thiru V. Chandrasekaran, Founder of Sri Vidya Mandir Group of Institutions, Patrons, Dr. N. Gunasekaran, Principal, Dr D. Kavitha, Vice Principal** and would like to congratulate the **Convener of the Conference Dr. R. Arivu Selvi**, Members of the Scientific and Technical Committee, Faculty Members, Research Scholars and PG Students of Physics for the successful conduct of the conference and wish the event every success.

(M N Ponnuswamy)

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DEPARTMENT OF PHYSICS

Dr.M.Selvapandiyan M.Sc., M.Phil., Ph.D
Professor and Head

Date: 15.02.2024

It gives me great pleasure to note that **PG & Research Department of Physics,** Sri Vidya Mandir Arts and Science College, Uthangarai in collaboration with Indian SpectroPhysics Association (ISPA), Chennai, India is organizing an **International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS - 2024)** in commemoration of National Science Day between 21 and 22 February 2024. An international Conference is well-timed one and my best wishes to the convener **Dr. R. Aivuselvi,** Head, **PG & Research Department of Physics,** Sri Vidya Mandir College of Arts and Science College, Uthangarai, Tamil Nadu for being a successful skipper in uniting her team to bring out this scientific mega event as a victorious one. Also I convey my heartfelt wishes to Honourable Secretary **Mr. V. Chandirasekaran** for taking effort and interest to motivate the faculties to organize a useful conference for the development of Students and as well as Nation. I extend my wishes to **Dr. N. Gunasekaran,** Principal for his passionate way of approaching the faculties and support to organize the **Advanced Materials and Spectroscopy** oriented conference

This conference, will hope, create an opportunity for Students, participants and young researchers to interact with Eminent Professors, Scientists and Scholars in the fields of Materials Science and Spectroscopy, share their ideas and progress. It will also initiate them into the ins and outs of research. I wish the conference a very insightful deliberation that will push the frontiers of knowledge and a grand success. I really congratulate **Prof. Dr. S. Gunasekaran, Founder President, ISPA,** Chennai, Tamil Nadu, India and his team for organizing series of conference for the development of young students and faculty members of Physics of SVM worked behind the screen of an International Conference.

(Dr.M.Selvapandiyan)

INTERNATIONAL CONFERENCE ON RESEARCH IN EMERGING ADVANCED MATERIALS AND SPECTROSCOPY

(ICREAMS - 2024)

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- Drug Design
- Instrumentation
- Characterization Methods
- MEMS Design
- Optoelectronic Devices
- Superconducting Materials
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- Theoretical Physics
- Crystal Growth
- Medical Physics
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Dr. Muthu Senthil Pandiyan, Chennai
Dr. J. Balavijayalakshmi, Coimbatore
Dr. B. Venkatram Reddy, Warangal
Dr. G. Anbalagan, Chennai
Dr. M. Selvapandiyan, Dharmapuri
Dr. L. Jothi, Namakkal
Dr. M. Jose, Tirupattur

Invited Speakers

Prof. Irena Kostova, Ph.D., D.Sc.

Professor, Faculty of Pharmacy
Medical University, Sofia
Bulgaria

Prof. Jiban Podder, Ph.D., F.B.A.S.

Professor, Department of Physics
Bangladesh University of Engineering and Technology
Dhaka, Bangladesh

Prof. M.N. Ponnusamy, Ph.D., D.Sc.

Emeritus Professor, Centre for Advanced Study in Crystallography and Biophysics
University of Madras, Chennai

Prof. S. Gunasekaran, Ph.D., D.Sc.

Dean (R&D)
St. Peter's Institute of Higher Education and Research
Chennai

Prof. Debashish Bhattacharyya, Ph.D.,

Deputy Director (Retd.)
Indian Institute of Chemical Biology
Jadavpur, Kolkata

Prof. C. K. Jayasankar, Ph.D., F.N.A. Sc.

Emeritus Professor, Former UGC-BSR Faculty Fellow
Department of Physics
Sri Venkateswara University, Tirupati

Prof. Byru Venkatram Reddy, Ph.D.

Professor, Department of Physics
Kakatiya University
Warangal

Prof. M. Selvapandiyan, Ph.D.,

Professor, Department of Physics
Periyar University Centre for PG & Research Studies
Dharmapuri

Dr. S. Srinivasan, Ph.D.,

Associate Professor, Department of Physics
Presidency College
Chennai

Dr. S. Kumaresan, Ph.D.,

Associate Professor, Department of Physics
Arignar Anna Government Arts College
Cheyyar

Dr. P. Janani, Ph.D.,

Instructional Designer Head (Academics)
Echtian Contents Private Limited
Mumbai

Food for Thought

On February 7, 1928, Krishnan confirmed the presence of "weak fluorescence" in a number of organic liquids and vapours. Two days later, Raman and Krishnan detected the new radiation in vapours of ether and amylene. On February 28, 1928 Raman and Krishnan examined the influence of the wavelength of the incident light on the phenomenon, To their surprise, they found that the modified scattering was separated from the scattering corresponding to the incident light by a dark space leading to the discovery of Raman Effect.

The apparatus used by Raman for his discovery would not have been more than Rs. 300. The discovery was not the result of an accident, but was the culmination of seven years of systematic and sustained work carried out with devotion by Raman and his band of students leading to the commemoration of National Science Day Celebration.

Call for Abstracts

The Organizing committee invites original research papers for oral and poster presentation. Authors are requested to send the abstract not exceeding 300 words in the prescribed font (Times New Roman, Font - 12 points and 1.5 lines spacing) to the mail svmcphyicreams2024@gmail.com on or before 10- 02- 2024 Papers will be accepted for presentation based on the recommendation of the panel of referees and the full length of the selected papers will be published in the proceedings with ISBN number. The full length paper will be published in the International Journal of Science, Technology and Humanities (INJSTH).

Last Date for Abstract submission	**: 29.01.2024**
Last Date for full Length Paper Submission	**: 10.02.2024**

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ISPA Awards

ISPA Veteran Scientist Award
ISPA Life Time Achievement Award
ISPA Dr. S. Gunasekaran Award
Best Oral/ Poster Presentation

Address for Communication

Dr. R. Arivuselvi, Convener , ICREAMS - 2024
Asst. Professor & Head, PG & Research Department of Physics
Sri Vidya Mandir Arts & Science College (Autonomous)
Katteri - 636902, Uthangarai.
Mobile : +91 7010865424, +91 97892 39583
Email: svmcphyicreams2024@gmail.com

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Katteri – 636 902, Uthangarai, Krishnagiri, Tamil Nadu, India

21 – 22 February, 2024

International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS – 2024)

In commemoration of National Science Day

Organised by

PG & Research Department of Physics

In association with

Indian SpectroPhysics Association (ISPA)

Chennai, India

A Grand Welcome to All

PG & Research Department of Physics

Sri Vidya Mandir Arts & Science College (Autonomous)

Katteri – 636 902, Uthangarai, Krishnagiri, Tamil Nadu, India

In association with

Indian SpectroPhysics Association (ISPA)

Chennai, India

Cordially invite you for the

International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS – 2024)

In commemoration of National Science Day

21 – 22 February, 2024

Time: 10:00 a.m.

Venue: SVMC Auditorium

Inaugural Session
21st February 2024

Inaugural Address

Prof. Irena Kostova, *Ph.D., D.Sc.*
Faculty of Pharmacy, Medical University
Sofia, Bulgaria

Presidential Address

Thiru. V. Chandrasekaran
Founder, SVM Group of Educational Institutions
Chief Patron, ICREAMS 2024

Keynote Address

Prof. M.N. Ponnusamy, *Ph.D., D.Sc.*
Emeritus Professor, CAS in Crystallography and Biophysics, University of Madras, Chennai

Address by President ISPA

Prof. S. Gunasekaran, *Ph.D., D.Sc.*
Founder President, ISPA
Conference President, ICREAMS 2024

Special Address

Prof. C. K. Jayasankar, *Ph.D.*
Emeritus Professor, Department of Physics
Sri Venkateshwara University, Tirupati

Dr. N. Gunasekaran, *Ph.D.*
Principal

Dr. D. Kavitha, *Ph.D.*
Vice Principal

Dr. R. Arivuselvi, *Ph.D.*
Convenor, ICREAMS 2024

Programme Schedule

Day 1 (21.02.2024)

Inauguration

10: 00 a.m. *Invocation*

10: 05 a.m. *Welcome Address*
Dr. R. Arivuselvi, Ph.D.
Convenor, ICREAMS 2024

10: 10 a.m. *Paramountcy of the Conference*
Prof. S. Gunasekaran, Ph.D., D.Sc.,
Founder-President, ISPA

10: 15 a.m. *Presidential Address*
Thiru. V. Chandrasekaran
Founder, Sri Vidya Mandir Group of Educational Institutions

10: 20 a.m. *Unveiling the Portrait of Sir CV Raman*

10: 25 a.m. *Inaugural Address*
Prof. Irena Kostova, Ph.D., D.Sc.
Faculty of Pharmacy, Sofia Medical University, Bulgaria

10: 35 a.m. *Release of Conference Proceedings*

10: 40 a.m. *Conferring ISPA Awards*

ISPA Veteran Scientist Award
Prof. Irena Kostova, Ph.D., D.Sc.
Faculty of Pharmacy, Department of Chemistry
Medical University, Sofia, Bulgaria

ISPA Life Time Achievement Award
Prof. A. T. Ravichandran, Ph.D.
Associate Professor, Department of Physics
National College, Tiruchirappalli

ISPA Ariviyal Mudhumunaivar Sethu. Gunasekaran Award

Prof. Deva Prasad Raju, Ph.D.
Professor & Head, Department of Physics
Sri Venkateswara University, Tirupati

Dr. K. Vijaya Babu, Ph.D.
Assistant Professor, Department of Optimetry
Centurion University, Vizianagaram, Andhra Pradesh

10: 50 a.m. *Special Address*
Prof. C. K. Jayasankar, Ph.D., F.N.A.Sc.
Emeritus Professor, Department of Physics
Sri Venkateswara University, Tirupati

10: 55 a.m. *Felicitation Address*
Dr. N. Gunasekaran, Ph.D.
Principal, SVMC

Dr. D. Kavitha, Ph.D.
Vice-Principal, SVMC

11: 00 a.m. *Keynote Address*
Prof. M.N. Ponnusamy, Ph.D., D.Sc.
Emeritus Professor, CAS in Crystallography & Biophysics,
University of Madras, Guindy Campus, Chennai

11: 10 a.m. *Vote of Thanks*
Dr. K. Venkatesan, Ph.D.
Organising Secretary, ICREAMS 2024

11: 15 a.m. *High Tea*

Technical Sessions

Day 1 (21.02.2024)

Technical Session – I

Chair Person: Prof. A. T. Ravichandran

11:30 a.m. – 12:10 p.m.

Prof. Irena Kostova, *Ph.D., D.Sc.*
Professor, Faculty of Pharmacy Medical University, Sofia Bulgaria
Density Functional Theory and Spectral Investigations of Reactive Sites, Molecular and Electronic Structures of Coumarins, Uracils and Their Bioactive Ln(III) Complexes

12:10 p.m. – 12:50 p.m.

Prof. M. N. Ponnusamy, *Ph.D., D.Sc.*
Emeritus Professor, CAS in Crystallography and Biophysics, University of Madras, Chennai
Crystallography and Biophysics for Drug Design

Lunch: 12:50 p.m. – 01: 45 p.m.

Technical Session – II

Chair Person: Prof. Deva Prasad Raju

01:45 p.m. – 02:25 p.m.

Prof. Byru Venkatram Reddy, *Ph.D.*
Professor, Department of Physics, Kakatiya University, Warangal
DFT - A tool for the study of structure, vibrational analysis and molecular parameters in conjunction with experimental spectroscopic techniques: The case of monohalogenated methyl- and methoxy-benzoic acids

02:25 p.m. – 03:05 p.m.

Prof. C K Jayasankar, *Ph.D., F.N.A.Sc.*
Emeritus Professor, Department of Physics, Sri Venkateswara University, Tirupati
Research and Developments in Emerging Advanced Materials: Spectroscopy of Rare Earth Doped Glasses

Tea Break: 03:05 p.m. – 03:20 p.m.

Technical Session III

Chair Person: Prof. K. Vijaya Babu

03:20 p.m. – 04:00 p.m.

Prof. S. Kumaresan, *Ph.D.*
Associate Professor, Department of Physics, Arignar Anna Government Arts College, Cheyyar
Spectroscopic and structural investigations on structural isomers of two and three hydroxyl benzenes: An attempt on traditional medicinal plants

04:00 p.m. – 04:40 p.m.

Dr. P. Janani, *Ph.D.*
Instructional Designer Head (Academics), Echtian Contents Private Limited, Mumbai
Continuous monitoring of hypothyroid disorder using blood in an adult woman patient using FTIR-ATR spectroscopic technique

Oral & Poster Presentation
(21.02.2024)

Chairpersons: *Dr. A. Prakasam and Dr. S. Vijayakumar*
Oral Session I *01:45 p.m. – 04:30 p.m.*
Chairpersons: *Prof. S. Thambidurai and Dr. M. Revathi*
Poster Session I *01:45 p.m. – 04:30 p.m.*

Day 2 (22.02.2024)

Technical Session – IV

Chair Person: Prof. M. N. Ponnusamy

09:00 a.m. – 09:40 a.m.

Prof. Jiban Podder, Ph.D., F.B.A.S
Professor, Department of Physics, Bangladesh University of Engineering and Technology, Bangladesh
Functional Metal Oxide Thin Films via a Simple Chemical Route for Energy Storage Applications

09:40 a.m. – 10:20 a.m.

Prof. S. Gunasekaran, Ph.D., D.Sc.
Dean (R&D), St. Peter's Institute of Higher Education and Research, Chennai
Tribute to Light Legendary – Sir C V Raman

Technical Session – V

Chair Person: Dr. S. Srinivasan

10:20 a.m. – 11:00 a.m.

Dr. Lozan Todorov, Ph.D.
Faculty of Pharmacy, Medical University, Sofia, Bulgaria
In Vitro Free Radical Scavenging Assays – A Brief Introduction

Tea Break: 11:00 a.m. – 11: 15 a.m.

11:15 a.m. – 11:55 a.m.

Prof. Abhijit Chakraborty, Ph.D.,
Professor, Department of Physics, University of Burdwan, Golapbag, West Bengal
Conformational Landscape in Tetrahydronaphthalene Derivatives and Their Clusters with Water and Ammonia

Technical Session VI

Chair Person: Dr. R. Robert

11:55 a.m. – 12:35 p.m.

Prof. M. Selvapandiyan, Ph.D.
Professor, Department of Physics, Periyar University Centre for PG & Research Studies, Dharmapuri
Activated Carbon Derived from Biomass for High Performance Electrode Materials

12:35 p.m. – 01:15 p.m.

Dr. S. Srinivasan, Ph.D.
Associate Professor, Department of Physics, Presidency College, Chennai
Simulation Study on Some Perovskite Solar Cells using SCAPS 1D Software

Lunch: 01:15 p.m. – 02: 00 p.m.

Technical Session – VII

Chair Person: Prof. M. Selvapandiyan

02:00 p.m. – 02:40 p.m.

Dr. N. Pugazhenthiran, Ph.D.
Assistant Professor, Department of Chemistry, Universidad Técnica Federico Santa María, Valparaíso, Chile
Photocatalytic Nanomaterials: Sustainable Innovations in Water Treatment for a Cleaner Future

Oral & Poster Presentation (22.02.2024)

Chairpersons: Dr. R. Robert and Dr. S. Jayaseelan
Oral Session II 10:30 a.m. – 12:00 noon
Chairpersons: Dr. P. Ramesh Babu and Dr. T. Sivanesan
Poster Session II 10:30 a.m. – 12:00 noon

Tea Break: 02:40 p.m. – 03: 00 p.m.

PG & Research Department of Physics

Sri Vidya Mandir Arts & Science College (Autonomous)

Katteri – 636 902, Uthangarai, Krishnagiri, Tamil Nadu, India

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International Conference on Research in Emerging Advanced Materials and Spectroscopy (ICREAMS – 2024)

In commemoration of National Science Day

Time: 03:00 p.m. **Venue: SVMC Auditorium**

21 – 22 February, 2024

Valedictory Function

Day 2 (22.02.2024)

03: 00 p.m.	***Welcome Address***
	Dr. K. Venkatesan, Ph.D.
	Organising Secretary, ICREAMS 2024
03: 05 p.m.	***Presidential Address***
	Thiru. V. Chandrasekaran
	Founder, Sri Vidya Mandir Group of Educational Institutions
03:10 p.m.	***Report of the Conference***
	Dr. K. M. Prabu, Ph.D.
	Organising Secretary, ICREAMS 2024
03:15 p.m.	***Address by ISPA President***
	Prof. S. Gunasekaran, Ph.D., D.Sc.
	Founder-President, ISPA
03:20 p.m.	***Valedictory Address***
	Prof. Abhijit Chakraborthy, Ph.D.
	Department of Physics, University of Burdwan, West Bengal
03:30 p.m.	***Felicitation***
	Dr. N. Gunasekaran, Ph.D.
	Principal, SVMC
	Dr. D. Kavitha, Ph.D.
	Vice Principal, SVMC
03:35 p.m.	***Prize Distribution & Feedback***
03:40 p.m.	***Vote of Thanks***
	Dr. R. Arivuselvi, Ph.D
	Convenor, ICREAMS 2024
03:45 p.m.	***National Anthem***

CONTENTS-I

INVITED TALK

	Dr. Lozan Todorov	
IT-09	CONFORMATIONAL LANDSCAPE IN TETRAHYDRONAPHTHALENE DERIVATIVES AND THEIR CLUSTERS WITH WATER AND AMMONIA **Prof. Abhijit Chakraborty**	13
IT-10	SIMULATION STUDY ON SOME PEROVSKITE SOLAR CELLS USING SCAPS 1D SOFTWARE **Dr. S. Srinivasan**	14
IT-11	SPECTROSCOPIC AND STRUCTURAL INVESTIGATIONS ON STRUCTURAL ISOMERS OF TWO AND THREE HYDROXYL BENZENES: AN ATTEMPT ON TRADITIONAL MEDICINAL PLANTS **Dr. Subramanian Kumaresan**	15
IT-12	PHOTOCATALYTIC NANOMATERIALS: SUSTAINABLE INNOVATIONS IN WATER TREATMENT FOR A CLEANER FUTURE **Dr. N. Pugazhenthiran**	16
IT-13	CONTINUOUS MONITORING OF HYPOTHYROID DISORDER USING BLOOD IN AN ADULT WOMAN PATIENT USING FTIR-ATR SPECTROSCOPIC TECHNIQUE **Dr. Janani Panneer Selvam**	17

CONTENTS-II

CONTRIBUTED PAPERS

IT-01

DENSITY FUNCTIONAL THEORY AND SPECTRAL INVESTIGATIONS OF REACTIVE SITES, MOLECULAR AND ELECTRONIC STRUCTURES OF COUMARINS, URACILS AND THEIR BIOACTIVE LN(III) COMPLEXES

Prof. Irena Kostova

Department of Chemistry, Faculty of Pharmacy, Medical University,

2 Dunav St., Sofia 1000, BULGARIA

E-mail: irenakostova@yahoo.com

Density functional theory (DFT) have become an efficient tool in the prediction of molecular structures, conjugations, hydrogen bonding harmonic force field, vibrational frequencies of bioactive organic molecules and their metal complexes. DFT approximation was applied for investigation of a series of biologically active ligands and their lanthanide(III) complexes to elucidate their structural and bonding features. Different basis sets were tested in the course of the calculations of the hydrogen bonds, electron density distribution, molecular electrostatic potentials, optimized geometries of the neutral and anionic species of the ligands and their complexes. The calculated parameters were applied for predicting the most probable sites for electrophilic attack for metal coordination.

Systematic spectral analysis of the ligands and metal complexes based on both calculated and experimental (FT-IR, FT-Raman, ^{1}H NMR and ^{13}C NMR) data confirmed the suggested metal–ligand binding modes. The recorded and theoretically predicted spectral bands of characteristic functional groups were in excellent agreement and can be used as data bank for further application in trace analysis of lanthanide(III) complexes.

The results from the pharmacological tests of the studied compounds, including their oxidative behavior and inhibitory cytotoxic effects, have shown that the lanthanide(III) complexes revealed

promising pharmacological propertieswhich in all the cases were more pronounced for the lanthanide(III) complexes than for the respective bioligands and inorganic salts.

Acknowledgments: The administrative support received by the European Union-Next Generation EU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No. BG-RRP-2.004-0004-C01 is greatly acknowledged.

IT-02

FUNCTIONAL METAL OXIDE THIN FILMS VIA A SIMPLE CHEMICAL ROUTE FOR ENERGY STORAGE APPLICATIONS

Prof. Jiban Podder, Ph.D, FRSC
Department of Physics
Bangladesh University of Engineering and Technology
Dhaka-1000, Bangladesh
E-mail: jpodder@phy.buet.ac.bd

Functional metal oxide films are widely used in various energy fields and information technologies including electronic and ionic conductors, photovoltaics, thermoelectrics, dielectrics and resistive switches. Solution based spray pyrolysis deposition process offers a potentially scalable and an inexpensive method to the other available thin film deposition techniques. In addition, the spray pyrolysis method has various advantages such as rapid film growth rates, high throughput, and reproducibility of the films. In spray pyrolysis, the reaction occurs from the gas phase at moderately high temperatures, and oxidation can occur in air. Such a technique has been used for successfully depositing some novel binary and ternary oxide films like ZnO, TiO_2, CuO, MnO_2, WO_3, and Sn_2O, etc. and transition metal doped films onto glass

substrates at moderate temperatures of about 200 to 450°C in air. This technique is used for the deposition of metal oxide by using the aqueous precursor solutions. The solution contains two reactive compounds, and the temperature of the substrate activates a chemical reaction between the two compounds. Adjust the pH of the solution to 3.0 by adding a few drops of HCl. The solution is prepared just prior to the commencement of the spray. A solution of the dissolved precursor is sprayed in a vector gas as fine droplets onto a heated substrate. The solvent is evaporated or decomposes into gaseous products. From a band gap engineering perspective, by controlling the composition of the material, the band gap can be tuned and considered an ideal material for optoelectronic devices. The surface morphology, structure, and optical properties of the deposited films are studied, and the suitability of these films as transparent conductive window materials for optoelectronic applications is discussed. In addition, this lecture gives an overview of the spray process used for thin film deposition and also addresses the accumulated experience of many years work in this area.

Keywords: Spray pyrolysis; Oxide thin films; Surface morphology; Optical transmission; Band gap energy.

IT-03

CRYSTALLOGRAPHY AND BIOPHYSICS FOR THE DESIGN OF DRUG

Prof. M. N. Ponnuswamy and P. Sugumar

Centre of Advanced Study in Crystallography and Biophysics,

University of Madras, Guindy Campus, Chennai-600 025, Tamilnadu, India.

Department of Physics, Agni College of Technology,

Thalambur, Chennai-600 130, Tamilnadu, India.

E-mail: mnpsy@hotmail.com

Crystallography and Biophysics are the main tools and plays a major role in the discovery of drugs. The drug molecules of three dimensional shapes docked inside the active aminoacids in the protein molecules. The kinds of interactions after docking enhance the functional activity of the drug molecules, so the kinetics mechanics play a role there. The methods to design the drug molecules will be discussed at length, some examples will be shown. The salient features of Crystallography in determining the structures and how useful the subject Biophysics derived data (Bioinformatics) will be elaborated.

IT-04

LIGHT LEGENDARY SIR CV RAMAN

Prof. Dr. S. Gunasekaran, Ph.D., D.Sc.

TANSA Awardee

Dean, Research & Development

St. Peter's Institute of Higher Education and Research, Avadi, Chennai – 600 054.

Founder President, Indian Spectrophysics Association

Former Head, Department of Physics, Pachaiyappa's College, Chennai – 600 030.

Former Registrar, Periyar University, Salem.

E-mail : deanresearchspu@gmail.com

Website: www.ispa.org

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. 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.

IT-05

RESEARCH AND DEVELOPMENTS IN EMERGING ADVANCED MATERIALS: SPECTROSCOPY OF RARE EARTH DOPED GLASSES

Prof.C.K. Jayasankar

Department of Physics, S.V. University, Tirupati – 517 502, India.

***Presenting author: ckjaya@yahoo.com**

Materials science teaches us what things are made of and why they behave as they do. Materials engineering shows us how to apply knowledge to make better things and to make things better. Materials science and engineering drives innovation in research, development and industry in everything from A (Archeology) to Z (Zoology). In this direction materials such as energy, magnetic, electrical, optical, etc. are found to be very potential due to wide variety of applications. Among these materials, rare earth based materials such as single crystals, polycrystallines, phosphors, glasses and glass-ceramics are found to be very attractive for laser gain media, optical fiber amplifiers, display devices, sensors, magnetics and so on. For characterization and optimization of physical, chemical and optical properties for specific applications, spectroscopic techniques are more powerful for finger print analysis and therefore widely are being used. In this direction, for the last four decades, our group is focusing on

preparation and characterization of wide variety of rare earth doped matrices. In this presentation, we discuss the series of rare earths and their characteristic properties in different glasses and glass-ceramics, highlighting the luminescence properties for the design of laser gain media and display devices.

Acknowledgments: The author (CKJ) is highly grateful to DAE-BRNS, Govt. of India (No.2009/34/36/BRNS/3174, dt.12-02-2010) for financial support and also thankful to UGC, New Delhi for the award of UGC-BSR Faculty Fellow (No. F.18-1/2011/(BSR) dated 24-11-2017).

IT-06

DFT - A TOOL FOR THE STUDY OF STRUCTURE, VIBRATIONAL ANALYSIS AND MOLECULAR PARAMETERS IN CONJUNCTION WITH EXPERIMENTAL SPECTROSCOPIC TECHNIQUES: THE CASE OF MONOHALOGENATED METHYL- AND METHOXY-BENZOIC ACIDS

Prof. B. Venkatram Reddy

Department of Physics, Kakatiya University, Warangal – 506009, Telangana, India.

E-mail:bvreddy67@yahoo.com

Spectroscopy is an experimentally non-invasive way of studying a molecular system that consists few dozen atoms to several dozen atoms existing in gas phase to solution to crystals at different physicochemical conditions to elucidate its molecular structure, dynamic behavior like chemical linkages, reactivity and mutual interactions among atoms and atomic charges

modulated by temperature and environmental effects using infrared (IR) and Raman spectroscopies.

Computational spectroscopy, born as a branch of quantum chemistry that exploits theoretical models, provides tools and computer codes, and validates procedures for the prediction, analysis, interpretation, and understanding of spectroscopic features and properties. It can act as a bridge between experiments and underlying physical properties, as it provides the theoretical expressions linking observable measurements and molecular properties. Combining broad computational studies with a focus on structure-property relationships can identify short-lived and unstable species (in either ground or excited states). Computational and experimental spectroscopy can also be used to benchmark each other. Since experimental spectroscopy is extremely sensitive to the electronic structure of a given system, it is one of the best ways to verify the reliability and accuracy of theoretical predictions and validate QC calculation results.

Exploiting the scope of the DFT, we have been investigating the organic compounds which exhibit biological activity and NLO behavior. Monohalogenated methyl- and methoxy-benzoic acids, a class of molecules having biological activity, were investigated spectroscopically for their structure and vibrational properties and results were published **(Journal of Molecular Structure 1298 (2024) 137078).**

Benzoic acid and its derivatives are being attracted by growing researchers for investigation due to their biological activity, which occur widely in plants and animals tissues. They are constituents of vitamin B-complex and lenticular pigments present in the eye lenses of humans and in certain diurnal animals. They are also widely used in the manufacture of pharmaceuticals and miticides as contrast media in urology, cholocystrographic investigations, etc. They also find usage in dyes, curing tobacco, fruit juices preservation, a large variety of esters as a mordant in cloth printing and as a reference standard in volumetric analysis. They are also used as a protective drug against UV radiation in the diagnosis of gastrointestinal disorders and therapeutically in fibrotic skin disorders. The derivatives of benzoic acids play a vital role in minimising the population of mosquitoes. They are also used as important inhibitors for bacteria growth and affect the catalytic activity of various enzymes.

Keeping in view of the biological importance of benzoic acid derivatives, the molecules 3-fluoro-2-methylbenzoic acid; 3-chloro-2-methoxybenzoic acid; and 3-bromo-2-methylbenzoic were investigated using experimental and quantum chemical theoretical approach for vibrational and electronic properties from the optimized structure. Becke three parameter Lee-Yang-Parr density functionals along with 6-311++G(d,p) basis set were employed to compute their geometric optimization, fundamental frequencies and molecular parameters. The detected FT-IR and FT-Raman spectra were compared with their simulated spectra and the rms error between the detected and simulated vibrational frequencies was found at 6.17, 7.22 and 6.76 cm^{-1} for FMA, CMA and BMA, respectively. All the vibrational fundamentals were assigned unequivocally using potential energy distribution (PED) obtained in the computations. ^{1}H and ^{13}C NMR chemical shifts were evaluated by integrating the gauge-independent atomic orbital (GIAO) method with DFT and compared with corresponding experimental values. TD-DFT approach was followed to compare the simulated absorption maxima (λ_{max}) in DMSO-d6 solvent with observed values and interpreted in terms of HOMO and LUMO. The global reactive descriptors were estimated from the associated energies of HOMO and LUMO which describe the reactivity and stability of the molecules. Molecular electrostatic potential (MEP) surface has been determined using the charge density distributions to demonstrate electrophilic and nucleophilic nature of the molecules. DFT computations also ascertained the applicability of the titled molecules as NLO materials from the computed values of dipole moment and hyperpolarizability. Thermodynamic parameters and rotational constants were also evaluated employing rigid rotor harmonic oscillator approximation. Natural bond orbital (NBO) analysis confirmed the charge delocalization due to intra-molecular interactions.

IT-07

ACTIVATED CARBON DERIVED FROM BIOMASS FOR HIGH PERFORMANCE ELECTRODE MATERIALS

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The increasing demand for energy storage devices with high power density, rapid charge – discharge cycles and environmental sustainability has stimulated the research into novel materials for supercapacitor electrodes. In this study, we investigate the utilization of activated carbon derived from coconut shell as a viable and eco – friendly alternative for energy storage applications. Synthesis of biomass derived activated carbon for energy storage applications involves a controlled process of carbonization and activation at 600° C for 1h. The resulting activated carbon exhibited a well – defined porous structure with a significant specific surface area, rendering it suitable for electrolyte ion adsorption in energy storage devices. The electrochemical performance of the coconut shell derived activated carbon was evaluated through various techniques, cyclic voltammetry, galvanostatic charge – discharge cycling and electrochemical impedance spectroscopy. This materials demonstrated excellent electrochemical properties such as high specific capacitance, rapid charge – discharge and long cycling stability. The findings contribute to the growing field of green energy storage technologies and offer insights into the development of high – performance, eco –friendly energy storage materials.

Keywords: Plant biomass; Carbonization; Cyclic voltammetry; Electrochemical Impedance Spectroscopy

IT-08

IN VITRO FREE RADICAL SCAVENGING ASSAYS – A BRIEF INTRODUCTION

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Free radicals are chemical species, bearing an unpaired electron that tend to be highly chemically reactive. Such species are constantly produced and eliminated in living organisms. A variety of physiological mechanisms exist for regulating their formation and elimination. Disrupted balance between generation of free radicals and the ability of the body to detoxify them is a phenomenon, called oxidative stress. Oxidative stress can be a "double-edged sword" – desired in some cases (immune defense or cancer treatment) and harmful in others, as an intrinsic component of a multitude of pathological processes – inflammatory, cardiovascular, neurodegenerative and others. One way to prevent, or alleviate oxidative stress is by the application of antioxidant compounds that scavenge free radicals (radical scavengers), thus preventing them from impairing the normal functions of biomolecules. The interactions between such compounds and physiologically significant reactive species can be investigated in vitrothrough the utility of a variety of model systems that generate these reactive species. In the current talk, the Speaker will describe the essence of a number of in vitro model systems for testing chemical compounds for potential radical-scavenging activity. Their behavior is observed with the aid of UV-VIS spectroscopy and chemiluminometry. They apply both "natural" reactive species, that normally occur in living organisms as well as synthetic ones (DPPH, ABTS). The Authors aim to inform the audience in a brief and concise manner about the general idea behind

each model system, their usefulness and practical limitations and would also share some practical experience, gathered in the laboratory.

IT-09

CONFORMATIONAL LANDSCAPE IN TETRAHYDRONAPHTHALENE DERIVATIVES AND THEIR CLUSTERS WITH WATER AND AMMONIA

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1,2,3,4 –tetrahydronaphthalene (THN) is characterized by its 'twisted' conformation of the saturated ring. Its nitrogen and oxygen substituted molecules show aa variety of conformations depending also on the place of substitution. In nitrogen substituted ones, this landscape becomes more complicated with the orientation of the associated H atom. On the other hand, the sulphur substitution displays the 'bent' conformation as the most stable one, which in rest of the derivatives are either a transition state or lie much higher in energy.

On the other hand the water and ammonia clusters of the nitrogen substituted derivative will be presented here showing a representative case of the interesting avenue of cluster studies in these molecules. The ammonia clusters show intermolecular proton transfer one of the clusters in the excited state. The various noncovalent interactions will be discussed leading to these clusters. The partial covalent nature in a few of the hydrogen bonds is observed in the hydrated clusters. The different intra and intermolecular interactions will also be discussed in the bare

molecules. These computations lead to reassignment of high resolution spectroscopic data of the molecules obtained through supersonic jet spectroscopy.

IT-10

SIMULATION STUDY ON SOME PEROVSKITE SOLAR CELLS USING SCAPS 1D SOFTWARE

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Sustainable energy sources are needed for the present and future scenario for harvesting energy at low cost and environment friendly. A solar cell or photovoltaic cell is an electrical device works on the principle called Photoelectric effect which utilize sun light from the atmosphere and convert it into useful energy. Most of the fabricated solar cell is Silicon solar cell due to its higher efficiency. However the fabrication process is somewhat sophisticated. Recently, a type of solar cell called Perosvkite is emerging into the market because of ease fabrication. A lead based perovskite solar cell exhibit highest efficiency of 25%. Due to toxicity of lead, researchers developed recently lead free perovskite structure solar cell. The present study focused to further improve the efficiency of lead free tin based solar cell by optimized device structure of different metal oxide as hole and electron transport layer to show its efficiency performance. Other influence key parameter on enhance its efficiency performance are to be explored and discussed in this paper using numerically simulated SCAPS software.

IT-11

SPECTROSCOPIC AND STRUCTURAL INVESTIGATIONS ON STRUCTURAL ISOMERS OF TWO AND THREE HYDROXYL BENZENES: AN ATTEMPT ON TRADITIONAL MEDICINAL PLANTS

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Indian traditional medicines are the oldest practice for the health care over years and still a practice alternative to new medicinal systems. This study aims at in identifying certain important medicines and its isomers which were extracted from traditional medicinal plants for the first time. The role of hydroxyl groups in benzene and their structure, physio-chmeical properties were discussed using theoretical and experimental methods. Spectroscopic and structural properties of hydroxyl group based structural isomers such as benzenetriol isomers, benzenediol isomers have been investigated by FT-IR, FT-Raman, NMR and UV-Vis analytical techniques with the help of quantum chemical calculations. The vibrational spectra were recorded in the mid IR region. The electronic spectra were recorded in the UV-Vis region. The ^{1}H and ^{13}C NMR spectra were recorded in Dimethyl sulfoxide (DMSO) at base frequency of 400 MHz for ^{1}H and 100 MHz for ^{13}C nuclei (4:1 ratio). Moreover, attempts have been made to identify pyrogallol from extract of Abrusprecatorius Linn and resorcinol from the extract of Cassia auriculatta flowers by using Gas Chromatography – Mass Spectrometry (GC-MS) characterization techniques and NIST (National Institute of Standards and Technology) library.

Keywords: FT-IR, FT-Raman, ^{1}H and ^{13}C NMR, UV-Vis, GC-MS

IT-12

PHOTOCATALYTIC NANOMATERIALS: SUSTAINABLE INNOVATIONS IN WATER TREATMENT FOR A CLEANER FUTURE

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One of the most serious problems currently facing the man kind throughout the world is freshwater scarcity. Millions of people including children lose their life annually due to water-borne diseases caused by the consumption of contaminated fresh water. Fresh water resources are predominantly polluted by effluents discharged from various industries that are toxic to aquatic environment and human beings. In addition, the accumulation of various synthetic organic compounds such as dyes, phenols, organochlorides, antibiotics and etc., are known to cause great harm to human health (carcinogenic, teratogenic and mutagenic) even when their concentration in water is less than 10^{-7} magnitude. Moreover, it is very difficult to mineralize the synthetic organic compounds wastes using the traditional treatment techniques, such as, adsorption, sedimentation, coagulation, evaporation, etc. due to their high solubility in water. Hence, problems related to water are expected to grow worse in the coming decades with freshwater scarcity occurring globally even in the regions currently endowed with fresh water-rich. Addressing these serious problems requires robust advanced nanotechnologies for purifying water polluted with synthetic organic compounds wastes in an economical way and with less energy consumption. Heterogeneous photocatalytic oxidation process with an aid of oxide semiconductor nanoparticles is of special interest, especially when visible portion of the solar light is used. The semiconductor nanomaterials as a catalyst facilitate large contact area on its surface for the adsorption of a greater number of target organic pollutant molecules. This ensures that the catalytic active sites can be effectively used for the degradation of organic pollutants. In view of the above facts, the current presentation will be discussed the state-of-the-art research

activities and latest advancements in the design of different nanostructured materials via various strategies, including hydrothermal/solvothermal, high temperature gas phase methods and ect., To overcome the large band gap of nanostructured semiconductor materials and rapid recombination of photogenerated charge carriers, modifications are carried out to manipulate its electronic band structure, including transition metal doping, noble metal doping, non-metal doping and incorporating graphene as a two-dimensional (2D) catalyst support. The advancements made in these aspects are thoroughly examined, with additional insights related to the charge transfer events for each strategy of the modified nanostructured semiconductor materials. Finally, a summary and some invigorating perspectives on the major challenges and new research directions for future exploitation in this emerging frontier for various environmental applications.

IT-13

CONTINUOUS MONITORING OF HYPOTHYROID DISORDER USING BLOOD IN AN ADULT WOMAN PATIENT USING FTIR-ATR SPECTROSCOPIC TECHNIQUE

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Fourier transform infrared-attenuated total reflectance spectroscopy has been found useful of monitoring the efficacy of an Ayurvedic drug Thyronil during the treatment in a

hypothyroid woman. In the present work, various biomarker ratios such as carbohydrate-glucose ratio (1162 cm^{-1} and 1083 cm^{-1}), LDL-glucose ratio (1466 cm^{-1} and 1083 cm^{-1}) lipid-protein ratio (2872 cm^{-1} and 1466 cm^{-1}) and lipid protein (1744 cm^{-1} and 14663 cm^{-1}) are considered to study the efficacy of the drug thyronil. Out of the considered biomarker ratios, the lipid protein (1744 cm^{-1} and 14663 cm^{-1}) ratio of the hypothyroid patient increased immediately after treatment and then decreased to the level of a healthy group compared to the other biomarker ratios. Fig. 1 represents the variation in the lipid-protein ratio as obtained from the absorbance at 1744 cm^{-1} and 1466 cm^{-1} after min-max normalization in the regions 2925 cm^{-1} and 1550 cm^{-1} respectively. The red dot denotes the values deduced for the healthy group. This parameter can be used as possible biomarker to indicate successful remission and suggest that FTIR-ATR spectroscopy may provide a rapid optical method for continuous monitoring or evaluation of a hypothyroid disorder.

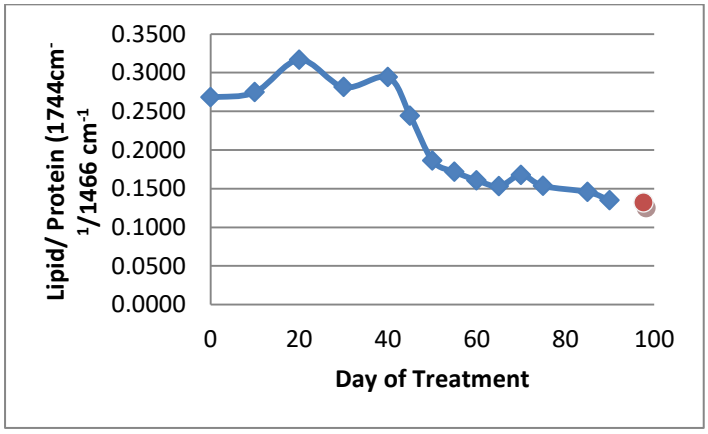

Fig.1 Variation in the lipid-protein ratio as obtained from the absorbance at 1744 cm^{-1} and 1466 cm^{-1} after min-max normalization in the regions 2925 cm^{-1} and 1550 cm^{-1} respectively. The red dot denotes the values deduced for the healthy group.

CP-1

CHEMICAL SYNTHESIS AND ENHANCED PHOTOCATALYTIC ACTIVITY OF NiO NANOPARTICLES

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Abstract

In recent years, Nickel Oxide has various applications such as fuel cell, magnetic materials, gas sensors, electrochromic film, catalysts, thermoelectric materials, waste water treatment and anode of organic light emitting diodes. Nickel oxide nanoparticles were synthesized using low cost chemical synthesis method. The formation of the NiO nanoparticles were studied by Fourier transform infrared spectroscopy. The face-centred cubic crystalline structure (JCPDS, No. 04-0835) of the material was confirmed by X-Ray Diffraction studies. The morphological studies were performed by Scanning Electron Microscope. The optical band gap energy of the material was found with the help of UV-Visible Spectroscopy. The photocatalytic activity of NiO nanoparticles has investigated the degradation of methylene blue dye.

Keywords: Nickel oxide, XRD, FTIR, SEM, UV-Visible Spectroscopy and Photocatalytic activity.

CP-2

INVESTIGATION ABOUT THE EFFECT OF ROTATION OF PHENYL RING ON PROTON TRANSFER IN (Z)-4-(HYDROXY (PHENYL) METHYLENE) ISOCHROMAN-1, 3-DIONE

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Abstract

The intra-molecular tautomerism between (Z)-4-(hydroxy(phenyl)methylene) isochroman-1, 3-dione (PHIC) and its tautomer 4-benzoyl-3-hydroxy-1H-isochromen-1-one (PHOC) is searched in the present work. In this tautomerisation pathway the movement of a proton between two O atoms within the target molecule is investigated. With the variation O···H bond distance in the proton transfer (PT) region two tautomers can be obtained by interconversion. A phenyl ring is attached to the molecule. Potential energy of the molecule depends on its orientation and torsional angle. All the DFT and ab-initio computational methods identify PHIC as the global minimum in ground state. PHOC is about 3.5 ±0.5 kcal/mole higher than PHIC on potential energy curve with the variation of O···H bond length. In the tautomerisation process the transition state (TS) is also characterised through the computations of variation of energy with intrinsic reaction co-ordinates (IRC). The transition state (TS) is located about 4.5 ±0.5 kcal/mole higher in energy than PHIC.

Figure: The optimised structure of phenol form with the PT region marked within the oval line and the dihedral angle marked responsible for the torsion of phenyl ring.

References:

1. Antonov L. Tautomerism: concepts and applications in science and technology. Wiley-VCH, Weinheim; 2016.
2. Zhao, J. Chen, Y. Cui, J. Wang, L. Xia, Y. Dai, P. Song, F. Ma Phys. Chem. Chem. Phys. 2015; 17:1142-1150.
3. Antonov L. Molecules. 2019; 24: 2252

CP-3

CONFORMATIONAL LANDSCAPE OF ISOTHIOCHROMAN IN S_0 : A COMPUTATIONAL STUDY

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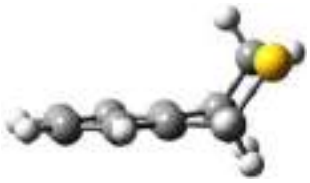
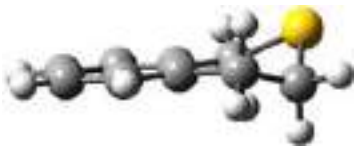
Abstract

1, 2, 3, 4 -tetrahydronaphthalene (THN) and its derivatives present various conformations with the twisted form of the saturated ring being the most stable one for the nitrogen and oxygen substituted one. Incidentally, the 'Bent' conformation is either a transition state (TS) or lies much higher in energy in these molecules. The sulphur substitution in isothiochroman yield interesting results. All the methods and basis sets indicate the 'Bent' conformation of isothiochroman, is the global minimum in the ground state. The respective 'twisted' form is higher by 60 ± 40 cm^{-1}. The suitable potential energy surface (PES) identifies all the minima and two TSs. The planar structure having C_s symmetry lie 4000 cm^{-1} higher in energy.



Bent



Twisted

Calculation of molecular electrostatic potential indicates the sights of electrophilic interactions and the small energy difference between the minima in isothiochroman predict an interesting interplay of intramolecular interactions. Natural Bond Orbital (NBO) analyses are included to identify the various intramlecular interactions. The orientation of lone pairs in this molecule play a much bigger role than the oxygen substitted one in determining the conformational pattern. Frontier molecular orbitals indicate the changes in the respective molecules on excitation. We also compare these results with the respective silicon and selenium

substituted THN derivatives. The maximum hardness principle is obeyed only by the transition states of isothiochroman. Minimum electrophilicity principle is completely violated here. The vibrational signatures are identified.

CP-4

FT-IR, UV-VIS, DRUG-LIKENESS AND MOLECULAR DOCKING STUDIES ON 3,7,11,15-TETRAMETHYL-2-HEXADECEN-1-OL

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A b s t r a c t

The organic compound of 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (3TMH) it's also known as Phytol commonly found in the chlorophyll pigment of plants. The title compound consists antimicrobial, anti-bacterial, antioxidant, anti-inflammatory, and anticancer properties. 3TMH compound has wide range of pharmaceutical applications were investigated by FT-IR, UV-Vis and DFT. Geometrical parameters, HOMO-LUMO and molecular electrostatic potential (MEP) map interpreted by B3LYP method with the 6-311++G(d,p) basis set. The NBO investigated by high stabilization between donor and acceptor in the molecules. The maximum absorption estimated by DT-DFT corelated with experimental UV-Vis spectra. The theoretical spectra of vibrational assignment with PED % carried out by Veda 04 well agreement with recorded FT-IR spectrum. The drug likeness obtains by online PKCM database satisfied five Lipinski's rule on title molecules. Additionally, molecular docking analysis by ligand-protein interaction of least binding energy on 3TMH compound against anti-cancer activity.

Keywords: Tetramethyl, DFT, Drug-likeness, Molecular docking

CP-5

SPECTROSCOPY, QUANTUM CHEMICAL CALCULATION, MOLECULAR DOCKING AND BIOLOGICAL INVESTIGATION OF 3-CYCLOHEXEN-1-OL, 4-METHYL-1-(1-METHYLETHYL)-

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Ab s t r a c t

The 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- is a natural drug synthesis from 100% medicinal plant of Hybanthus enneaspermus. The C3MM molecules structure identified through GC-MS results. The geometry optimized structure parameters on the C3MM molecule have been interpreted at the same level of B3LYP/6-311++G (d,p) good agreement with the XRD database. The NBO used to analysis inter-intra and donor, acceptor molecular interaction, the first-order hyperpolarizability were also completed. The DFT were computed energy gap reported which is good biological activity and MEP used to predict the chemical reactivity site of the title molecules. The TD-DFT using model IEFPCM carried out UV-Vis maximum absorptions are good agreements with experimental value and the recorded FT-IR spectra correlated with the theoretical spectra with PED carried out Veda 04. The molecular docking studies exhibit strength of protein-ligand (C3MM) complex on receptor respectively.

Keywords: C3MM, IEFPCM, XRD

CP-6

GREEN SYNTHESIS, SPECTRAL CHARACTERIZATION, DFT,DRUG-LIKENESS, MOLECULAR DOCKING EVALUATION OFDECOSANOIC ACID, METHYL ESTER BY ANTI-CANCER EFFICIENCY

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Ab s t r a c t

Decosanoic acid, methyl ester (DAMS) has been used to examine pharmacological efficiency by many scientist to developments the effect of anti-cancer cells. The title chemical structure identified using GC-MS analysis from extract of Aegle marmelos. The natural DAMS compound has estimated by B3LYP/6-311++G (d,p) technique in DFT calculations. HOMO-LUMO, MEP and electron transition are interpreted by same level with solute-solvent interaction to find strength and stability of molecules. NBO analysis provided well explanation of localized bond and lone pair, high stabilization energy of title molecules. The spectral characterization of FT-IR and UV-Vis have correlated with stimulated vibrational assignment (PED %) and maximum absorption by TD-DFT method in IEFPCM level. The topological analysis of ELF, LOL and RDG are interpreted by following softwareMultiwfn 3.8. Furthermore, the evaluations of anticancer, pharmacological qualities obtain by using molecular docking and drug-likeness observation on DAMS molecules.

Keywords: Drug-likeness, Molecular Docking, ELF, LOL and RDG

CP-7

SYNTHESIS AND OPTIMIZATION OF CORNCOB – DERIVED ACTIVATED CARBON FOR HIGH – PERFORMANCE ELECTRODE MATERIALS FOR SUPERCAPACITOR APPLICATIONS

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Activated carbon derived from corncob are the promising electrode material for supercapacitor applications due to their specific porosity, low cost and electrochemical stability. Synthesis of activated carbon from corncob through impregnation of KOH and H_3PO_4 at different ratios. The impregnated samples are activated at 500° C for 2h. X – Ray Diffraction (XRD) analysis of prepared activated carbon shows amorphous and disordered structure. The calculated BET surface area of activated carbon is 152 m^2/g with micro and mesoporous in nature. In GCD, the estimated specific capacitance of the electrode material about 347 F/g at 2 A/g in 1M Na_2SO_4. The specific energy density and power density of corncob activated carbon material are 48 Wh/ Kg at 2 A/g and 999 W/ Kg respectively.

Keywords: Corncob; Activated carbon; Galvanostatic Charge – Discharge (GCD); Brunauer – Emmett – Teller (BET) ; Supercapacitor

CP-8

SYNTHESIS AND CHARACTERIZATION OF NANO METAL MIXED P-ANISIDINE POLYMER

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Abstract

Anisidine ($CH_3OC_6H_4NH_2$) is obtained in the resonance form of ortho, meta, and para anisidine. Poly (ρ-anisidine) (PPA) is a derivative of polyaniline presented with methoxy (-OCH_3) substituent group at para position of phenyl ring(C_6H_5). Nowadays conjugated polymer plays an important role in novel technology application mainly in electrode material, an experimental work was performed to obtain more insight into the crystallization process of Poly (ρ-anisidine) (PPA) with silver nano particle(nAg). Synthesis of (PPA/nAg) were taken place by chemical oxidative polymerisation method in the presence of ammonium persulfate (APS).

Formation of synthesised polymer nanocomposites were confirmed by using FT-IR and XRD. X-ray Diffraction (XRD) shows that the peak obtained at 2θ values is 7.42^0 shows PPA is amorphous in nature. Mixing of Poly p anisidine with silver nano particles lead to intercalation PPA and nAg and its shows the improved crystalline nature of polymer. Average crystalline Size of obtained polymer nanocomposites (PPA/nAg) is 22.61 nm was calculated. FTIR spectra of prepared polymer nanocomposites were analysed, the intense peak appeared in the range of 513 cm^{-1} which corresponds to the stretching vibration of Ag-O group which conform the presence of silver nano particle within polymer chain. Peak at 1561 cm^{-1} and 1486 cm^{-1}consist of benzenoid and quinonoid form of PPA chain. Peak at 1344cm^{-1} and 3214cm^{-1} is attributed to C-N and N-H stretching mode indicated the presence of PPA. Morphological structure studies were carried out by Scanning Electron Microscope (SEM). Elemental composition of PPA/Ag were studied using Energy dispersive X-ray (EDX). Polymer nanocomposites are widely used in the application of electrode material, solar cell, fuel cells etc.

Keywords: ρ-anisidine, silver, oxidative polymerization.

CP-9

INFLUENCE OF INTRAMOLECULAR HYPERCONJUGATIVE CHARGE TRANSFER ON MOLECULAR CONFORMATION: TETRAHYDRONAPHTHALENE AND TETRAHYDROISOQUINOLINE

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Abstract

Conjugation and hyperconjugation mechanisms play crucial roles in explaining the conformers of cyclohexene derivatives.Hyperconjugation, is assessed using Natural Bond Orbital

(NBO) theory, has been identified as a significant factor in substituted cyclohexenes with exocyclic double bonds. Specifically, the interaction between the lone pair of substituents and the anti-bonding orbitals of the endocyclic bonds played a key role in determining the conformers. The effect of hyperconjugation is explored on the conformational patterns of tetrahydronaphthalene (THN) and tetrahydroisoquinoline (THIQ). This comparison provides insights into the influence of the lone pair of nitrogen (N) atom [N(LP)] when a CH2 group in THN is substituted with an NH group in THIQ.Conformational changes primarily occur in the sp^3 hybridized saturated ring of both molecules. Therefore, assessing the charge transfer from different bonding to various anti-bonding orbitals within the saturated ring allows for an estimation of changes in the saturated ring. The total energy (E_{NBO}) associated with the charge transfer in the saturated ring of THN and THIQ is of the same order, consistent with the relative energies of the conformers. The significant role of charge transfer to different bonds is observed in the presence of N(LP) as well as with its orientation. As the lone pair is a more powerful donor than σ or π bonding orbitals, charge transfers are primarily controlled by the lone pair and its orientation. The investigation further reveals that the changes in twisting angles and the transition between twisted and bent structures are dictated by the change of E_{NBO} with changes of lone pair orientations.

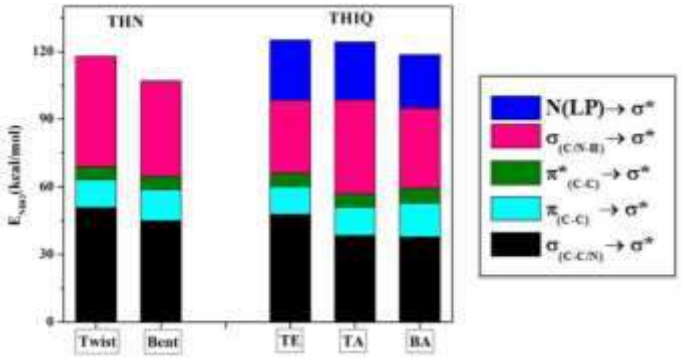

Fig. Total E_{NBO} (kcal/mol) including different type orbitals interactions of different conformers of THN (Twist & bent) and THIQ (TE, TA, & BA) molecules.Computations are performed with MP2 method with aug-cc-pVDZ basis set.

CP-10

TRANSFORMATION OF CONFORMATIONAL LANDSCAPE ON SUBSTITUTION IN TETRAHYDRONAPHTHALENE IN S_0 : A THOROUGH COMPUTATIONAL INVESTIGATION

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Abstract

In this study we substituted 1,2,3,4-tetrahydronaphthalene (THN) so that the substituent is in conjugation with the unsaturated ring. Oxygen, Nitrogen and Sulphur atoms were chosen as substituent to have chroman, tetrahydroquinoline (THQ) and thiochroman molecules respectively. THN had earlier shown to possess two equivalent conformers in S_0 where the saturated ring was twisted. Two equivalent minima corresponding to the equivalent twisted conformations appeared at the bottom of the well in chroman, with the bent form as the transition state. In thiochroman, two inequivalent conformations are observed, one of them is a twisted structure as in chroman and the new one is a bent conformer. The potential energy curve is symmetric around the origin of the dihedral angle representing the relative orientations of the two rings. A number of TS's are also observed. The relative energies varied slightly with the method of computations. Nitrogen substituted substance, THQ showed two low energy twisted conformers corresponding to the different orientations of the H atom of the NH group. The bent conformer also appeared as a TS. Frontier molecular orbitals are calculated to observe the changes in molecules on excitation. Molecular electrostatic potential gives an idea of intermolecular interactions of these molecules with solvents and indicates the sights of electrophilic interactions.The computed spectra show low frequency vibrations appearing at different positions in the different conformers as well as in molecules. We suggest some experiments to corroborate our findings.

CP-11

SYNTHESIS AND CHARACTERIZATION OF POLY-P-ANISIDINE MIXED COPPER NANOPARTICLES TO ENHANCE THE CONDUCTIVITY.

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Abstract

Poly-p-anisidine ($C_7H_9NO)_n$, is a conducting polymer derived from the polymerization of p-anisidine monomers. It belongs to the family of Polyaniline derivatives. The environmental stability of Poly-p-anisidine (PPA) is an important consideration for its practicaluse. In this work Poly-p-anisidine is mixed with Copper (Cu) nanoparticle by Chemical Oxidative Polymerization process using Ammonium Persulfate (APS) as an oxidizing agent and Dimethyl formamide (DMF)as a solvent. The FT-IR spectra of synthesized sample PPA/Cu were analyzed in the region 400-4000 cm^{-1} to identify the vibrational characteristics. The peaks at 3570cm^{-1},3355 cm^{-1}, 1581 cm^{-1},1477 cm^{-1}, 516 cm^{-1} and 636 cm^{-1} were attributed to N-H, O-H, C=C, C-N, Cu-O and C-H stretching vibrations within the polymer chain. Using X-ray Diffraction (XRD) technique the broad peak of PPA conducting polymer were analysed and suggested that it was due to its amorphous nature. By mixing the Cu nanoparticle into PPA, the crystalline nature of polymer nanocomposite was observed and the calculated average crystalline size was 34.798nm. Morphological structure of PPA/Cu was characterised using Scanning Electron Microscopy. The elemental composition of PPA/Cu was carried out using EDX spectrum. It showed 26% of Cu nanoparticle, distributed in the polymer matrix.

Keywords: Poly-p-anisidine,Conducting polymer, PPA/Cu nanocomposite.

CP-12

INVESTIGATION OF INTRAMOLECULAR PROTON TRANSFER IN 5,6-DIHYDROQUINOLIN-8-OL IN THE S_0 AND S_1 STATES

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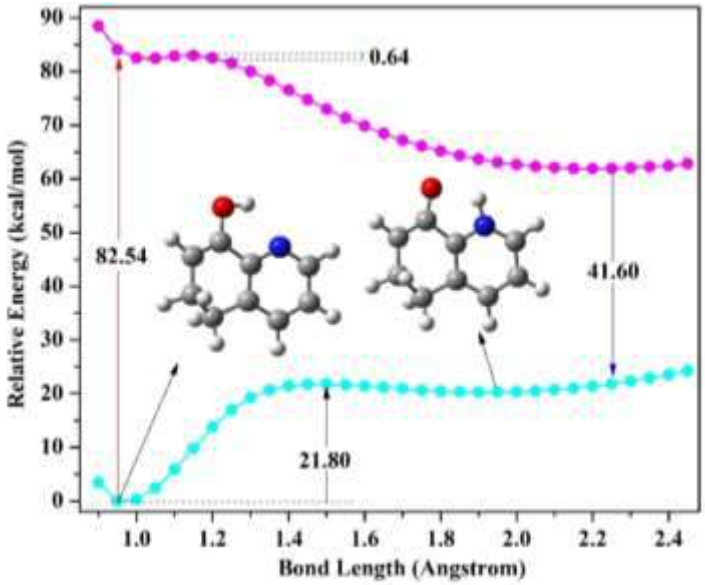
Abstract

The hydroxyquinoline family play an important role due to their photophysical properties. Among these they are a possible candidiate for a facile excited state intra and intermoleular proton transfers (ESIPT) both in isolation aswell as in their hydrated clusters.. In this article the intramolecular proton transfers in both ground (GSIPT) and excited (ESIPT) states are probed in 5,6-dihydroquinolin-8-ol (8-DHQ) which bears a close resemblance to 8-hydroxyquinoline (8-HQ). The enol form is the global minimum in S_0 , while the keto one in S_1 confirming ESIPT. The N···O distance reduces in both the molecules on excitation confirming the presence of a strong non covalent intramolecular interaction (NCI). This NCI is further investigated through quantum theory of atoms in molecules (QTAIM) and Natural Bond orbital (NBO) analyses. The presence of a Bond Critical Point (BCP) and the respective values of electron density (ρ_C) of the individual structures give us a measure of the strength of NCI. The transition states (TS) are indentified and the respective intrinsic reaction coordinate (IRC) computations show the evolution of 8-DHQ from TS. The barrier for PT reduces on excitation, though it is more in 8-DHQ than 8-HQ. The partial saturation of the ring and related non-planarity might be the reason behind this.



CP-13

SPECTROSCOPIC STUDIES OF P_2O_5 + TEO_2 + $SRCO_3$ + MGF_2 DOPED DY^{3+} ION FOR W- LED APPLICATIONS

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Abstract

The fluoride-based telluride phosphate (FBTP) glasses are doped with Dysprosium ions are prepared by using the method conventional melt quenching. For synthesized PTSM glasses physical parameters were evaluating, moreover, the structural, optical, and fluorescence properties were analyzed/studied by XRD, FTIR, EDAX, photoluminescence study analysis, and optical absorption. The optical band gap is estimated based on the tauc's curve extracted from the absorption spectrum, and the value obtained shows a non-linear behaviour with the concentration of doping ions. The intensity parameters (Ω2, Ω4, Ω6.) were evaluated using Judd – Ofelt theory and which follows Ω2 > Ω4 > Ω6 trend. From the emission spectra, the FBTP Dy glasses doped with 1.0 mol% Dysprosium ions (FBTPDy10) attains the higher emission peak intensity among the prepared glasses. The $^6H_{15/2} \rightarrow {}^6F_{11/2}$ transition emitting the radiation at 473 nm was more intense than the other transition and attains a higher value for optical gain bandwidth, Stimulated emission cross-section and branching ratio. The emission spectra are used to evaluate by colorimetric analysis of the 1931 CIE color coordinates, Y/B intensity ratio, and CCT values to see the adaptability of the fluoride-based telluride phosphate glasses to solid-state white light LED applications.

Keywords: Phosphate glasses, Dysprosium ions, Photoluminescence, w-LED, Optical bandgap

CP-14

GREEN SYNTHESIS OF ZINC OXIDE NANOSTRUCTURES USING CENTELLA ASIATICA, JUSTICIA ADHATODA AND CARDIOSPERMUM HALICACABUM

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Abstract

In materials science, “green” synthesis has gained extensive attention as a reliable, sustainable, and eco-friendly protocol for synthesizing a wide range of nanomaterials including metal /metal oxides nanomaterials, hybrid materials, and bioinspired materials. As such, green synthesis is regarded as an important tool to reduce the destructive effects associated with the traditional methods of synthesis for nanoparticles commonly utilized in laboratory and industry. In this review, we summarized the fundamental processes and mechanisms of “green” synthesis approaches, especially for metal and metal oxide [e.g., gold (Au), silver (Ag), copper oxide (CuO), and zinc oxide (ZnO)] nanoparticles using natural extracts. The Zinc oxide (ZnO) nanoparticles were synthesized using Centella asiatica, Justicia adhatoda and Cardiospermum halicacabum leaf extracts. The prepared samples are characterized by using FT-IR, UV-Vis, SEM, EDAX.

CP-15

SOL-GEL AUTO-COMBUSTION SYNTHESIS AND CHARACTERIZATIONS OF NANOCRYSTALLINE COBALT COPPER ALUMINATE ($Co_{0.7}Cu_{0.3}Al_2O_4$)

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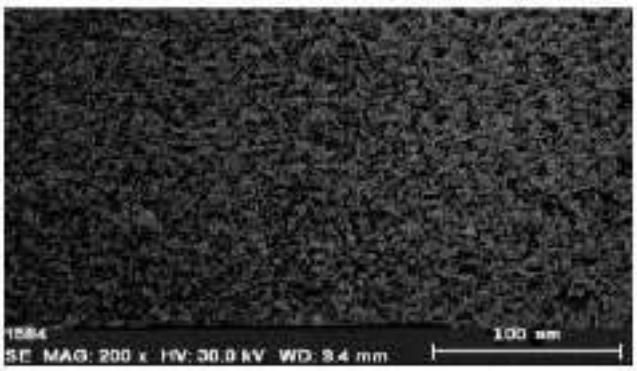
Abstract

The mixed metal oxides such as spinel structure oxides (AB_2O_4) constitute one of the most interesting classes of inorganic metalloid materials. They have fundamental physical and chemical properties. The Nanocrystalline Cobalt Copper Aluminate ($Co_{0.7}Cu_{0.3}Al_2O_4$) should be prepared by auto combustion method using cobalt nitrate, aluminium nitrate and glycine. The prepared nanoparticles were characterized by XRD, FTIR, FE-SEM and EDAX analysis. Among the spinel oxides, copper and cobalt aluminates possess interesting properties for technological application. The Nanocrystalline Cobalt Copper Aluminate ($Co_{0.7}Cu_{0.3}Al_2O_4$) has been employed in various fields such as ceramic pigment, optical properties, catalysts in reactions, photo catalyst for degradation of pollutants such as carbon monoxide, sensors for gas and volatile organic compounds, hydrogenation, and removal of H_2S and NH_3.



CP-16

IMPACT OF PRICKLY PEAR CACTUS ON STRUCTURAL, OPTICAL AND BIOMEDICAL PROPERTIES OF 8 – HYDROXY QUINOLINE NANOMATERIALS

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Abstract

The transformative impact of prickly pear cactus extracts on the structural, optical, and biomedical characteristics of 8-hydroxyquinoline nanomaterials. Through a meticulous synthesis process, the integration of prickly pear cactus components results in distinct modifications to the nanomaterials' structure, imparting unique optical properties. The investigation extends to the biomedical domain, exploring the potential of these hybrid nanomaterials for applications in medicine. By unraveling the intricate interplay between 8-hydroxyquinoline and prickly pear cactus, this study not only advances our understanding of nanomaterial design but also paves the way for the development of innovative and bio-compatible nanomaterials with promising applications in optical and biomedical fields.

Keywords: 8- Hydroxyqunoline, Prickly Pear Cactus, X-Ray Diffraction, FT-IR and UV-visible spectra.

CP-17

BIOSYNTHESIS AND CHARACTERIZATION OF ZINC OXIDE NANOPARTICLES USING *CARDIOSPERMUM HALICACABUM* PLANT LEAVES

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Abstract

The synthesis of Zinc oxide nanoparticles using a plant-mediated approach is presented in this work. The nanoparticles were successfully synthesized using the Zinc Nitrate and plant extract of the medicinal plant *Cardiospermum halicacabum***.** Zn $(NO_3)_2.6H_2O$ was made to react with the plant extract and the reaction temperature was maintained at 80 °C. The yellow coloured paste obtained was wholly dried, collected, and packed for further analysis. The scanning electron microscope images reveals the formation of small spherical ZnO nanoparticles (NPs) in the form of clusters whose diameter ranges between 20 and 30 nm with an average diameter of 25 nm. The energy-dispersive X-ray spectrum of the ZnO NPs indicated presence of Zn and O elements. XRD analysis revealed the formation of Wurtzite-type hexagonal ZnO crystal structured and high crystalline nature of ZnO. The Fourier-transform infrared spectrum of the ZnO NPs exhibited strong absorption bands at 463 and 489 cm^{-1} that proves the formation of hexagonal wurtzite structured ZnO. The photocatalytic performance of the greenly synthesized ZnO NPs showed almost complete decolorization of methylene blue dye at 80 min of natural sunlight irradiation. Hence, the *Cardiospermum halicacabum* leaf extract can be regarded as a

sustainable natural resource towards green synthesis of ZnO NPs for photocatalytic applications. This green synthesis method was found to be cost-effective and eco-friendly.

Keywords: Green synthesis; Cardiospermum halicacabum leaf extract; Zinc oxide nanoparticles; Photocatalytic performance

CP-18

GREEN SYNTHESIS OF ZINC OXIDE NANOPARTICLES USING *COCCINIA GRANDIS* LEAF EXTRACT AND THEIR CHARACTERIZATION

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Abstract

The research work involves the development of better and reliable method for the bio-fabrication of Zinc oxide nanoparticles through green method using Coccinia grandis leaf extract as an effective chelating agent. The crystalline structure, morphology, chemical composition and optical properties of ZnO nanoparticles were studied using various characterization techniques such as scanning electron microscopy (SEM), X-ray diffractometer (XRD), Energy-dispersive X-ray spectroscopy (EDAX), and UV visible Spectroscopy analysis. SEM images exhibited formation of ZnO nanoparticles with spherical shape. XRD analysis revealed the formation of Wurtzite-type hexagonal ZnO crystal structured and high crystalline nature of ZnO. EDAX spectra clearly indicated peaks corresponding to Zn and O elements that confirm the formation of

pristine ZnO nanoparticles through this green synthesize route. The bandgap energy 3.51 eV was calculated from UV visible Spectroscopy analysis.

Keywords: Green synthesis; Coccinia grandis leaf extract; Zinc oxide nanoparticles; Bandgap energy.

CP-19

STRUCTURAL GROWTH DYNAMICS OF POTASSIUM PARA NITROPHENOL BASED THIRD ORDER NONLINEAR HYBRID NANOCATALYSIS FOR ELECTRICAL AND MECHANICAL OPTIMIZATION

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Abstract

A potential, second order NLO optical hybrid nanocatalysis Potassium Para Nitro Phenol (KPNP) was grown by the slow evaporation technique. The grown semi organic non linear optical (NLO) crystals were subjected to various studies such as single crystal X-ray diffraction, Ultraviolet–Visible spectrum, Fourier transform infrared spectra, photoluminescence, Second Harmonic Generation, laser damage threshold (LDT) studies, Microhardness, Z-scan and dielectric studies. The potassium para nitrophenol (KPNP) crystal belongs to triclinic system with volume 737 Å. The optical cut off wavelength of the grown crystal was found to be at 208 nm which represents the grown sample as potential material for optical electronic device fabrication. The various functional groups present in KPNP grown crystal was confirmed by FT-IR spectroscopic. The optical properties of grown crystal was measured by Laser Damage threshold (LDT) of Q- switched pulsed Nd:YAG laser having the wavelength 1064 nm, pulse width 6 ns and repetition rate 10 HZ system with pulse energy range 1.5 mJ. The powder second harmonic generation (SHG) analysis was carried out for powder KPNP sample using the modified Kurtz and Perry Powder technique. The SHG efficiency of KPNP crystal was found to be 5.1 times that of KDP crystal. The mechanical

strength of title compound was measured by Vicker's microhardness method. The third order NLO properties of the material were calculated by Z-scan study. The dielectric studies were performed at different temperatures and frequencies to analyze the electrical properties. Photoconductivity results exhibit that the negative photoconductive nature of the crystal.

Keywords: Powder crystal XRD, UV-Vis, FT-IR, Mechanical studies, Photoconductivity.

CP-20

STRUCTURAL GROWTH DYNAMICS OF POTASSIUM PARA NITROPHENOL BASED THIRD ORDER NONLINEAR HYBRID NANOCATALYSIS FOR ELECTRICAL AND MECHANICAL OPTIMIZATION

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Uthangarai - 636902, India

Abstract

A potential, second order NLO optical hybrid nanocatalysis Potassium Para Nitro Phenol (KPNP) was grown by the slow evaporation technique. The grown semi organic non linear optical (NLO) crystals were subjected to various studies such as single crystal X-ray diffraction, Ultraviolet–Visible spectrum, Fourier transform infrared spectra, photoluminescence, Second Harmonic Generation, laser damage threshold (LDT) studies, Microhardness, Z-scan and dielectric studies. The potassium para nitrophenol (KPNP) crystal belongs to triclinic system with volume 737 Å. The optical cut off wavelength of the grown crystal was found to be at 208 nm which represents the grown sample as potential material for optical electronic device fabrication. The various functional groups present in KPNP grown crystal was confirmed by FT-IR spectroscopic. The optical properties of grown crystal was measured by Laser Damage threshold (LDT) of Q- switched pulsed Nd:YAG laser having the wavelength 1064 nm, pulse width 6 ns and repetition rate 10 HZ system with pulse energy range 1.5 mJ. The powder second harmonic generation (SHG) analysis was carried out for powder KPNP sample using the modified Kurtz and Perry Powder technique. The SHG efficiency of KPNP crystal was found to be 5.1 times that of KDP crystal. The mechanical

strength of title compound was measured by Vicker's microhardness method. The third order NLO properties of the material were calculated by Z-scan study. The dielectric studies were performed at different temperatures and frequencies to analyze the electrical properties. Photoconductivity results exhibit that the negative photoconductive nature of the crystal.

Keywords: Powder crystal XRD, UV-Vis, FT-IR, Mechanical studies, Photoconductivity.

CP-21

GROWTH, STRUCTURAL, SPECTROSCOPIC, LINEAR AND NONLINEAR OPTICAL CHARACTERIZATIONS ON 2, 3- DIAMINOPYRIDINIUM 4-CARBOXY BUTANOATE (DPCB) SINGLE CRYSTAL

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Abstract

Optically good quality organic single crystals of 2, 3- Diaminopyridinium 4-carboxy butanoate (DPCB)were grown using methanol solvent. The crystal structure and crystalline nature of the compound were identified using X-ray diffraction technique. Structural confirmation of the crystal was carried out using ^{1}H-NMR and ^{13}C-NMR characterization studies. UV plot showed visible region transparency of the grown crystal. Dielectric, DC conductivity, photoconductivity, photoluminenscence results were taken for the grown crystal. Additionally, third order nonlinear optical (NLO) efficiency of the crystal is found employing pumped diode laser of wavelength 532 nm.

Key words: Crystal growth, Nonlinear, Band gap, Optical, Dielectric studies

CP-22

GROWTH AND CHARACTERIZATION OF AND COPPER DOPED LITHIUM SULPHATE CRYSTAL

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Abstract

The Novel organic component of Cu doped Li_2SO_4single crystals have been grown from slow evaporation solution growth technique at room temperature employing water as solvent. The crystalline structure and nature of Cu doped Li_2SO_4were elucidated by X-ray diffraction studies. The unit cell parameters for the crystal of Cu doped $Li_2SO_4$are, a = 5.45 Å, b = 4.87 Å, c = 8.01 Å and α= 89.05 °, β=105.95°, ν= 89.05°. However, the functional groups confirmation of expected crystalline compound was successfully carried out using FTIR spectrum. The UV-Visible transmission and absorption spectrum of title compound in the region from 190 nm - 1100 nm. Lower values of absorption in between 200 nm and 800 nm wavelength range in the UV trace exposed valuable properties of title crystal which could be beneficial in designing opto-electronic devices. The lower-cut off wavelength of the crystal occurred at 383 nm and its optical band gap 3.24 eV. Using Z-Scan studies the third order parameters of title compounds were analysed.

CP-23

GROWTH AND CHARACTERIZATION OF INORGANIC MATERIAL DOPED PICRIC ACID SINGLE CRYSTAL

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Abstract

The Novel organic component of Lithium doped Picric acidsingle crystals have been grown from slow evaporation solution growth technique at room temperature employing water as solvent. The crystalline structure and nature of Lithium doped Picric acidwere elucidated by X-ray diffraction studies. The unit cell parameters for the crystal of Lithium doped Picric acidare, a = 5.75 Å, b = 4.67 Å, c = 8.61 Å and α= 88.05 °, β=106.95°, ν= 88.05°. However, the functional groups confirmation of expected crystalline compound was successfully carried out using FTIR spectrum. The UV-Visible transmission and absorption spectrum of title compound in the region from 190 nm - 1100 nm. Lower values of absorption in between 200 nm and 800 nm wavelength range in the UV trace exposed valuable properties of title crystal which could be beneficial in designing opto-electronic devices. The lower-cut off wavelength of the crystal occurred at 383 nm and its optical band gap 3.24 eV.

CP-24

STRUCTURAL, MORPHOLOGICAL, AND MAGNETIC PROPERTIES OF RARE-EARTH DOPED STRONTIUM FERRITE NANOPOWDERS SYNTHESIZED BY SOLUTION COMBUSTION METHOD

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Abstract

Perovskites are a family of crystals that show promising properties for applications in nanotechnology. Multiferroics exhibit more than one primary ferroic ordering—ferromagnetism, ferroelectricity, ferroelasticity or ferrotoroidicity. Among the permanent magnets hard ferrites,

particularly M-type hexagonal ferrites have special place by virtue of their low cost and reasonable magnetic properties. Ferrite magnets are used for a number of applications ranging from magnetic holding tools to motors and generators. The Multiferroic Strontium ferrite with Gd doped strontium ferrite nano powders having composition 5% and 9% were successfully synthesized by solution combustion method using citric acid as fuel at a temperature as low as 250˚C. As prepared samples annealed at 1000˚C for 2hrs and they were examined by powder XRD for phase identification and to determine its crystallite size. The surface morphology was carried out using SEM and it is found to have more homogenous distribution. The elemental analysis is carried out using EDAX and it confirms the presence of the elements. The magnetic property is carried out using vibrational sample magnetometer. The divalent Gd^{3+} ions doped with Strontium ferrite improves the ferromagnetic property than that of the undoped sample. An enhancement in magnetization by Gd doping is observed which also increase the Coercivity. Dopant concentration, phase purity, small particle size, and grain size are all mentioned as possible mechanisms for improving the aforementioned qualities

Keywords: Multiferroic , Perovskite, strontium ferrite , Gd, Ferromagnetic.

CP-25

INVESTIGATION OF ELECTROCHEMICAL PERFORMANCE OF TIN ZINC SULFIDE ($SNZN_2S_4$) SYNTHESIZED VIA MICROWAVE – ASSISTED TECHNIQUE

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Abstract

The highly active SnZn2S4 (TZS) nanocomposite has been prepared in a little time at 100˚C by using microwave-assisted technique synthesis process. According to advance the activity, zinc tin acetate hydroxide prepared using microwave treatments is used for the

preparation of TZS in above synthesis method. Sulfidation of Zn- Sn acetate hydroxide with thioacetamide was performed in the occurrence of alcohol to produce SnZn2S4 nanocomposite. The $SnZn_2S_4$ nanocomposite demonstrated tremendous physiochemical properties with advanced electrochemical performances. The resultant product have been characterized using X-ray Diffraction (XRD), Transmission Electron Microscope (TEM), Fourier Transform Infrared (FTIR), Surface Area Determination (BET) and Electrochemical Analysis. Due to the superior faradic redox reaction, enhanced surface area and incomparable mass transfer environment, the nanocomposite demonstrated a better charge/discharge stability, high specific capacitance and long-term cycling existence. Bring together asymmetric super capacitor assembled with $SnZn_2S_4$ nanocomposite working a high energy density and power density. The long–period cycle existence with capacitance maintenance would satisfy the growing require for energy-related devices. The exclusive $SnZn_2S_4$nanocomposite not only convey capable roles in energy storage but in addition stand for an unconstrained potential of hetrostructures materials.

CP-26

INVESTIGATION OF INORGANIC NONLINEAR OPTICAL POTASSIUM PENTA BORATE TETRA HYDRATE (PPBTH) SINGLE CRYSTALS GROWN BY SLOW EVAPORATION METHOD

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Abstract

Borates family crystals were plays vital role in the field of non linear optics (NLO) due to needs of wide range of applications. In this report, NLO crystals (potassium penta borate tetra hydrate ($KB_5H_8O_{12}$) are grown by slow evaporation method at room temperature (28^o C) and studied their physical properties. The harvested single crystals are transparent with the dimension of 12 x 10 x 6 mm^3 and colourless. X-ray diffraction of single crystals reveals that the grown

crystal belongs to orthorhombic system with non-centrosymmetric space group Pba2. All the absorbed functional groups are present in the order of inorganic compounds expect 1688 cm^{-1} because of water (O – H - O blending) molecule present in the pristine. Crystals show transparent in the entire visible region with 5.9 eV optical band gap and also it shows excellence in second order nonlinear optical properties. Crystals can withstand upto 154°C without any phase changes which is observed using thermal (TGA/DTA) analysis.

Key Words : Slow evaporation method; nonlinear optical materials; non-centrosymmetric; Kurtz-Perry powder test; TG-DTA.

CP-27

CRYSTALLIZATION OF INORGANIC NONLINEAR OPTICAL ZINC DIMAGNESIUM CHLORO SULPHATE (ZDMCS) SINGLE CRYSTAL

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Abstract

The growth of inorganic zinc dimagnesium chloro sulphate (ZDMCS) nonlinear optical material from low temperature evaporation technique at ambient temperature has been reported. The dimension of harvested crystal is 29 x 10 x 2 mm^3 and is possess rectangular shape morphology. The single crystal X-ray diffraction studies confirmed that the grown crystal belongs to the system of trigonal. The S- Cl stretching vibrations and Mg^{2+} ions present in the sample were observed by FTIR spectrometer. The cut - off wavelength of the grown crystal is about 203 nm is found by UV-visible absorption spectrum. The nonlinear optical efficiency was determined by powder Kurtz Perry technique. EDAX spectrum confirms the presence of elements within the material. Dielectric nature of the sample was analyzed for the frequency range 50 Hz - 5 MHz at different temperatures. The mechanical behaviour of the title compound was investigated using Vicker's microhardness tester.

Keywords: Crystal growth; optical materials; FTIR; UV-Visible; Vicker's microhardness test.

CP-28

SYNTHESIS OF Bi_2MoO_6 – Ag_2MoO_4 NANOCOMPOSITE FOR PHOTOCATALYTIC AND ANTIBACTERIAL APPLICATIONS

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Abstract

The novel Bi_2MoO_6 – Ag_2MoO_4 nano photocatalyst for the removal of toxic dyes was prepared through Hydrothermal route. In the synthesis, there are two steps. First, $Bi(NO_3)_3$ and Na_2HoO_4 have been taken in the same ratio and dissolved in 100ml deionized water, Then, by stirring, drying and calcination process, we got Bi_2MoO_6. Second, Bi_2MoO_6 and Na_2HoO_4 have been taken in the same ratio and dissolved in 50 ml deionized water. After that 0.2M of $AgNO_3$ was added. Then by sonication, drying and calcination process, we got Bi_2MoO_6–Ag_2MoO_4 nanocomposite. Then Powder X-ray diffraction was done and the obtained XRD patterns confirm the phase formation of Bi_2MoO_6–Ag_2MoO_4. The morphology of the prepared Bi_2MoO_6–Ag_2MoO_4 nanocompostie has been studied from SEM micrographs. Photocatalytic activity and antibacterial applications have been studies.

CP-29

STUDIES ON PURE AND IRRADIATED Cu_2ZnSnS_4 FOR ENERGY APPLICATIONS

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INTRODUCTION:

Extensive research has been conducted on copper indium gallium selenide (CIGSe) as a light-absorbing material, however the widespread production of CIGSe solar cells is hindered by the scarcity and high costs associated with rare metals such as indium and gallium. In response to these challenges, researchers have identified copper zinc tin sulfide (CZTS) as a promising alternative absorber material. CZTS comprises readily available, less toxic, and cost-effective elements, while still exhibiting material properties comparable to CIGSe.

As a quaternary chalcogenide and direct bandgap semiconductor with an optimal bandgap of approximately 1.5 eV and a significant absorption coefficient, CZTS has obtained special attention for its distinctive properties.

These features make CZTS particularly noteworthy for applications focused on low-cost and environmentally friendly energy solutions.

OBJECTIVE:

- To synthesis CZTS NP using a simple solution based chemical method.
- To enhance the properties of synthesized CZTS NP by Microwave irradiation.
- To study the physical & optical properties of prepared pure and irradiated CZTS NPs.

Method of preparation:

Copper Chloride Dihydrate, Zinc Chloride, Stannous Chloride Dihydrate, and Thiourea (in a molar ratio of 2:1:1:4) are dissolved in distilled water to create a precursor solution. The solution is stirred for 45 minutes. Subsequently, the solution is transferred into a 100ml stainless steel autoclave with a Teflon liner and placed in a muffle furnace at 200°C for 20 hours. After the hydrothermal reaction, the autoclave is allowed to cool naturally. The resulting precipitate is washed four times with Ethyl alcohol and then dried at 80°C under vacuum conditions. The obtained black powder is collected for further characterizations.

Outcomes:

- Synthesis of pure and Microwave irradiated CZTSwith chemical route has been successfully achieved. CZTS NP synthesized by simple solution-based approach is cost effective and can be scaled up at large level.
- Based on X-Ray Diffraction obtained, it can be concluded that the compound shows Tetragonal symmetry, Kesterite structure – $I\bar{4}2d$. The sharp intense peaks in all cases confirms the good crystalline nature of NPs and the peaks originated from (112), (200), (220) and (312) are reflections of tetragonal (kesterite) CZTS (International Center for Diffraction Data, JCPDS 26-0575).
- The SEM analysis shows that the compound is in nanoscale and EDAX analysis confirms the presence of Cu, Zn, and SnS in the lattice.
- The UV-Vis spectrum shows a strong absorption peak at the wavelength range from 400 to 800 nm. The optical bandgap was estimated by plotting $(ahv)^2$ as a function of hv.
- The Raman spectra of pure CZTS and irradiated CZTS were studied. The vibration frequency at 332 cm^{-1} confirms the formation of pure kesterite phase CZTS

CP- 30

FACILE FABRICATION, STRUCTURAL, MORPHOLOGY, OPTICAL AND ELECTROCHEMICAL INVESTIGATIONS OF LI-DOPED ZNO@AC NANORODS

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Abstract

Due to global population growth and increasing energy consumption, recent years have seen a significant rise in the development of renewable and environmentally friendly resources for energy storage. In this behavior, supercapacitors have emerged as fascinating options for energy storage applications. Lithium doped zinc oxide at activated carbon (Li-ZnO@AC) was synthesised by a short-term microwave-autoclave. The samples were analysed via X-ray powder diffractometry, scanning electron microscopy, and spectroscopic techniques such as UV-vis, Fourier transform infrared, and photoluminescence, electrochemical properties were investigated using cyclic voltametric, EIS technique. Li-ZnO@AC nanorods reveal the hexagonal phase, and the XRD data were used to calculate the crystalline size determined from the various Scherrer models, WH plot, SSP, and HW plot. Surface morphology is investigated by SEM it shows rod shape. FTIR spectrum to identify the various functional groups and molecular vibrations. More than 80% optical transparency was found using UV-Vis spectroscopy, which exhibited a 240 nm reduced UV cutoff. The optical band gap was determined using Tauc's relation, the purity of Li-ZnO@AC nanorods in the Urbach tail method. Transmission spectrum data were used to analyze the refractive index and other optical characteristics. Intense PL was also seen with some spectrum manipulation, most likely with emission photon energy. The specific capacitance of the Li-ZnO@AC electrode was determined at a scan rate of 1 mV/s. The frequency-dependent properties of it were investigated through electrochemical impedance spectroscopy (EIS).

Keywords: Li-ZnO@ACXRD, WH plot, SSP, HW plot, Urbach tail, Optical band gap, etc.,

CP-31

FACILE GREEN SYNTHESIS, CHARACTERIZATION, STRUCTURAL AND OPTICAL PROPERTIES OF ZNO NPS FROM THE ORANGE PEEL EXTRACT

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Abstract

In green synthesis, natural plant extracts are often employed as reducing agents for the synthesis of metal oxide nanoparticles. Because green NP synthesis is economical, has a shorter duration, reduces energy consumption, and is ecologically friendly, it is important. Zinc oxide nanoparticles (ZnO NPs) have numerous applications in fields of biological, optical, medical, electrical, cosmetics, environmental protection, drug delivery, and antibacterial drugs. The present investigation employs the sol-gel technique to prepare orange peel extracts, which produce ZnO NPs in an environmentally benign manner. Powder X-ray diffraction (XRD) was used to analyse the structural and other crystalline properties of ZnO NPs. The materials were discovered to have adopted a hexagonal crystal structure. Using the XRD data, the average particle size, dislocation density, and starin value calculated from W.H plot. The surface morphology of the material was investigated by SEM.FTIR is employed to determine various functional groups. UV-visible spectroscopy is used to investigate the optical absorption properties. The cut-off wavelengths were found to be 386 nm. It is determined that the optical bandgap energy (Eg) near the edge of the absorption band is 3.33 eV. The ZnO NPs generate blue and red colours, according to the photoluminescence (PL) spectrum. So, ZnO NPs are the best options for the manufacturing of solar cells, panels, sensors, LEDs, etc., based on the results of the UV-Vis and PL spectroscopic examinations.

Keywords: ZnO, NPs, WH plot, Optical band gap, PL, LEDs, etc.,

CP-32

MAGNETIC AND MAGNETOCALORIC PROPERTIES OF COMBUSTED NI-DOPED $LAMNO_3$ PEROVSKITES

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Abstract

In the past few years, the exploration of magnetocaloric phenomena has grown significantly, resulting in the identification of a broad range of materials, encompassing intermetallics and oxides. This study focuses on the comprehensive analysis of $LaMn_{1-x}Ni_xO_3$ (x=0, 0.2, 0.4, 0.6, 0.8) through various characterization techniques. The investigation involves X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), and Vibrating Sample Magnetometry (VSM). XRD analysis reveals the crystal structure and lattice parameters of the samples. SEM provides insights into surface morphology. EDX confirms the successful incorporation of Ni as the dopant and validates compositional adjustments. VSM measurements offer a detailed understanding of the magnetic and magnetocaloric behaviour of the $LaMn_{1-x}Ni_xO_3$ compounds. The results through these techniques provides a comprehensive assessment of the structural, morphological, compositional, magnetic and magnetocaloric properties of $LaMn_{1-x}Ni_xO_3$ nanoparticles, highlighting their potential for magnetic refrigeration applications.

Keywords: Perovskites, Mn site doping, Magnetic properties, Magnetocaloric properties

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CP-33

FACILE CO-PRECIPITATION ASSISTED SYNTHESIS AND CHARACTERIZATION OF ZINC OXIDE - TIN OXIDE NANOCOMPOSITES AND THEIR PERFORMANCE EVALUATION AS PHOTO ANODES IN DYE-SENSITIZED SOLAR CELL

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Abstract

A co-precipitation route was followed to produce zinc oxide-tin oxide nanocomposites (ZnO-SnO2 NCs) by changing molar proportion between precursor salts. The characterization tools, viz. XRD, UV–Vis spectrophotometer, SEM, and EDAX were utilized to inspect structural, optical, morphological, and elemental features of ZnO-SnO2 NCs. The XRD patterns exhibited diffraction angles corresponding to hexagonal wurtzite ZnO and tetragonal rutile SnO2. The ZnO-SnO2 NCs showed absorption from 300 nm to 700 nm, owing to the presence of visible light reactive SnO2 in the ZnO–SnO2 NCs. The SEM images displayed ZnO–SnO2 NCs

with diverse morphology as a consequence of the incorporation of Sn2+ ions and the corresponding EDAX spectra confirmed their purity. The dye-sensitized solar cell (DSSC) integrated with ZnO–SnO2 NC photo anodes showed consid- erable variations in photovoltaic parameters due to the influence of their band gap and morphology.

Keywords : XRD, SEM, EDAX .

CP-34

PREPARATION AND CHARACTERIZATION OF COBALT TUNGSTATE GRAPHITIC CARBON NITRIDE NANOHYBRID FOR ENERGY STORAGE APPLICATION

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Abstract

Cobalt tungstate-graphitic carbon nitride ($CoWO_4$-'x' g-C_3N_4) nanostructures were synthesized through a cost-effective hydrothermal method. Structural, vibrational and morphological properties of the prepared samples were characterized by powder X-ray diffraction, Fourier transform infrared spectroscopy and scanning electron microscopy analysis. The results revealed the formation of monoclinic crystal structure and flower-like morphology of $CoWO_4$-'x' g-C_3N_4) nanostructures. Among the prepared samples, the $CoWO_4$-'x' g-C_3N_4 (x=1.0) electrode material has exhibited high surface area, increased electrical conductivity and enhanced electrode-electrolyte ion transportation efficiency. The $CoWO_4$-'x' g-C_3N_4) electrodes materials with composition 'x' of g-C_3N_4 (x = 0.5, 1.0 2.0) with were subjected to electrochemical investigations. When evaluated for supercapacitors, the $CoWO_4$-'x' g-C_3N_4 (x= 1.0) electrode material disclosed a remarkable electrochemical performance with a high specific capacitance of 1108 Fg^{-1} at 2 A g^{-1} and improved life cycling performance. These findings paved the way for $CoWO_4$-'x' g-C_3N_4 electrode materials for supercapacitor application.

Keywords: Cobalt tungstate; Graphitic carbon nitride; Hydrothermal method; Energy Storage

CP-35

SYNTHESIS OF PURE AND SILVER DOPED CERIUM OXIDE IN THE CONTEXT FOR WASTEWATER TREATMENT UNDER SOLAR LIGHT EXCITATION

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Abstract

Anthropic pollution in water resources is a current problem, therefore, new technologies or compounds are required for the treatment, for example, of industrial, textile, medical wastewater, among others. In that sense, the silver-doped cerium oxide (CeO-Ag) nanoparticles were produced by co-precipitation method. Various characteristics procedures such as XRD, UV-Vis, FT-IR, SEM, EDX, and XPS and were applied for the structure determination and morphology of synthesized CeO-Ag nanoparticles. CeO nanoparticles are expected to possess simultaneous antimicrobial activity and photocatalytic activity. Further, the activity of CeO can be enhanced with noble metal, here silver (Ag) was used as the dopant to enhance its activity. Hence, Ag doped CeO was synthesized as a nanocomposite which works under the excitation of sun light and used as a substance in the treatment of wastewater. From the characterization techniques its was observed that the formed pure CeO and Ag doped CeO are impurity-free and possesses a size in nanometer range. Further it was noted that it produces reactive oxygen species (ROS) which are responsible for the improved antimicrobial activity and photocatalytic activity.

Keywords: antimicrobial activity, nanocomposite, cerium oxide, silver, photocatalyst, solar light

CP-36

STUDY OF PHASE SHIFT IN COPPER SULPHIDE DUE TO DIFFERENT PH AND DIFFERENT SOLVENT

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Abstract

Using a straightforward co-precipitate technique, Copper Sulphide was produced for each sample at a mole concentration of 0.5 M sodium Sulphide as an anion source and 0.2 M copper acetate as a cation source. The bath temperature was kept between 70 and 90 degrees Celsius. Twenty milliliters of TEA were utilized as a complexing agent, and for the all samples, a deep black precipitate with a greasy texture was obtained on top of the precursor. Samples of copper Sulphide were made both with and without aqueous ammonia, and the results showed that this had a major effect on the final compound. Water was used to prepare the solution for the first four precursor samples, and ethanol and water were used in equal amounts for the remaining two samples. All the filtered and cleaned powder samples annealed at 200 degrees Celsius were subjected to photoluminescence study, XRD, SEM with EDX, TEM, and XPS. The typical studies clearly show that the addition of ammonia to change the pH was a significant factor in the manipulation of the composition, surface morphologies, and sample structure. In the first Batch first and third samples, which were made without ammonia, had a bulky, greenish-black

color and a Cu_2S phase. However, when ammonia was added under the same conditions, the result was a smooth, dark-black powder that had a phase transition from Cu_2S to CuS and was entirely in water as the solvent. However in next batch, the fifth and sixth samples with the same amount of ethanol and water found to have opposite results from the first batch, producing Cu_2S phase instead of CuS while adding ammonia.

Keywords: Co-precipitation, Nanomaterials, Phase shift.

CP-37

EXPLORING THE INFLUENCE OF TAPIOCA EXTRACTS ON THE STRUCTURAL, OPTICAL, AND BIOMEDICAL CHARACTERISTICS OF 8-HYDROXYQUINOLINE NANOMATERIALS

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Abstract

This research delves into the transformative impact of tapioca extracts on the structural, optical, and biomedical attributes of 8-hydroxyquinoline nanomaterials. Through a meticulous synthesis process, tapioca components are integrated into the nanomaterials, inducing significant modifications to their structure and conferring distinctive optical properties. The investigation extends to the biomedical realm, where the potential of these hybrid nanomaterials for medical applications is explored. By elucidating the complex interplay between 8-hydroxyquinoline and tapioca, this study not only advances our comprehension of nanomaterial design but also lays the groundwork for the development of innovative and biocompatible nanomaterials with promising prospects in optical and biomedical fields.

CP-38

FT-IR, NMR AND UV– VIS SPECTRA, 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. FTIR spectra were recorded in the region of 400 – 4000 cm^{-1} and UV-Vis absorption spectrum of Pravastatin has been recorded in powder form in the region 190 -1400 nm. 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. Molecular docking and molecular dynamics have been performed for Anti- lipidemic drug.

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

CP-39

INVESTIGATIONONSILICADIOXIDE(SiO_2)NANOPARTICLESFORTHEUTILISATIONINGLASSINDUSTRY

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Abstract

The increasing demand for new materials with superior thermal, mechanical, and chemical abilities has drawn significant attention to silica nanoparticles qualitatively. Silica dioxide nano polymers have been utilized frequently in the manufacture of glass due to their high thermal stability. The sol-gel technique is one of the simplest methods to synthesize silica nanoparticles as the technique can produce uniformly distributed structures of high purity with less aggregation. The present research focuses on synthesising and analysing silica dioxide nanoparticles characteristics using various spectroscopic techniques such as UV-Vis spectroscopy, FTIR-ATR spectroscopy, Thermo gravimetric analysis, Dynamic light scattering technique, Powder X-ray diffraction technique and Scanning electron microscopic technique. The cut-off wavelength of silica dioxide nanoparticles was observed at 240 nm in the UV region using UV-Vis spectroscopy, and the band gap energy was found to be 5.1 eV. From the FTIR-ATR technique the polymeric Si-O-Si asymmetric stretching, symmetric stretching and bending vibration was observed at 1068 cm^{-1}, 792 cm^{-1} and 580 cm^{-1} respectively. Thermo gravimetric analysis (TGA) revealed that SiO_2 nanoparticles have a relatively high thermal strength and due to low thermal conductivity, no exothermic peaks werefounduntil1000°C.Theparticlesizeanalyser calculatedthe averagesizedistributionof thenanoparticles,and theresultsshow that the distributionwas uniform within thenanometre range (1- 100 nm). The crystal phase was studied by verifying the Powder X-ray diffraction technique results with the JCPDS data (Q = Quartz – JCPDS # 46-1045) and the sharppeaks correspond to crystalline phase of silica dioxide. The result from scanning electron

microscopic technique (SEM) showed that the silica dioxide nanoparticles have tetragonal shape with an average size of 68.5 nm. The EDAX technique results verified the elemental composition of SiO_2 nanoparticles with a weight percentage of 17.82%. The results promise that the Silica dioxide nanoparticles serve as an excellent insulator with high thermal stability and can be used in glass industries.

Keywords: Sol gel analysis, Thermal stability, Insulator, glass coating.

CP-40

CHEMICAL SYNTHESIS AND ENHANCED PHOTOCATALYTIC ACTIVITY OF NIO NANOPARTICLES

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Abstract

In recent years, Nickel Oxide has various applications such as fuel cell, magnetic materials, gas sensors, electrochromic film, catalysts, thermoelectric materials, waste water treatment and anode of organic light emitting diodes. Nickel oxide nanoparticles were synthesized using low cost chemical synthesis method. The formation of the NiO nanoparticles were studied by Fourier transform infrared spectroscopy. The face-centred cubic crystalline structure (JCPDS, No. 04-0835) of the material was confirmed by X-Ray Diffraction studies. The morphological studies were performed by Scanning Electron Microscope. The optical band gap energy of the material was found with the help of UV-Visible Spectroscopy. The photocatalytic activity of NiO nanoparticles has investigated the degradation of methylene blue dye.

Keywords: Nickel oxide, XRD, FTIR, SEM, UV-Visible Spectroscopy and Photocatalytic activity.

CP-41

SCREENING AND MOLECULAR DOCKING THE BIOACTIVE CONSTITUENT OF BRASSICA OLERACEA CAPITATA TO ERADICATE HELICOBACTER PYLORI

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Abstract

Peptic Ulcer is an inflammatory disease in the gastrointestinal mucosae. One of the main causes for Peptic Ulcer is the presence of a bacteria Helicobacter pylorus in the stomach. Presence of an enzyme Urease on Helicobacter pylorus makes it to survive comfortably and spread colonies in an acidic environment. Hence for resolving Peptic Ulcer, eradication of Helicobacter pylorus by inhibiting Urease is an important task. There are various synthetic drugs prescribed for eradicating Helicobacter pylorus. But they are suspected to be chemicals having many side effects and adverse effects.

Now a days, some of the secondary metabolites present in the plants and vegetables are acting as ligands for biological targets and perform as drugs. Brassica oleracea capitata is one such leafy vegetable considered for our study. GC-MS studies have been carried out to identify the bioactive constituents present in the ethanolic extract of Brassica oleracea capitata. Indole along with 76 other bioactive constituents are identified.in the mixture. Molecular docking studies have been carried out for Indole present in the ethanolic extract and the standard drug Acetohydroxamic acid for inhibiting the enzyme Urease of Helicobacter pylorus. The docking score and the Glide energies of Indole and Aceto hydroxamic acid are compared.

CP-42

EXPLORING AC FREQUENCY OF STEEL WIRES OF VARIOUS THICKNESS USING SONOMETER: A COMPARATIVE STUDY

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Abstract

This study focuses on the investigation of alternating current (AC) frequency characteristics exhibited by steel wires of varying thicknesses. Employing a sonometer setup, we aim to discern the AC frequency response of these wires, shedding light on their electrical properties. By subjecting the wires to controlled vibrations and measuring the resulting frequencies, we intend to unveil how wire thickness influences AC frequency. Through rigorous experimentation and analysis, our study endeavours to offer insights into the electrical behaviour of steel wires across different dimensions. The comparative analysis will serve to highlight any discernible patterns or anomalies in the AC frequency spectra, potentially uncovering valuable implications for wire manufacturing and applications. This research underscores the significance of understanding AC frequency dynamics in steel wires, providing a foundation for optimizing their performance in various industrial and engineering contexts.

CP-43

SPECTROSCOPIC, DENSITY FUNCTION THEORY AND MOLECULAR DOCKING STUDIES ON1-ACETYL-4-HYDROXYPHENYL PIPERAZINE

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Abstract

1-Acetyl-4-hydroxyphenyl piperazinepiperazine acid is a new organic material used widely in the drug industry. The optimized molecular geometry, vibrational frequencies, and infrared intensities in the ground state were carried out by using the density functional theory (B3LYP) method with a 6-311++G(d,p) basis set. A detailed interpretation of the infrared spectrum of the title compound is reported. The vibrational frequencies are calculated and compared with experimental FT-IR and FT-Raman spectra. AIM topological studies have been carried out on the molecule. Quantum chemical studies like NBO, HOMO LUMO, MEP, and contour maps were calculated. Drug-likeness and molecular docking of the title compound with different proteins were calculated and it acts as an antifungal agent.

Keywords: DFT; FT-IR; NBO; MEP; Molecular Docking

References:

[1] G. Keresztury, in: J.M. Chalmers, P.R. Griffith (Eds.), Raman Spectroscopy: Theory in Handbook of Vibrational Spectroscopy, vol. 1, John Wiley & Sons Ltd., New York, 2002.

[2] S.A.K. Elroby, M.S.I. Makki, T.R. Sobahi, Rifaat H. Hilal, Int. J. Mol. Sci. 13 (2012) 4321.

CP-44

BIO SYNTHESIS OF COPPER OXIDE NANOPARTICLES USING CITRUS SINENSIS PEEL EXTRACT

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Abstract

For the first time, copper oxide (CuO) was synthesized through a green route using C. sinensis peel extract. The prepared CuO nanoparticles were characterized using X-ray diffraction (XRD), Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR). The results revealed the successful synthesis of CuO nanoparticles by simple biological approach may provide a useful tool in the field of nanotechnology.

Keywords: Bio Synthesis; Citrus sinensis peel; CuO nanoparticles

CP-45

BIO SYNTHESIS OF ZINC OXIDE NANOPARTICLES USING CASSIA AURICULATA FLOWER EXTRACT

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Abstract

Zinc Oxide (ZnO) was synthesized through a green route using C. sinensis peel extract. The prepared ZnO NPs were characterized using X-ray diffraction (XRD), Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR). The results revealed the successful synthesis of ZnO NPs by easy natural approach may give a valuable tool in the field of nanotechnology.

Keywords: Bio Synthesis; Cassia auriculata flower; ZnO nanoparticles

CP-46

GREEN SYNTHESIS OF COBALT OXIDE NANOPARTICLES USING CITRUS SINENSIS PEEL EXTRACT

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Abstract

In this study, Cobalt Oxide (Co_3O_4) was synthesized through a green route using C. sinensis peel extract. The prepared Co_3O_4 NPs were characterized using X-ray diffraction (XRD), Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR). The results revealed the successful synthesis of Co_3O_4 NPs by easy natural approach may give a valuable tool in the field of nanotechnology.

Keywords: Green Synthesis; Citrus sinensis peel; Co_3O_4 nanoparticles

CP-47

BIOGENIC SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE AND ZINC OXIDE NANOPARTICLES USING CALOTROPIS GIGANTEA LATEX EXTRACT

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Abstract

The present investigation portrays the biogenic synthesis of iron oxide and zinc oxide nanoparticles mediated by the latex extract of Calotropis gigantea. Synthesized samples were tested for their structural, optical, morphological, antibacterial, and antioxidant properties. The structure of iron oxide and zinc oxide was confirmed as rhombohedral and hexagonal phases using XRD analysis. Various functional molecular bonding was identified using an FTIR spectrometer and the metal oxide bond between Fe-O and Zn-O was obtained at 619cm^{-1} and 632cm^{-1}. Morphological studies showed a spherical distribution of the particles with few agglomerates. The band gap of the prepared samples was calculated using a Tauc plot and found to be 5.17eV and 2.85eV respectively. The composition of the elements was identified using EDAX analysis. Antimicrobial assay studies against gram-positive and gram-negative bacteria E.coli and S.aureus were carried out with 50µl and 100µl concentrations and the zone of inhibition was good in comparison with the reference for both samples. The antioxidant activity of the synthesized samples was tested concerning a mixture of methanol and ascorbic acid with different concentration levels and results depicted that iron oxide nanoparticles have appreciable scavenging activity over zinc oxide nanoparticles.

Keywords: Iron Oxide, Zinc Oxide, Calotropis gigantea, Antibacterial, Antioxidant.

CP-48

SYNTHESIS, GROWTH AND CHARACTERIZATION OF L-TYROSINE GUANIDINE CARBONATE SINGLE CRYSTAL FOR NLO APPLICATIONS

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Abstract

A new Non-linear optical material L-tyrosine Guanidine Carbonate single crystal is synthesized by the slow evaporation solution growth technique at room temperature using water as a solvent. Good transparent LTGC crystal is sized. Single crystal X-ray diffraction reveals the crystal belongs to the Tetragonal P structure and a space group of P41212. The sharp intense peak in Powder XRD analysis confirms the good crystalline nature and purity of the crystal. The presence of various functional groups and their modes of vibration were identified by FTIR spectral analysis. The UV-Vis spectroscopic study shows that the lower cut-off wavelength is 234.6 nm with wide transparency range and very low absorbance. The optical band gap spectrum shows the energy gap of the crystal is about 5.6 eV. The LTGC was subjected to fluorescence analysis and it was ascertained that the maximum emission was in the green region at 532.4 nm. The mechanical behavior was studied by Vickers microhardness test. The presence of second harmonic generation for the grown crystal was confirmed by Kurtz Perry powder technique and it was found to be 1.5 times greater than that of standard KDP value which proves the Non-linear optical behaviour of the crystal. All these studies indicate that the LTGC crystal has NLO properties that can be used in the field like laser technology, optoelectronics, optical communication and Signal processing.

Key words: Single crystal XRD, Microhardness, Fluorescence, SHG

CP-49

GROWTH AND CHARACTERIZATION OF SULFAMIC ACID AND COPPER SULFATE SINGLE CRYSTAL

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Abstract

Blue emissive properties of Sulfamic acid and Copper sulfate single crystal is synthesized by the slow evaporation solution growth technique at room temperature using de-ionized water as a solvent. Good SACS crystal is sized. Single crystal X-ray diffraction reveals the crystal belongs to the Triclinic structure and space group P-1. The sharp, intense peak in powder XRD analysis confirms the good crystalline nature and purity of the crystal. The presence of various functional groups and their modes of vibration were identified by FTIR spectral analysis. The UV-Vis spectroscopic study shows that the lower cut-off wavelength is 230 nm with a wide transmittance range and very low absorbance. The optical band gap spectrum shows the energy gap of the crystal is about 5.36 eV. The SACS was subjected to fluorescence analysis, and it was ascertained that the maximum emission was in the blue region at 493.10 nm. The electrical properties were assessed by dielectric studies. The mechanical behavior was studied by the Vickers microhardness test.

Key words: Powder XRD, Single crystal XRD, Dielectric Studies, Fluorescence

CP-50

SYNTHESIS AND CHARACTERIZATION NANO $LiFePO_4$/C CATHODE MATERIALS

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Abstract

Li-ion batteries have a much higher energy density than that of lead-acid, Ni-Cd and Ni-MH batteries, large-scale lithium ion batteries have great potential for use in future electric vehicles and dispersed energy storage systems.$LiFePO_4$/C nano-sized cathode material were synthesized by solgel process which $LiFePO_4$ particles were embedded in amorphous carbon. The carbon does not affect the olivine structure of $LiFePO_4$. Some physical and chemical properties of the products were characterized by X-ray powder diffraction (XRD), SEM techniques. The effect of morphology and electrochemical properties of the composites were thoroughly investigated. It is revealed that the carbon layer coated on the surface of $LiFePO_4$ and the amorphous carbon wrapping and connecting the particles enhanced the electronic conductivity and rate performance of the cathode materials.

Keywords: Li-ion Battery, XRD, SEM

CP-51

PHOLCIDAE COBWEB EXTRACT AS A NOVEL BIOMATERIAL FOR THE ECO-FRIENDLY SYNTHESIS OF ZnO AND CuO NANOPARTICLES.

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Abstract

Biosynthesis is an alternative to conventional physical and chemical synthesis methods. Green synthesis of nanoparticles is gaining importance due to its cost-effectiveness, reduction of toxic chemicals, and extensive antimicrobial activity. In this current investigation, we synthesized Zinc oxide and Copper oxide nanoparticles using Pholcidae cobweb extract which

act as a biomaterial for the synthesis of desired nanoparticles from the precursor material by preparing cobweb extract by heat-assisted method. Prepared samples were characterized using various analytical techniques including XRD, FTIR, UV-Visible, SEM, EDAX, and antimicrobial studies. The structure was found to be hexagonal and Monoclinic for ZnO and CuO with an average crystalline size of 29nm and 97nm. From the UV-visible studies and based on the Tauc plot the band gap was 5.6 eV and 4.7eV. Molecular bonding of Zn-O and Cu-O was identified from the FTIR with the absorption peak at 470.50 cm^{-1} and 688.16 cm^{-1}. The elemental composition and surface morphology of the sample were analyzed and showed a uniform spherical structure in the case of ZnO and uneven distribution in CuO. Antibacterial studies with the selected species of Pseudomonas aeruginosa and Bacillus. Sub showed good results in the zone of inhibition at various concentration levels and the overall study showed that the synthesized specimen may find suitable applications against disease-causing pathogens.

Keywords: Zinc oxide, Copper oxide, biomaterial, Pholcidae cobweb, antimicrobial

CP-52

BIOSYNTHESIS AND CHARACTERIZATION OF ZnO AND CuO NANOPARTICLES USING *STRYCHNOS POTATORUM* SEED EXTRACT

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Abstract

The current study demonstrates the environmentally friendly method of synthesizing Copper oxide and Zinc oxide nanoparticles from seed extract of Strychnos potatorum. The specimens were prepared using $Zn(NO_3)_2.6.H_2O$ and $CuSO_4.5H_2O$ as precursors and the seed

powder of Strychnos potatorum as mediators. Prepared samples have been characterized using X-ray diffraction analysis, Fourier transforms infrared spectroscopy, UV-visible spectroscopy, SEM, and EDAX, antimicrobial and antibacterial studies. The structural morphology of ZnO and CuO nanoparticles was confirmed by XRD and the average crystalline sizes were found to be 13 nm and 36 nm, respectively. The molecular bonding formation was established by FTIR spectroscopy studies and the metal oxide bond between Zn and O nanoparticles is confirmed by the peaks at 687 cm^{-1} and 499.5 cm^{-1}, whereas for Cu-O nanoparticles are confirmed by the peaks at 529 cm^{-1} and 589 cm^{-1}. The cut-off wavelength of ZnO and CuO was found to be 231nm and 262nm and the band gap was calculated using Tauc plot and was calculated to be 5.1eV and 5.02eV.SEM results revealed that both the samples have some agglomerates with uneven distribution of particles which is due to the interaction of the phytochemicals with the precursor material. It showed some irregular cubes and spherical-shaped particles. Elemental composition was confirmed by EDAX analysis and the desired compound was present in the sample. The synthesized ZnO and CuO NPs were tested against Pseudomonas aeruginosa and Bacillus subtilis bacteria and the zone of inhibition was increased as the concentration of the sample increased and the overall investigation reports that the material found its application in the optoelectronic devices due to its remarkable optical properties and as a drug delivery material against disease-causing pathogens.

Keywords: Zinc Oxide, Copper Oxide, Strychnos potatorum, Structural, Antibacterial

CP-53

FTIR AND ESR SPECTROSCOPY – A VALUABLE TOOL TO STUDY OF DROUGHT TOLERANCE MECHANISM IN RICE (ORYZA SATIVA L.)

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Abstract

The drought stress management is one of the most significant challenges in the agricultural and crop research field. Hence, the present study focused on drought stress given to two varieties of rice (Oryza sativa L.) ADT-45 and ADT-49 and analyzed growth characteristics, physiological, biochemical changes, FT-IR and ESR spectroscopy analysis. The results showed that shoot, root height, fresh and dry mass, and RWC decreased as well as photosynthetic pigments, chlorophyll a and b were recorded low values in drought-induced plants compared to control of two varieties of rice and, FTIR spectroscopy was used to investigate the response of progressive drought. In this study, FTIR can provide valuable insights into drought responses of plants and may be useful for identifying novel drought tolerance traits. The free radical formation validated by electron spin resonance (ESR) in drought plants. ESR spectroscopy was an assured method for identifying tolerant and sensitive rice varieties in this study. Our results confirmed that drought affected the growth and physiological metabolism in two varieties of rice and ADT-49 relatively tolerant than ADT-45 which was either sensitive to drought stress or drought escape by complete their life cycle by early.

Keywords: Water stress, Oryza sativa, enzymatic antioxidants, ESR, FTIR.

CP-54

GREEN BIOSYNTHESIS OF ZNO NANOPARTICLES BY PHYLLANTHUS ACIDUS LEAF EXTRACT THEIR PHOTOCATALYTIC ACTIVITY TOWARD METHYLENE BLUE DEGRADATION

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Abstract

Synthesis of zinc oxide nanoparticles by green synthesis technique using phyllanthus acidus leaf extract is reported in this communication. Very stable nanoparticles of zinc oxide are obtained using zinc nitrate and phyllanthus acidus leaf extract. We explored the role of biological components, essential phytochemicals as reducing agent as well as capping agent and also as solvent system. XRD, FESEM, UV–vis spectroscopy and FTIR spectroscopy were used to investigate the structural, optical and vibrational properties of synthesised ZnO NPs. The pristine hexagonal wurtzite structure is confirmed by the XRD results. FESEM confirms the formation of spherical NPs. The EDAX analysis reveals the purity of ZnO NPs. The presence of Zn-O stretching vibration in the prepared NPs is revealed by FTIR analysis. UV–vis curve shows the optical response of ZnO nanoparticles and having the optical bandgap 3.24 eV. Photocatalytic ability of as synthesized samples was examined for the degradation of methylene blue. The percentage degradation of methylene blue using nanocomposite was 95 % in 80 min. This enhanced photocatalytic ability of nanocomposite make it a potential candidate for removal of organic pollutants from waste water.

Keywords: Biosynthesis; phyllanthus acidus; ZnO NPs; Photocatalytic activity; methylene blue

CP-55

GREEN SYNTHESIS OF ZnO NANOPARTICLES AND THEIR STRUCTURAL, OPTICAL AND ANTIBACTERIAL ACTIVITY

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Abstract

Development of plant based nanoparticles has many advantages over conventional physico-chemical methods and has various applications in medicine and biology. In present study, zinc oxide (ZnO) nanoparticles (NPs) were synthesized using leaf extracts of Syzygium cumini. 0.02 M zinc acetate dihydrate was used as a precursor in leaf extracts of respective plants for NPs synthesis. The structural and optical properties of NPs were investigated by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscope (SEM), and ultraviolet-visible spectrophotometer (UV-Vis). The antibacterial potential of ZnO NPs was examined by Agar well diffusion method method against two clinical strains of Escherichia coli (E. coli) and Staphylococcus aureus (S. aureus) based on the zone of inhibition. Change in color of the reaction mixture from brown to white indicated the formation of ZnO NPs.

Keywords: Biosynthesis; Syzygium cumini; ZnO NPs; Antibacterial activity

CP-56

Ni DOPING EFFECT ON THE STRUCTURAL AND OPTICAL PROPERTIES OF ZnO NANOPARTICLES PREPARED BY CHEMICAL CO-PRECIPITATION METHOD

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Abstract

The wet chemical precipitation method has been used to synthesize $Zn_{(0.04)}$ $Ni_{(0.01)}O$ nanoparticles. The morphological and optical properties of Ni-doped ZnO samples annealed at 350ºC are characterized by X-ray diffraction (XRD), reveals that Ni-doped ZnO crystallites were in hexagonal wurtzite crystal structure with secondary phase (NiO) was detected with a sensitivity of XRD measurement with increasing in the dopant concentration. FTIR spectroscopy furnishes additional evidence on functional groups. The outcome Field emission scanning electron microscopy (FE-SEM) results indicated the presence of hexagonal rods like nanostructures. Further, the optical energy bandgap obtained by Tauc plot. Room temperature Antibacterial studies reveal that the Ni-doped ZnO nanoparticles possess improved antibacterial activity against both gram-positive (Escherichia coli) and the gram-negative (Enterococcus faecalisis) bacterial strains than the pure ZnO nanorods.

Keywords: Coprecipitation; Nanocomposite; Antibacterial activity

CP-57

GREEN SYNTHESIS OF SNO_2 NANOPARTICLES USING PHYLLANTHUS ACIDUS PLANT LEAF EXTRACT AND ITS PHOTOCATALYTIC ACTIVITY OF METHYLENE BLUE DYE

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Abstract

Tin oxide (SnO_2) nanoparticles were prepared using Phyllanthus acidus plant leaf extract by calcining stannous chloride precursors at 350°C by green synthesis method. Synthesized SnO_2 NPs were confirmed via characterization techniques such as UV–visible spectroscopy (UV), X-ray diffraction (XRD), Scanning Electron Microscope (SEM) and Energy Dispersive X-ray analysis (EDAX). The results show that the synthesized SnO_2 nanoparticles have spherical morphologies, cassiterite crystal phases, and band gap values of 3.5 eV, respectively. Further we have undergone catalytic degradation of organic dye named methylene blue (MB). Photocatalytic activities of the as-synthesized products revealing that MB solution is almost completely degraded after 80 min under sunlight irradiation.

Keywords: green synthesis; Phyllanthus acidus; photocatalysis; methylene blue

CP-58

GREEN SYNTHESIS OF SNO_2 NANOPARTICLES USING PHYLLANTHUS ACIDUS PLANT LEAF EXTRACT AND ITS PHOTOCATALYTIC ACTIVITY OF METHYLENE BLUE DYE

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Abstract

Nanomaterials have significantly affected the different disciplines of science especially agriculture, medicine, environment, and energy production. So far, numbers of nanomaterials with promising features have been synthesized relying on physical, chemical, and biological processes. The nanocrystalline Copper Aluminate ($CuAl_2O_4$)should be prepared by sol-gel auto combustion method using copper nitrate, aluminium nitrate and glycine. The prepared nanoparticles were characterized by XRD, FTIR, FE-SEM and EDAX analysis. Further we have undergone catalytic degradation of organic dye named methylene blue (MB). Photocatalytic activities of the as-synthesized products revealing that MB solution is almost completely degraded after 80 min under sunlight irradiation.

CP-59

STRUCTURAL PROPERTIES AND CATALYTIC ACTIVITY OF A NOVEL gC3N4 DOPED CuO NANOPARTICLES

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Abstract

Investigating highly active, extremely stable, and environmentally friendly photocatalytic materials is the main problem with wastewater treatment.Scientists around the world favor graphitic carbon nitride (g-C3N4, GCN) due to its many advantages, including its ideal bandgap of approximately 2.7 eV, affordable cost, non-poisonous nature, and decent stability.In order to synthesis CuO/g-C3N4 nanocomposite for the treatment of wastewater, a straightforward Co Precipitation synthesis method was employed in this work.Using Fourier transform infrared

spectroscopy (FTIR) and X-ray diffraction (XRD), the formation of CuO and g-C3N4 were verified. The morphology of prepared CuO/g-C3N4 nanoparticles were studied using SEM analysis.The impact of CuO loading on g-C3N4's optical characteristic was ascertained through spectral analysis of ultraviolet-visible absorption.Thus, methyl orange and congo red were broken down using the prepared nanomaterial as the photocatalyst.Furthermore, following the formation of CuO/g-C3N4 heterojunctions, photostimulated e-/h+ pairs have shown a very good recombination rate. By coupling with transition metal oxides, the process for making CuO/g-C3N4 heterojunction catalysts gives the impression of increased rate of photocatalytic activity in the azo dyedegradation.

Keywords: CuO/g-C3N4, coprecipition method, Photo catalyst, •OH radicals, Azo dyes.

CP-60

CRYSTAL GROWTH, OPTICAL, FUNCTIONAL AND STRUCTURAL ANALYSIS AMMONIUM MALATE (AM) SINGLE CRYSTAL

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Abstract

Single crystal of Ammonium Malate (MA) has been grown by slow evaporation method at ambient temperature. The UV- Visible spectroscopy reveals that the crystal is transparent in the entire visible region with band gap energy of 4.2 eV. The SHG output of AM was recorded by Kurtz Perry technique and it is greater than that of KDP crystal.FTIR analysis was used to confirm the presence of various functional groups in the grown crystal. Powder crystal X-ray diffraction studies have proved that the title compound is belongs to the monoclinic system. In the overview of optical property of the grown crystal can be used for optoelectronics and photonic device fabrication.

CP-61

GROWTH, OPTICAL, FUNTIONAL AND STRUCTURAL PROPERTIES OF LITHIUM MALATE (LM) SINGLE CRYSTAL BY SLOW EVAPORATION TECHNIQUE

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Abstract

In the present work, the growth of Lithium Malate (LM) single crystal is reported. The crystals were grown by slow evaporation solution method using water as a solvent. The crystalline structure has been investigated using powder XRD analysis. From the UV-Visible spectroscopy, the cutoff wavelength and band gap energy of the grown crystal were determined. The cutoff wavelength of the crystal is 292 nm and band gap energy of the grown crystal is found to be 4.25eV. Hence the grown crystal was under the category of insulating material. A Fourier transform infrared spectral study was performed to identify the functional group present in the crystal. In the overview of optical property of the grown crystal can be used for optoelectronics and photonic device fabrication

CP-62

Synthesis, Growth, UV – Visible, FTIR and PXRD Characterization of Strontium Borate (SB) Single Crystal by Slow Evaporation Solution Growth Technique

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Abstract

In the present work, an inorganic Strontium borate (SB) single crystal was grown by slow evaporation solution growth technique. The grown crystals were characterized by UV-Visible, FTIR and powder X-ray diffraction analysis.The linear optical study from UV-Visible spectroscopy revealed the good transparency of the grown crystal in wide wavelength range

which suits the crystal for various electro optic applications. The presence of various functional groups in the grown sample was estimated by FTIR analysis. The lattice parameters were evaluated by powder X-ray diffraction analysis.

CP-63

CRYSTAL GROWTH, OPTICAL, FUNCTIONAL AND STRUCTURAL ANALYSIS AMMONIUM MALATE (AM) SINGLE CRYSTAL

R. Arivuselvi*, D. Santhiya, G. Divya, S. Sumithra

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Abstract

Single crystal of Ammonium Malate (MA) has been grown by slow evaporation method at ambient temperature. The UV- Visible spectroscopy reveals that the crystal is transparent in the entire visible region with band gap energy of 4.2 eV. The SHG output of AM was recorded by Kurtz Perry technique and it is greater than that of KDP crystal.FTIR analysis was used to confirm the presence of various functional groups in the grown crystal. Powder crystal X-ray diffraction studies have proved that the title compound is belongs to the monoclinic system. In the overview of optical property of the grown crystal can be used for optoelectronics and photonic device fabrication.

CP-64

CRYSTAL GROWTH AND CHARACTERIZATION OF MPMC SINGLE CRYSTAL USING METHANOL AS A SOLVENT BY SLOW EVAPORATION TECHNIQUE

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Abstract

In the present work, magnesium paranitrophenol manganese chloride (MPMC) single crystal where successfully grown by the slow evaporation technique using methanol as a solvent. The lower cut of wavelength was found to be 207 nm with a good optical transmittance window cover in the entire visible-NIR region. The optical band gap 5.60 eV was determined using Tauc's plot. The fundamental groups of the grown material have been identified by FTIR analysis. The lattice parameters of the grown crystals were determined by powder crystal X- Ray diffraction analysis. Photoluminescence study was carried out to determine the light emission property of MPMC crystal.

Keywords: Slow Evaporation technique; UV-Visible; Optical band gap; Photoluminescence study.

CP-65

SYNTHESIS, GROWTH, UV – VISIBLE, FTIR AND PXRD CHARACTERIZATION OF STRONTIUM BORATE (SB) SINGLE CRYSTAL BY SLOW EVAPORATION SOLUTION GROWTH TECHNIQUE

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Abstract

In the present work, an inorganic Strontium borate (SB) single crystal was grown by slow evaporation solution growth technique. The grown crystals were characterized by UV-Visible, FTIR and powder X-ray diffraction analysis.The linear optical study from UV-Visible spectroscopy revealed the good transparency of the grown crystal in wide wavelength range which suits the crystal for various electro optic applications. The presence of various functional groups in the grown sample was estimated by FTIR analysis. The lattice parameters were evaluated by powder X-ray diffraction analysis.

CP-66

FACILE SYNTHESIS OF NOVEL FOOD PACKAGING FILM FROM NATURAL STARCH BASED MATERIAL AND ITS ANTIMICROBIAL ACTIVITY

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Abstract

Natural starch from elephant food yam based PLA films have been widely used for food packaging application because of its antibacterial activity and cooling material. yam is easily available, low cost with excellent antimicrobial property. Elephant food yam was fabricated using poly lactic acid (PLA) with 1% percentages by one step solvent casting method. The natural starch-based PLA films were characterized by UV to determination of impurities of the sample, FTIR is an analytical technique used to identify organic (and some cases inorganic) materials and to find the Characterization of crystalline materials was analyzed throught XRD. The surface morphology of the natural food packaging films was analyzed through SEM. This natural food packaging films showed good chemical and physical properties compare to artificial film and has enhanced antibacterial activity with various microorganisms.

Keywords: PLA, FTIR, antimicrobial and SEM

CP-67

FABRICATION OF DYE-SENSITIZED SOLAR CELLS (DSSCS) USING NATURAL DYE EXTRACTS FROM CAMELLIA SINENSIS LEAF

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Abstract

Dye-sensitized solar cells (DSSC) represent a relatively new photovoltaic technology with great potential: investment costs for initiating production are low and manufacturing costs below 0.5 US$/$W_{peak}$ are predicted. Furthermore, DSSC offers the possibility of various colors and attractive designs, such as semitransparent modules. Record solar cell efficiencies are 11% for DSSC containing liquid redox electrolyte and 6% for DSSC with solid hole conductors. Promising stability data suggesting more than 20 years lifetime has been achieved. In this work a prototype of the dye-sensitized solar cell based on a natural organic dye from blackberry was studied. The samples have been characterized by Fourier Transform Infrared (FTIR), UV-Visible Spectroscopy, Scanning Electronic Microscopy and IV was recorded. The vibration assignments, intensities and wave number (cm^{-1}) of dominant peak were obtained from FTIR spectral analysis. Probable assignments of the bands were made with respect to the components present in the samples. The microphotograph obtained from scanning electron microscopy (SEM) .The UV/Vis spectra show that an absorption peak, occurring due to Surface Plasmon Resonance (SPR).The cell was fabricated using technologies available at NIT. The I-V characteristics with open circuit voltage,fill factor and efficiency of DSSC are calculated.

CP-68

Electron Transport in Triphenylamine context of Dye Sensitized Solar Cells: A DFT Study

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Abstract

Dye-sensitized solar cells (DSSCs) have drawn a significant interest due to their low production cost, light weight, better flexibility in design, and better tunability. Herein, two metal free organic dyes based on Donor-π-Acceptor types architecture having triphenylamine (TPA) as Donor, thiopen (T) and furan (F) as Spacer, Pyridyl (A1), and Carboxylic acid (A2) as the acceptor unit as are successfully designed for fabrication of DSSCs. To tune the optical

properties, structural engineering has been carried out. Various structural, electronic and optical parameters are calculated for the designed dyes. Our study reveals that dyes substituted with electron withdrawing groups possess lower values for both TPA-T-A1 and TPA-T-A1 groups of dyes. Moreover, the TPA-F-A1 and TPA-F-A1 values of all the dyes confirm the spontaneity of the electron injection and dye regeneration processes with respect to the conduction band of the TiO_2 surface and redox potential of the I^-/I^3 redox couple. The absorption properties also manifest the red shift behavior of the designed dyes. Hence, our study provides a good recommendation for further designing of dyes to enhance the performance of DSSCs.

Keywords: DSSCs, Acceptor, DFT, Electron Injection and Dye Regeneration.

CP-69

INVESTIGATION OF STRUCTURAL, OPTICAL AND ELECTROCHEMICAL BEHAVIORS OF CDMGAG@MWCNT NANOCRYSTAL BY MICROWAVE IRRADIATION-SYNTHESIS PROCESS

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Abstract

Multiwalled carbon nanotubes (MWCNTs) are three-dimensional nanomaterials that have numerous desired features. The materials possess high mechanical tensile modulus and strength, excellent electrical conductivity, and good thermal conductivity. CdMgAg@MWCNT nanocrystals were fabricated by the microwave irradiation-synthesis process (MISP). This method has produced well-structured nanocrystals easily, and the process was done in a very short period of time. The final product was collected in a dark crimson color. The structural analysis of the obtained nanomaterial has been revealed by XRD. The particle size has been

calculated by the Scherrer formula; an average particle size is 32.61 nm.To investigate the inherent strain and particle size using XRD peak broadening examinations, W-H plot techniques were applied. The crystallographic formula exhibits crystal properties, which confirm that the material has a cubic structure. The spectroscopy studies of UV-Vis spectroscopy given the cut off wavelength nearby 200 nm , the band gap energy is 5.47 eV and the PL spectra emitted red shift strongly. Electrochemical analysis The Cyclic Voltameter method given specific capacitance of the nanomaterial is 282.06 F/g. SEM study illustrates the morphology of the synthesized nanomaterial at different size range. The excellent electrochemical properties of CdMgAg@MWCNT composites contribute to their identification as high performance materials for supercapacitor electrodes.

Keywords: MISP, XRD, W-H plot, PL, MWCNT, etc.,

CP-70

ESTIMATION OF AVERAGE CRYSTALLITE SIZES, LATTICE PARAMETERS, VOLUME OF THE UNIT CELL, MICROSTRAIN, AND DISLOCATION DENSITY BY THE SYNTHESIS OF ZnO NANOPARTICLES

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Abstract

In this study,Zinc oxide nanoparticles (ZnO NPs) were synthesizedbychemical precipitation method. The prepared products werecharacterized by the X-ray diffraction, and

scanning electron microscope (SEM) with energy dispersive spectra (EDS) analysis. Structural behavior of the nanoparticles was studied by the XRD and it was found that ZnO NPs samples were hexagonal Wurtzite structure with no other phase. The effect of ZnO sample was clarified by calculatingaverage crystallite sizes, lattice parameters, volume, microstrain, and dislocation density. The morphology and the particle size were studied using SEM analysis. The prepared sample elements are confirmed by EDS analysis.

Keywords: Zinc OxideNPs, structural, chemical precipitation method.

CP-71

THE SYNTHESIS AND CHARACTERIZATION OF MOS_2 NANOFLOWERS DRAPED G-C_3N_4NANO SHEET (G-C_3N_4 / MOS_2 / TIO_2) TERNARYCOMPOSITE FOR THE EFFICIENT PHOTOCATALYTIC APPLICATIONS

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Abstract

In this study composite of g-C_3N_4 / MoS_2 / Tio_2Nano rod like composites synthesized using hydrothermal procedure. The structural, morphological and optical properties of the synthesized materials are studied by X-Ray Diffraction, Fourier Transform Infrared Spectroscopy, Field Emission Scanning Electron Microscope, Energy Dispersive X-Ray Analysis and UV –Vis Spectroscopy. The characterization by various methods clearly confirmed that the flower-like MoS_2 was loaded on the g-C_3N_4nanosheets and that the successful construction of the hetero junction widened the visible light absorption range. The waste water

contaminated by methyl dyes was purified using the product. The results show that a small amount of MoS_2 combined with g-C_3N_4 significantly improves the photo catalytic activity and increases the degradation rate as expected. So the composite can be employed as a catalyst for the removal of methyl dyes from industrial wastes.

Keywords:g-C_3N_4;MoS_2; Methyl Dyes; Photocatalysis; Clean Environment.

CP-72

CRYSTAL GROWTH, STRUCTURAL, SPECTRAL, OPTICAL, MECHANICAL AND NLO STUDIES OF ORANGE AZO DYE DOPED GLYCINE (OAG) SINGLE CRYSTALS

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Abstract

Single crystals of Orange Azo dye doped Glycine (OAG) has been successfully grown by the slow evaporation technique. Good optical quality crystal of OAG with well dimension is obtained. The structural information and crystal purity of the grown crystals were confirmed by Powder X-Ray diffraction analysis. The vibrational modes of the molecules and the presence of functional groups present in OAG were identified using FT-IR technique. The UV – Visible spectrum of OAG crystal shows that the grown crystals have wide range of optical transparency in the whole visible region. The mechanical strength of OAG crystal was estimated by Vickers micro hardness Analyzer. The Meyer index value (n) point out the grown crystal belongs to soft-material category. The stiffness constant (C_{11}) was calculated by the Wooster's empirical relation.The second-order nonlinear optical property of the fine powdered sample of OAG crystal was investigated by Kurtz-Perry powder technique and the relative second harmonic

generation efficiency was found to be higher than that of reference inorganic material potassium dihydrogen phosphate (KDP).

CP-73

HETEROGENEOUS-HOMOGENEOUS CHEMICAL REACTIONS OF OLDROYD-B FLUID FLOW OVER A STRETCHABLE SHEET WITH CATTANEO-CHRISTOV

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Abstract

This paper discusses the steady 2D hydro-magnetic radiative flow, mass and heat transfers of an Oldroyd-B liquid towards a stretchy surface along with heterogeneous and homogeneous reactions including heat generation. The heat flux is established on Cattaneo-Christov concept. Appropriate similarity transformations are applied to transmute nonlinear PDE to ODE. The homotopy setup is helped to crack the nonlinear ordinary system. The contributions of several physical constants are examined and discussed. The Opposite trend is got in the velocity graph for growing values of Deborah numbers.

Keywords: Oldroyd-B liquid; Thermal radiation; Magnetohydrodynamics;Cattaneo-Christov heat flux; Heterogeneous-homogeneous reactions.

CP-74

FACILE PREPARATION OF ALUMINIUM OXIDE THIN FILMS ON ALUMINIUM SUBSTRATE BY CHEMICAL OXIDATION METHOD

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Abstract

Aluminium oxide (Al_2O_3) thin films were prepared through a room temperature chemical oxidation of Al plate in a reaction solution containing dual oxidants (sodium hydroxide (NaOH) concentration and potassium persulfate ($K_2S_2O_8$)). The formed Al_2O_3 thin films were characterized through X-ray diffraction (XRD), UV-Vis-NIR spectrophotometer and Fourier transform infrared (FTIR) spectrometer analyses. The XRD profiles of the Al_2O_3 thin film samples prepared at different concentrations of $K_2S_2O_8$ and constant concentration of NaOH disclosed very low intense diffraction peaks of the hexagonal Al_2O_3. The UV-Vis-NIR reflection spectra of Al_2O_3 thin film samples formed on Al showed nearly more or less comparable absorbance in the visible region, nevertheless they showed considerable dissimilarities in the reflectance value in the NIR region. The mean reflectance of the Al_2O_3 thin film samples prepared using different $K_2S_2O_8$concentration of 30 and 60 mM were 34.36 and 32.30%, respectively with their corresponding solar absorptance (α) values were 0.78 and 0.82. The increase in the formation of the Al_2O_3 phase while increasing the concentration of the $K_2S_2O_8$in the reaction medium from 30 mM to 60 mM increases the solar absorptance value. The FTIR spectra of Al_2O_3 thin film samples exhibited peaks between 440 and 660 cm^{-1}, due to the characteristic stretching vibrations of Al–O bond in the Al_2O_3.The solar selectivity values calculated for the Al_2O_3 thin film samples prepared using $K_2S_2O_8$ concentration of 30 and 60 mM were 7.1 and 10.3, respectively.

Keywords: Chemical oxidation method; Dual oxidants; Aluminium Oxide; Thin film; Solar selective absorber

CP-75

ANALYSING THE DRUG USING FTIR, DPT AND UV SPECTROSCOPY

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Abstract

Spectroscopy is the use of absorption, emission, or scattering of electromagnetic radiation by matter to qualitatively or quantitatively study the matter or to study physical processes. Vibrational spectroscopy has significant contributions towards the studies of structure and physico chemical properties of crystals and molecular system. Recently spectroscopic studies of benzene and its derivatives have been motivated by their biological and pharmaceutical importance. This article deals with spectroscopic investigation of Carbamazepine of pharmaceutical and biological interest using FTIR, FTRaman and UV-Vis spectral measurements. To study the structure these pharmaceutical compounds, the FTIR spectrum of the compound has been recorded over the region 4000-400 cm -1. A satisfactory assignment of the fundamental vibrations has been made according to the position, shape, nature and relative intensity. The quality analysis of the chosen compound has been analyzed using UV-Vis spectroscopy.

Key words: FTIR, DPT and UV

CP-76

DENSITY FUNCTIONAL THEORY (DFT) CALCULATION OF METFORMIN TABLET

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Abstract

Metformin is one of the important anti-diabetic drugs. DFT calculations have been performed to study properties of adsorption of metformin onto **[**M/g-$C_3N_4]^{+,+2,+3}$, where M: Li, Na, K, Be, Mg, Ca, B, Al, and Ga. Optimized structures of all systems were calculated using the DFT method. The results were used to calculate the absorption energy (E_{ads}) with the PBE0-D3(BJ)/def2-TZVP method. The adsorption energy values for the most stable configurations are 19.1–131.6 kcal/mol. By adsorption of metformin on [M/g-$C_3N_4]^{+,+2,+3}$ surfaces, the ionization potential values of [M/g-$C_3N_4]^+$**,** M: Li, Na and K are low, which means that the stability of M: Li, Na and K systems are higher than the other systems (groups 2 and 3). The [M/g-$C_3N_4]^+$ complexes have been seen as interesting adsorbents of metformin molecule.

Key Words: DFT, Metformin.

CP-77

DISCRIMINATION OF HEALTHY AND THYROID AFFECTED PERSONS USING HAIR SAMPLES THROUGH FTIR-ATR.

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Abstract

Fourier Transform Infrared spectroscopy – Attenuated Total Reflectance (FTIR–ATR) provides excellent data quality combined with high reproducibility, with minimal user-induced variations and no sample preparation. Spectra from heterogeneous biological systems, including the integumentary system, can be associated with hundreds or thousands of biomolecules. We developed a new approach by using Machine-Learning (ML) tools to leverage the potential and enhance the selectivity of the instrument, create classification models, and provide invaluable information saved in human hair with statistical confidence. Here, we report chemometric analysis of FTIR-ATR spectra for the discrimination of healthy and Thyroid affected human hair for the analysis of Thyroid levels. In particular, here we consider Glucose\Lipid ratio as the

indication of Thyroid function. It shows a cellular effect or cellular response to Thyroid hormone.

Key words: FTIR – ATR , Chemometric analysis , Thyroid , Glucose/Lipid.

CP-78

FTIR-ATR AND UV-VISIBLE SPECTROSCOPICANALYSIS ON METFORMIN HYDROCHLORIDE

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Abstract

Metformin hydrochloride is an antidiabetic drug. The FTIR-ATR spectra of the compound has been recorded and a qualitativeanalysis on the vibrational bands has been carried out. The light absorption activity in the UV-visible region of the drug under different storage conditions has also been analyzed. Further, the absorption ratio referred to as Qvalue used in confirmatory test of identity is evaluated from the UV-visible spectra of the compound. The characteristic vibrational frequenciesof the drug have been identified and assigned using FTIR-ATR spectrum.Acomparison after the samplestored in the ideal conditions and are exposed to environmental hazards are made.

Key Words: FTIR-ATR , UV-Visible spectra, Metformin Hydrochloride, Vibrational analysis.

CP-79

DISCRIMINATION OF DIABETES WITH HEALTHY SUBJECTS USING NAIL SAMPLES USING FTIR-ATR SPECTROSCOPY

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Abstract

FTIR makes use of mainly two phenomena namely beer lamberts law & total internal reflection. In ATR sampling, the infrared (IR) light travels through a crystal, is totally internally reflected at least once at the crystal-sample interface; and the reflected light travels to the FTIR detector. During the internal reflection, a part of the IR light travels into the sample, where it can be absorbed. This is called the evanescent wave. The penetration depth of the evanescent wave into the sample is defined by the refractive index difference between the sample and the ATR crystal. To account for different sample types and different path length requirements, several materials with different refractive indices are used as ATR sensors. For liquids and pastes, a small drop of the sample is placed onto the ATR crystal. The measurement is taken, and, after completion, the crystal can be wiped clean using a light solvent. For my project Iam using FINGERNAILS as sample for the discrimination of people with diabetes & normal cholestrol levels using FTIR ATR.

Keywords: FTIR ATR, infrared regions, Total internal reflection, beer lamberts law, sample types & methodolgy, discrimination of diabetes using fingernails

CP-80

ASSAY PHOTO STABILITY CALCULATION OF METFORMIN TABLET

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Abstract

Ultraviolet spectroscopy or UV/vis spectrophotometry refers to absorption spectroscopy or reflectance spectroscopy in part of the ultraviolet and the full, adjacent visible regions of the electromagnetic spectrum. A UV-vis spectrophotometer is an analytical instrument that measures the amount of uv and visible light that is absorbed by a sample.It consists of many applications including quantitative and qualitative analysis of sample. Photostability studies of drugs and drug products are an integral part of the product development process in the pharmaceutical industry. These studies are carried out to ensure quality, efficacy, and safety of the formulated products during manufacture, storage, and use. It highlights the role of the photochemistry in the photo stability studies, describes the functional groups important for the photo reactivity of drugs, explains photophysical processes, and deals with the kinetics of photochemical reactions. The various modes of photo degradation of drugs with examples of selected compounds are presented. The biological consequences of the effect of light on the drug degradation are described. In my project for the assay photo stability calculation, I am using metformin Tablet as sample.

Key Words: UV and Visible spectroscopy, Metformin sample.

CP-81

COMPARATIVE STUDY OF THYROID HAIR SAMPLE WITH NAIL SAMPLE AND CHOLESTEROL HAIR SAMPLE WITH NAIL SAMPLE FTIR-ATR.

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Abstract

Fourier Transform Infrared spectroscopy – Attenuated Total Reflectance (FTIR–ATR) provides excellent data quality combined with high reproducibility, with minimal user-induced variations and no sample preparation. Spectra from heterogeneous biological systems, including the integumentary system, can be associated with hundreds or thousands of biomolecules. We developed a new approach by using Machine-Learning (ML) tools to leverage the potential and enhance the selectivity of the instrument, create classification models, and provide invaluable information saved in human hair with statistical confidence. Here, we report chemometric analysis of FTIR-ATR spectra for the discrimination of healthy and Thyroid affected human hair for the analysis of Thyroid levels. In particular, here we considerGlucose\Lipid ratio as the indication of Thyroid function. It shows a cellular effect or cellular response to Thyroid hormone.

FTIR makes use of mainly two phenomena namely beer lamberts law & total internal Reflection. In ATR sampling ,the infrared (IR) light travels through a crystal, is totally internally Reflected at least once at the crystal-sample interface; and the reflected light travels to the FTIR Detector. During the internal reflection, a part of the IR light travels into the sample, where it can Be absorbed. This is called the evanescent wave. The penetration depth of the evanescent Wave into the sample is defined by the refractive index difference between the sample and the ATR crystal. To account for different sample types and different pathlength requirements, several materials with different refractive indices are used as ATR sensors. For liquids and Pastes, a small drop of the sample is placed onto the ATR crystal. The measurement is taken, and, after completion, the crystal can be wiped clean using a light solvent .For my project I am Using FINGERNAILS as sample for the discrimination of people with cholesterol & normal levels.

Key words: FTIR – ATR ,Hair and Nail sample ,Comparation ,Thyroid, Cholesterol

CP-82

STRUCTURAL CHARACTERIZATION OF SILVER NOPARTICLES LOADED TITANIA NANOSPHERES NANOCOMPOSITE: ENHANCED PHOTOVOLTAIC PERFORMANCE OFDYE-SENSITIZED SOLAR CELL

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Abstract

Silver nanoparticles loaded TiO_2 nanospheres (Ag@TiO_2 NSs) nanocomposite has been synthesized by green synthesis route. The prepared nanocomposites samples are analyzed by DRS, XRD, FESEM and HRTEM techniques. It was found out that the prepared Ag@TiO_2 NSs nanocomposites exhibits strong light harvesting. The photovoltaic performance evaluation of Ag@TiO_2 NSs nanocomposites photoanode in dye-sensitized solar cells and evaluated under standard simulated solar light illumination of 100 mW cm^{-2}. The Ag@TiO_2 NSs photoanode loaded with 3 mM Ag has exhibited higher power conversion efficiency (η) of 4.82 % with a short-circuit photocurrent density (J_{sc}) of 11.92 mA $cm^{-2}$and open circuit voltage (V_{oc}) of 0.72 V. This improvement in the photovoltaic performance can be attributed to high dye loading, enhancement in visible light harvesting property and fast photo-generated electrons transfer prompted by the plasmonic Ag NPs.

Keywords: Ag@TiO_2 NSs, DRS, XRD, FESEM and HRTEM

CP-83

INVESTIGATION ON STRUCTURAL, ELEMENTAL, THERMAL, MECHANICAL, LINEAR, AND NONLINEAR OPTICAL NATURE OF POTASSIUM PENTABORATE TETRAHYDRATE INORGANIC SINGLE CRYSTALS

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Abstract

Potassium pentaborate tetrahydrate (PPBTH) is an inorganic nonlinear optical single crystal. It was grown by slow evaporation solution growth method at room temperature and physical properties there are studied. The lattice parameters of grown crystal were determined using single-crystal and powder X-ray diffraction analysis. The functional group of various vibrational modes was assigned using FTIR spectrum. The optical transmittance, optical band gap, optical constants, and extinction coefficient were determined by recording UV–Vis–NIR spectrum. The fluorescence study confirmed the green emission of PPBTH. Vickers hardness test estimates the mechanical properties for various loads. This material exhibited the soft material category. The magnetic properties of PPBTH were studied by vibrating sample magnetometer. Thermal behaviours of the grown crystals have been investigated using TGA/DTA analysis. The nonlinear optical studies confirm the second harmonic generation signal of the grown sample.

CP-84

GREEN SYNTHESIS OF COPPER NANOPARTICLE USING NERIUM OLEANDER FLOWER EXTRACT AND ITS CHARACTERIZATION

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Abstract

The investigation aims the synthesis of copper oxide Nanoparticle (CuO NPs) using Nerium odorum soland plant extract at room temperature. This method is completely a green method, free from toxic and harmful solvent. The CuO NPs were synthesized by mixing copper sulphate dehydrate (CuSO4.5H2O) and aqueous Nerium odorum soland flower extract. The biosynthesized copper oxide nanoparticles were characterized by UV-vis spectroscopy, Fourier-transform infrared spectroscopy (FT- IR) and scanning electron microscopy SEM), DLS (Dynamic light scattering) XRD (X-ray diffraction). The existence of the CuO NPs was revealed by UV-vis spectroscopy. The FTIR spectra of control (leaf extract) and synthesized CuO NPs identified the functional groups of the active components. SEM images brought out that the particles were spherical in shape, and the size was found to be ranging under 1μm. DLS, XRD are characterized by CuO Nanoparticle.

Keywords: Copper nano particle, Nerium odorum soland extract, SEM, XRD.

CP-85

SYNTHESIS AND AMPLE APPLICATIONS OF METAL BASED NANOMATERIALS DERIVED FROM NATURAL PRODUCTS

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Abstract

Plants have the ability to assist as biological factories for the creation of stable nanoparticles in bulk at a faster rate. Numerous physical, chemical, and biological methods are available for the syntheses of nanoparticles. But many of chemical and physical methods have become less popular due to using hazardous chemicals or their high costs, respectively. The ‘green’ environment friendly processes in chemistry and chemical technologies are becoming progressively popular and are much desirable as a result of worldwide problems allied with environmental concerns.

Keeping in view of the aesthetic sense, biosynthesis of nanoparticles from natural products appears to be a more significant in developing a hasty, clean, nontoxic, and eco-friendly technology. Moreover, the use of the plant extracts as reducing, stabilizing and coating agent is an interesting eco-friendly approach leading to high efficiency. Owing to the rich biodiversity of plants, their potential use toward the synthesis of these metal nanoparticles is yet to be explored. The objectives of our present work are:

- To synthesize of various biogenic nanomaterials from natural products.
- Various techniques will be used to characterize the synthesized nanomaterials.
- To study their potential applications in various fields.

CP-86

STRUCTURAL AND ELECTROCHEMICAL STUDIES OF NICKEL SULFIDE NANOPARTICLES USING SINGLE SOURCE PRECURSOR BY MICROWAVE IRRADIATION METHOD

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Abstract:

Nickel sulfide nanoparticles were synthesized by microwave-irradiation method using nickel diethyldithiocarbamate complex as single source precursor and Octadecylamine (ODA) as topping agent. The prepared Ni9S8 nanoparticles were orthorhombic crystalline structure confirmed by powder X-ray diffraction, FTIR spectroscopy were confirmed by functional group analysis, scanning electron microscopy (SEM) image shows that the prepared nanoparticles were feather like in structure and energy dispersive spectroscopy (EDS) with mapping analysis. The qualitative phase and morphology study of the nanoparticles is likewise seen in the investigation. The prepared Nickel sulfide nanoparticles were investigated with electrochemical studies for supercapacitor energy storage applications.

Keywords: Metal sulfide precursor, microwave-irradiation method, Octadecylamine, dithiocarbamates, supercapacitor.

CP-87

SYNTHESIS AND CHARACTERIZATIONS OF ZINC SULFIDE NANOPARTICLES BY HYDROTHERMAL METHOD FOR ENERGY STORAGE APPLICATION

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Abstract:

The development of energy storage materials with high capacity and rapid charging and discharging ability have become the most important and major issues of concern in recent years. In this study, a Zinc sulfide (ZoS) Nanoparticles (NPs) was successfully synthesized by hydrothermal method using Zn(Ddtc)2 complex as single source precursor and Octadecylamine (ODA) as capping and shape directing agent.

The prepared sample was characterized through powder x-ray diffraction analysis [XRD] which clearly shows the crystalline structure of the Zinc Sulfide (ZnS). Fourier transform infrared spectroscopic analysis [FTIR] was confirmed the characteristic vibration of prepared ZnS NPs. The surface morphology, elemental composition and purity of Zinc Sulfide were investigated through scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) technique equipped with mapping analysis. The redox behavior, charge discharge mechanism was done through cyclic voltammetry and galvanostatic charge-discharge studies; the optical property was studied by using UV–Vis spectrophotometer. Thermal stability of as prepared sample was studied by TG/DTA analysis. Electrical transport studies of the prepared nanocomposite have been analyzed for various temperatures. The prepared ZnS NPs was examined with electrochemical activity in aqueous medium.

Keywords: ZnS Nanoparticles, Hydrothermal method, cyclic voltammetry, chargedischarge analysis.

CP-88

HARMONIC VIBRATIONAL SPECTROSCOPY OF 1,3 DIPHENYL PROPENONE

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Abstract

The Fourier Transform Infrared (FTIR) and Fourier transform Raman (FTRaman) spectra of 1,3-Diphenyl Propenone were recorded in the regions 4000-400 cm-1 and 4000-100 cm-1, respectively, in the solid phase. Molecular electronic energy, geometrical structure, harmonic vibrational spectra was computed at the DFT/ 6-31G(d,p) and three parameter hybrid functional Lee-Yang-Parr/6-31G(d,p) levels of theory. The vibrational studies were interpreted in terms of potential energy distribution (PED). The results were compared with experimental values with the help of scaling procedures. Most of the modes have wave numbers in the properties of Mulliken population analysis have been calculated. Besides, thermodynamic properties were performed.

CP-89

SYNTHESIS OF BIOINSPRIED ORGANIC INORGANIC HYBRID COMPOUNDS

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Abstract

The physical and chemical properties of inorganic and organic hybrid materials have tremendous impact on key technologies such as energy generation and storage, information, medicine and automotive engineering organism produce various organic-inorganic hybrid materials, which are called biominerals. This biominerals organized structures from nanometer to macroscopic length scales, resulting in their remarkable. Physical and chemical properties that

cannot be obtained by simple accumulation of their organic and inorganic constituents. The fundamental molecular studies on silica iron oxide and calcium carbonate biomineralizarion describe material synthesis based on these mechanisms.

Theses model materials can be used to identify the key micrstrutural features that should quid the synthesis of bio inspired ceramic based composites with unique strength and toughness. Looking to the future there is no doubt that these new generations of hybrid materials, born from the very fruitful in these research fields.

The objectives of our present work are

• To synthesize of bioinspired organic inorganic hybrid compounds.

• To study their application in various fields.

CP-90

STUDIES ON SYNTHESIS, GROWTH AND CHARACTERIZATION OF SECOND HARMONIC NON-LINEAR OPTICAL ORGANIC 4-DIMETHYLPYRIDINIUM-4-CHOLOROBENZOLATE CRYSTAL BY SLOW EVAPORATION SOLUTION GROWTH TECHNIQUE

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Abstract

Organic materials of 4-Dimethylpyridinium-4-Cholorobenzolate (4DMP4CB) were successfully grown by the slow evaporation method. The solubility was found to be low in water and so the crystallization 4DMP4CB was performed from its aqueous solution. The powder XRD spectrum shows the good crystalline nature of the grown crystal. The FTIR spectrum result confirms the various functional groups present. The optical transmittance with their cutoff wavelength has been identified by UV-Vis-NIR studies. Thermo gravimetric analysis and differential thermal analysis have also been carried out, and thermal stability shown good

quality. Second Harmonic Generation (SHG) on powder sample has been measured using the Kurtz and Perry technique. The micro hardness measurements were used to investigate the mechanical property of the grown crystal. The dielectric studies were performed at different temperatures and frequencies to analyze the electrical properties. Nonlinear optical (NLO) property confirms the SHG efficiency for the grown crystal.

Keywords: XRD, FTIR, UV-Vis studies, Thermal stability, SHG, grown crystal.

CP-91

UV, XRD, NMR AND PHOTOLUMINANCE CHARACTERIZATIONS OF NONLINEAR OPTICAL 2, 3- DIAMINOPYRIDINIUM 4-CARBOXY BUTANOATE (DPCB) SINGLE CRYSTAL

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Abstract

Optically good quality organic single crystals of 2, 3- Diaminopyridinium 4carboxy butanoate were grown using methanol solvent. The crystal structure and the crystalline nature of the compound were find using X-ray diffraction technique.The functional group of 2, 3-Diaminopyridinium 4-carboxy butanoate were find by FTIR Structural confirmation of the crystal was carried out using 1H-NMR and 13CNMR characterization studies. UV plot showed visible region transparency of the grown crystal. Dielectric, DC conductivity, photoconductivity, photoluminenscence results were taken for the grown crystal. Additionally, third order nonlinear optical (NLO) efficiency of the crystal is found employing pumped diode laser of wavelength 532 nm.

Key words: Crystal growth, Nonlinear, Band gap, Optical, Dielectric studies

CP-92

GROWTH AND CHARACTERIZATION OF BARIUM CHLORIDE DOPED WITH ORGANIC COMPOUNDS

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Abstract

The crystal growth of barium chloride doped with organic ompounds, cadmium chloride, thiourea in 1:1:1 molar ratio was dissolved in distilled water and the mixed materials were stirred well for 4 hours for homogenization. Then the solution was filtered in a beaker and covered with perforated polyethylene. The prepared solution was allowed to evaporate by slow evaporation technique at room temperature. After 10 days good quality white transparent crystals were obtained. Its dimension was found to be 12 mm x 7 mm x 2 mm. The grown crystals were subjected to various characterization techniques. The crystal system has been identified and lattice dimensions have been measured by X- Ray analysis. The functional groups of grown crystals were qualitatively examined by FTIR analysis. Its optical characters have been assessed by UV- Spectral transmission analysis. Further the hardness and fluorescence nature of the sample were analysed and reported.

CP-93

STRUCTURAL CHARACTERIZATION OF SILVER NANOPARTICLES LOADED TITANIA NANOSPHERES NANOCOMPOSITE: ENHANCED PHOTOVOLTAIC PERFORMANCE OF DYE-SENSITIZED SOLAR CELL

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Abstract

Silver nanoparticles loaded TiO2 nanospheres (Ag@TiO2 NSs) nanocomposite has been synthesized by green synthesis route. The prepared nanocomposites samples are analyzed by DRS, XRD, FESEM and HRTEM techniques. It was found out that the prepared Ag@TiO2 NSs nanocomposites exhibits strong light harvesting. The photovoltaic performance evaluation of Ag@TiO2 NSs nanocomposites photoanode in dye-sensitized solar cells and evaluated under standard simulated solar light illumination of 100 mW cm–2. The Ag@TiO2 NSs photoanode loaded with 3 mM Ag has exhibited higher power conversion efficiency (η) of 4.82 % with a short-circuit photocurrent density (Jsc) of 11.92 mA cm−2and open circuit voltage (Voc) of 0.72 V. This improvement in the photovoltaic performance can be attributed to high dye loading, enhancement in visible light harvesting property and fast photo-generated electrons transfer prompted by the plasmonic Ag NPs.

Keywords: Ag@TiO2 NSs, DRS, XRD, FESEM and HRTEM

CP-94

TEMPERATURE EFFECT TO INVESTIGATE OPTICAL AND STRUCTURAL PROPERTIES OF AZO NANOSTRUCTURES FOR OPTOELECTRONICS

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Abstract

A novel method to synthesize technique is used to deposit nanostructured Aluminium (Al) doped zinc oxide (ZnO) on p-Si substrate. Atomic forces microscopy (AFM), X-ray diffraction (XRD), Ultraviolet–diffusion reflectance spectroscopy (UV–DRS) and Field emission - scanning electron microscopies (FE-SEM) are utilized to investigate the influence of annealing temperature in the range of 200®Cto 500®C on the morphological, optical, structural and topographical characteristics of Al NPs-doped ZnO (AlZnO) nanostructure. The average reflectance is proven by the reflectance spectra to be in the wavelength range of 180–900 nm, and the absorption spectra provided the optical energy gaps of nanostructured Al-ZnO The

optical band gaps and Al-ZnO's annealing temperatures were directly linked at 3.40–3.67 eV as demonstrated by UV–Vis. Crystalline and grain size are correlated with annealing temperature variations from, thus providing more homogeneous and covered surface morphology. In this case, AZO nanostructures play a significant role in the near future. The surface nanostructures' high quality and versatile characteristics ensures its promising role in optoelectronics future researches.

Keywords: Al-ZnO, doping Al, annealing temperature, optical properties

CP-95

INVESTIGATIONS ON STRUCTURAL, OPTICAL AND MAGNETIC PROPERTIES OF DY SUBSTITUTED LAFEO3 PEROVSKITES

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Abstract

In the present investigations, perovskite type ceramic compounds of La1xDyxFeO3 (x=0, 0.1) have been prepared by High temperature solid state reaction method (HT-SSR). The X-ray diffraction (XRD) analysis indicates the single phase perovskite compounds. The Fourier transform infrared spectra confirms the Me-O vibrations of the synthesized compounds. Surface morphology of the compounds analysed using scanning electron microscopy (SEM) and elemental distributions were performed using EDS with mapping. The optical absorption was recorded at room temperature and energy bandgap (Eg) values are calculated using tauc's plot. The obtained optical band gap values of Pure LaFeO3 and Dy substituted LaFeO3 is 2.09 eV and 2.41 eV respectively. The pristine LaFeO3 compound shows the canted antiferromagnetic nature, After the Dysprosium substituted LaFeO3 sample exhibit paramagnetic nature at room temperature. From the M-H loop, saturation magnetization (Ms), remnant magnetization (Mr),

coercivity (Hc) and anisotropy constant (K1) values are calculated. The Dy3+ substituted with LaFeO3 is greatly influenced by the magnetic parameters.

Keywords: LaDyxFe1-xO3 perovskites; solid-state reaction; Optical bandgap; magnetic behaviour.

CP-96

GREEN SYNTHESIS AND CHARACTERIZATION OF COPPER NANOPARTICLES USING *ARTABOTRAYS HEXAPETALUS* LEAF EXTRACT

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Abstract

Nanoparticles being the smallest unit of nanotechnology now play an important role in our lives in different fields. The present study examines the synthesis of Cu Nanoparticles using a green synthesis method using a medicinal plant. The aqueous solution of *Artabotrays Hexapetalus* (*A. hexapetalus*) leaf extract and CuSO4 was carried out in the preparation process. The formation of copper nanoparticles is confirmed by a change of colour from pale green to dark brown which, mainly due to the properties of this phenomenon and the surface, acts as a plasma resonance. The detailed characterization of CuNps is performed by XRD, UV, FTIR, SEM & EDAX. The average grain size and structure of the material is calculated from the XRD analysis. X-ray diffraction patterns for pure and CuSO4 doped with leaf extract, prepared as a sample of powder. The main peaks appeared at 32.9°, 35.3°, 38.3°, 41.9°, 46.2°, 48.5°, 61.3°, 65° and 78°. Diffraction peaks can be easily indexed to CuSO4 phases, which are in good agreement with the reported values of the JCPDS. It is evident from the FTIR study that various expected functional groups are present in the sample. UV-Vis is used for optical properties and calculates the band gap energy. UV-Visible spectrum absorbance peak of CuNps at around 371.50 nm and its band gap energy was calculated as (3.33) eV. SEM & EDAX was used to investigate the morphology of prepared CuNPs. In conclusion, the synthesis of nanoparticles

with aqueous *A. hexapetalus* leaf extract is simple, fast, environmentally friendly and inexpensive.

Keywords: Green synthesis, Copper nanoparticles, *A. hexapetalus*, XRD, FTIR, UV, SEM, EDAX.

CP-97

MAGNETIC, DIELECTRIC AND NLO PROPERTIES OF L-LEUCINE PHTHALIC ACID SINGLE CRYSTAL

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Abstract

Single crystals of L-LPA were obtained by slow evaporation of an aqueous solution containing L-Leucine (C6H13NO2) and Phthalic acid (C8H6O4) in the 1:1 stochiometric ratio. The Kurtz and perry powder technique is had been used to measure The relative SHG activity of the (L-LPA) crystal. The efficacy of NLO crystals largely depends on its surface quality for its ability to withstand high power intensities in addition to their linear and nonlinear optical properties, Magnetic analyses of L-Luecine Phthalic acid (L-LPA) single crystals was studied.

The variation of εr and dielectric loss with frequency are discussed. Fully grown needle shaped crystals appearing inside the gel column and the harvested crystals. These crystals belong to the monoclinic crystal system with the non-centrosymmetric space group, the prominent peaks as (101), (112) and (300) were observed. The good crystallinity nature of the grown crystals was confirmed by sharp XRD pattern peaks. **Keywords:** biomaterial, adsorption, heavy metals, isotherms

CP-98

GREEN SYNTHESIS OF COPPER OXIDE NANOSTRUCTURE USING *CURCUMA LONGA* EXTRACT

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Abstract

In this report, green synthesis of copper oxide nanoparticle utilizing *Curcuma longa* is elucidated for the first time. The *C. longa* extract serve a dual role as reducing and capping agent during the fabrication of copper oxide nanoparticles. The copper oxide particles were characterized by scanning electron microscopy (SEM). Structural characterizations were analyzed by X-ray diffraction (XRD) pattern and Fourier transform infrared (FTIR) spectrum of CuO additionally proves formation of monoclinic CuO. Energy dispersive X-ray (EDAX) spectroscopy analysis demonstrated pristine nature of CuO nanostructures.

Keywords: Green Synthesis; Curcuma longa extract; Nanostructures

CP-99

GREEN SYNTHESIS OF COPPER OXIDE NANOSTRUCTURE USING BLACK VITEX LEAF EXTRACT

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Abstract

NPs are attracting wide attention from varied disciplines of science due to their immense application in diverse field. In this report, green synthesis of copper oxide nanoparticle utilizing *Black vitex leaf* is elucidated for the first time. The copper oxide particles were characterized by scanning electron microscopy (SEM). Structural characterizations were analyzed by X-ray diffraction (XRD) pattern and Fourier transform infrared (FTIR) spectrum of CuO additionally proves formation of monoclinic CuO. Energy dispersive X-ray (EDAX) spectroscopy analysis demonstrated pristine nature of CuO nanostructures.

Keywords: Green Synthesis; Black vitex leaf extract; Nanostructures

CP-100

Mg FERRITES SYNTHESISED BY SOL-GEL AUTO COMBUSTION METHOD: STRUCTURAL, DIELECTRIC AND MAGNETIC BEHAVIOUR OF SPINEL STRUCTURE (MGFE2O4)

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Abstract

In this present work, we have synthesised Magnesium ferrites (MgFe2O4) by Auto combustion method. The aqueous materials Magnesium nitrate, Ferric nitrate involved for synthesised and a glycine used as a chelating agent. The prepared sample is calcinated at 850oC

for 8 hours. We have done the different structural and physical properties characterized for prepared MgFe2O4. Powder XRD studies confirmed the crystal structure, FTIR shown the presence of various functional groups, FE-SEM demonstrated the surface morphology of the prepared sample, EDAX proved the percentage of chemical composition of Mg ferrites. Dielectric constant, dielectric loss, Cole-Cole plots and AC Conductivity for the Mg Ferrites for various frequencies at different temperatures. The magnetic parameters such as saturation magnetization(Ms), coercivity(Hc) and remanence(Mr) are studied for prepared sample. The behaviour of Mg Ferrite is ferromagnetic nature at room temperature (30oC) which is applied in many industrial applications.

Keyword: FE-SEM, Maxwell-wagner, Interfacial, Ferromagnetism

CP-101

FLUORESCENCE EMISSION, LIFE TIME, THERMAL PROPERTIES OF TRANS-STILBENE MIXED DIPHENYLACETYLENE SCINTILLATOR CRYSTAL

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Abstract

Diphenylacetylene (DPAC) is a promising organic scintillator material for fast neutron detection. Solubility measurement was carried with two different solvents such as toluene and methanol. Stilbene mixed diphenylacetylene (DPACS) was successfully harvested from toluene with the dimensions of 42 x 12 x 8 mm3. X-ray diffraction confirms the monoclinic crystal structure of grown with the obtained lattice parameters. The vibrational characteristic functional group was identified by FTIR studies. UV-Vis spectral analysis of the grown DPACS crystal reveals good optical transparency in visible and near IR region. The thermal behaviour and melting point of the sample was analysed by TGA-DSC. Chemical etching analysis was carried

out on the crystal surface at ambient temperature to see the dislocations and growth pattern of the crystal. Fluorescence broad emission peak was observed and the prompt and delayed fluorescence lifetimes of the DPACS were calculated.

Keywords: Organic Scintillator Crystal, Fast Neutron Detector, Trans-stilbene, Solubility of Diphenylacetylene, Fluorescence emission and Decay time, Thermal analysis.

CP-102

GREENER APPROACH ON ZNO NANOPARTICLES USING SESBANIA GRANDIFLORA LEAF EXTRACT AND ITS BACTERICIDAL ACTIVITY

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Abstract

Our massive biodiversity encourages scientists to explore innovative ideas. One of the rapid emerging fields is 'NANOTECHNOLOGY'. Yet there are different methods available, plant- mediated synthesis is the toxic free, elegant and simple instrumented method. Sesbania grandiflora is noteworthy for its multifaceted benefits. The anti-glycation property of this leave extract is remarkable. This paper is about the biosynthesis of zinc oxide nanoparticles from sesbania grandiflora leaf extract. Synthesized Nanoparticles were confirmed by various characterization techniques like X ray diffraction (XRD), Fourier Transform infrared spectroscopy (FTIR), Scanning electron microscope (SEM) with Energy Dispersive X-ray spectroscopy (EDAX) profile, UV-vis spectroscopy and antimicrobial activity. The average crystalline size found by Scherrer formula was 15 nm with hexagonal phase. The surface morphology and the transparency of the sample is determined by SEM and EDAX. The strong absorption peak at 340nm achieved the bandgap energy of 3.6 eV. Different chemical constitutions present in leaf extract made a way for antibacterial activity. Optimal activity of the synthesize sample was observed.

Keywords: ZnO NPs, Sesbania Grandiflora, X-RD analysis, Antibacterial Activity.

CP-103

BIO SYNTHESIS OF COPPER OXIDE NANOPARTICLES USING COFFEE SEEDS EXTRACT WITH ITS ANTIBACTERIAL ACTIVITY

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Abstract

The present work is concerned on the green synthesis of Copper Oxide nano particles from the extract of Coffee seeds. The synthesized sample was characterized for structural, functional, surface morphological, optical properties and anti-bacterial activity. From the XRD, the average crystalline size of the synthesized CuO NPs was found to be 15.26 nm. The functional present in the synthesized CuO NPs were confirmed in the FTIR spectrum. The band gap energy of the synthesized CuO NPs was found to be 1.19 eV from UV analysis. SEM analysis was used to find the surface topography. The synthesized CuO NPs exhibits flower like structure. Anti-bacterial activity of CuO NPs showed significant inhibition against both grampositive and gram-negative bacterial activity.

Keywords: Copper Oxide nanoparticles, Coffee seeds, X-RD Analysis, Antibacterial Activity.

CP-104

GROWTH AND CHARACTERIZATION OF PRISTINE AND DOPED SULPHAMIC ACID SINGLE CRYSTALS

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Abstract

The sulphamic acid crystal doped with L- histidine was grown using a solvent evaporation technique. X-ray diffraction experiments confirmed the orthorhombic structure. The optical transmission is an increase by the dopant in the whole visible region with a low cut-off wavelength is less than 220 nm. TG and DTA studies determined the title crystals are thermal stability up to 210 (pure) and 207 (1mol %). The enhancement in the hardness of the crystal after L- histidine doping was confirmed by the hardness test. The photoconductivity sensitivity of grown crystals is 0.101, and 0.371 for pure and 1 mol% respectively. The laser damage threshold analysis show that the L- histidine doped SA crystals have a high LDT 32 and 35 GW/cm2 than pure (17 GW/cm2) and KDP (27 GW/cm2) crystal. It is claimed that the L-histidine doped SA is a promising material for the improvement of device fabrication applications.

Keywords: Single crystal; Optical material; Laser damage threshold; Thermal property, Photoconductivity.

CP-105

SYNTHESIS OF MIXED IRON MAGNESIUM OXIDE (FEMGO) NANOPARTICLES FOR DEGRADATION OF METHYL ORANGE AND DYE REMOVAL FROM INDUSTRIAL WASTE WATER

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Abstract

Groundwater and agricultural soils are polluted for some reason such as solid waste, industrial waste, medical waste, but textile and industrial dyes are mixed in rivers and lakes are one of the main causes of water and soil pollution. The metal oxides were used to decompose wastewater and toxic dyes. Most of the researchers used metal oxides likeTiO2, ZrO2, ZnO2 CuO and etc. In the present work, mixed iron magnesium oxide **(**FeMgO) nanoparticles were synthesized using thermal plasma arc discharge method. The prepared powders were

characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and UV–VIS spectroscopy. Moreover, the adsorption actions of the nanoparticles were evaluated by the removal rates of methyl orange (MO) and waste water (WW). SEM-EDS studies revealed that the nanoparticles consisted of mixed oxide such as magnesium oxide (MgO) and iron oxide (FeO) particles. XRD revealed that the standard crystal size was calculated to be 25 nm. The synthesized nanoparticles had a strong adsorption activity for methyl orange (MO) and waste water (WW), degradation within 14 min and 120 min, respectively. Hence, the present study proposes that the FeMgO nanoparticles can be employed for the removal of dyes from wastewater.

Keywords: plasma arc discharge, FeMgO nanoparticles, industrial waste water and dye adsorption.

CP-106

COW DUNG EXTRACT AS A LOW-COST AND NATURAL SENSITIZER FOR DYE-SENSITIZED SOLAR CELL: A NOVEL INITIATIVE FOR WASTE TO ENERGY CONVERSION APPROACH

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Abstract

Cow dung extracts are prepared using ethanol and methanol as solvents. Electronic absorption spectra of cow dung extracts have exhibited broad absorption in UV and visible region of the solar spectrum between 300 and 730 nm. The absorption of cow dung extracts showed variations in intensity and absorption peaks at different wavelengths, which can be attributed to presence of diverse photosynthetic pigments corresponding to polarity of applied solvents. The observed pigments of chlorophyll *a*, chlorophyll *b* and carotenoids in the cow dung extracts can be ascribed to the feeding behavior of the cow. The FTIR and UV-vis absorption results disclosed that the sensitization of ZnO photoanode is mainly due to the chlorophylls present in the cow dung extract. The methyl group in the chlorophyll molecules can from an ideal bond with ZnO

nanoparticles that facilitates electron transfer from the chlorophyll molecules to the conduction band of ZnO. The solar cells sensitized with cow dung extract in methanol has delivered highest energy conversion efficiency of 0.102% with a short-circuit photocurrent density of 595 μA/cm2, open-circuit photovoltage) of 0.45 V and a fill factor of 0.38, which could be ascribed to presence of relatively a greater number of photosynthetic pigments.

Keywords: Dye-sensitized solar cell; Cow dung extract; Natural sensitizer; Photosynthetic pigments; Photovoltaic performance

CP-107

BOOSTING THE SPECIFIC CAPACITANCE OF NICKEL OXIDE/REDUCED GRAPHENE OXIDE COMPOSITE FOR SUPERCAPACITOR APPLICATION

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Abstract

Supercapacitors (SC) have made much attractive to future electronic applications owing to their unique property such as high storage ability at a short time span and more cycle durability. The energy density and capacitance of SC should depend on the choice of electrode materials. In this work, the nickel oxide (NiO)@reduced graphene oxide (rGO) composite electrode materials were synthesized by hydrothermal method. Structural property of NiO@rGO composite were examined by X-ray diffraction pattern and Raman spectroscopy. In the Raman spectra, The G-band (sp2 vibration mode of carbon-carbon bonding) was shifted from 1590 cm-1 to 1581 cm-1 compared to GO, it is due to the charge transfer between the carbon and NiO [1]. The surface morphology of the samples was investigated by FESEM, TEM, and STEM analysis, where plate-like NiO was attached on the surface of rGO sheets.The electrochemical and specific capacitance

of NiO@rGO electrode materials was studied and it shows better performance when compared with the NiO electrode.

CP-108

GREEN SYNTHESIS OF CUO NANOPARTICLES WITH BACTERICIDAL ACTIVITIES USING *FILAMENTOUS ALGAE* EXTRACT

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Abstract

Biological strategies for nanoparticle synthesis using microorganisms, enzymes, and plants or plant extracts are advised as attainable ecofriendly alternatives to chemical and physical strategies. In this paper, Copper oxide nanoparticles were synthesized by using copper nitrate and *F. algae* extract. The morphological characterizations were analyzed by scanning microscopy (SEM). Structural characterizations were analyzed by X-ray diffraction (XRD) pattern. Energydispersive X-ray (EDAX) qualitative analysis demonstrated pristine nature of CuO nanostructures. Hence, this work complete that the potential bactericidal activity exhibited by CuO nanostructures against gram-positive and gram-negative microorganism strains.

Keywords: Green Synthesis; Filamentous algae; CuO nanoparticles; Antibacterial activity

CP-109

GREEN SYNTHESIS OF COPPER OXIDE NANOSTRUCTURE USING *LETTUCE RED* LEAF EXTRACT

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Abstract

In present days, green synthesis of copper oxide (CuO) nanoparticles has received considerable attention due to nontoxic, low-cost and eco-friendly. For the first time CuO nano structures was develop using the extract of Lettuce red (L.red).

The morphological characterizations were analyzed by scanning electron microscopy (SEM). Structural characterizations were analyzed by X-ray diffraction (XRD) pattern. Energy-dispersive X-ray (EDAX) spectroscopy analysis demonstrated pristine nature of CuO nanostructures.

Keywords: Green Synthesis; Lettuce red leaf; Nanostructures

CP-110

FACILE SYNTHESIS OF MOLYBDENUM DISULFIDE AND ITS APPLICATIONS

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Abstract

In this work, the nanostructure Molybdenum disulfide (MoS2) nanoparticles were successfully synthesized for various temperatures like (140oC, 160oC, 180oC,

200oC) by using facile hydrothermal method. The prepared nanoparticles have been observed systematically by the advanced techniques such as X-Ray diffraction (XRD), Fourier Transform Infrared Spectra (FTIR), and Scanning Electron Microscopy (SEM). The structural analysis of the prepared nanoparticles was observed from XRD. From FTIR, the functional groups of the synthesized nanoparticles have been studied. The surface morphology of the prepared nanoparticles was captured through SEM.

Keywords: MoS2, XRD, FTIR, SEM

CP-111

TIGHT FOCUSING PROPERTIES OF DOUBLE RING SHAPED LONGITUDINALLY POLARIZED MULTI GAUSSIAN BEAM

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Abstract

Tight focusing of double ring shaped longitudinally polarized multi gaussian beam with cosine phase plate is studied numerically based on vector diffraction theory. For higher-order, radially polarized mode beams as well as a fundamental mode (RTEM01*) beam, the strong longitudinal component forms a sharper spot at the focal point under a high-NA focusing condition. In particular, double-ring-shaped radially polarized mode (R-TEM11*) beams can effectively reduce the focal spot size because of destructive interference between the inner and the outer rings. The mathematical expressions for the focused fields are derived. Simulation results show that the focused fields and phase distributions at focus are largely influenced by both the cosine parameter and beam diameter of the incident beams. Moreover, focal spot with flattopped, two focal spots patterns can be flexibly achieved by carefully choosing the cosine parameter (C) and the ratios of the pupil diameter to the beam diameter (β) which confirms the potential of such beams in wide applications, such as optical tweezers, lithography, and material processing.

Keywords: Vector diffraction theory, High NA Lens, Multi Gaussian beam, Optical trapping.

CP-112

SYNTHESIS AND CHARACTERIZATION OF PURE & DOPED AMMONIUM DIHYDROGEN ORTHOPHOSPHATE CRYSTALS BY SLOW EVAPORATION METHOD

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Abstract

Synthesis of pure and doped Ammonium Di hydrogen Orthophosphate crystals were synthesized by slow evaporation method. The synthesized crystals were characterized by XRD, FTIR and UV-visible spectroscopy. The XRD pattern showed that the synthesized ammonium di hydrogen orthophosphate crystal was of tetragonal structure. Colorless and transparent crystals were obtained. The FTIR trace reveals the presence of functional groups. From the UV-Vis spectrum shows the cut off wave length of pure and doped crystals are 220nm, 216nm & 215nm. Therefore, the doped crystal improved its transparency and this crystal may be suitable for optical devices.

Keywords: Ammonium dihydrogen orthophosphate, slow evaporation method, XRD, FTIR, UV-visible Spectroscopy.

CP-113

SYNTHESIS AND CHARACTERIZATION OF STUDIES OF NICKEL DOPED CERIUM OXIDE NANOPARTICLES BY SOL GEL METHOD

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Abstract

Unhoped and Ni doped CeO_2 nanoparticles were synthesized using sol-gel method the obtained products were characterized by (XRD),(FTIR),(SEM) and (UV-VIS) The XRD analysis indicated that the synthesized nanoparticles have the orthorhombic structure. The surface morphology of synthesized materials was investigated by using SEM. The other Properties were analyzed by FTIR and UV-VIS Spectroscopy.

Keywords: CeO2 Nanoparticles, Sol gel, XRD, UV-Vis, FTIR, and SEM.

CP-114

BIOSYNTHESIS OF ZINC OXIDE NANOPARTICLES VIA LEAF EXTRACTS OF *PHYLLANTHUS ACIDUS* AND THEIR CHARACTERIZATION

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Abstract

The nanostructures synthesized using the green chemistry method have recently attracted the attention of scientists due to their significance in many scientific domains. This work provides an overview of the biosynthesis of zinc oxide using the aqueous leaf extract of *Phyllanthus acidus* (Pa-ZnO NPs). The synthesized Pa-ZnO NPs were characterized by X-ray diffraction analysis (XRD), scanning electron microscopy (SEM), and Fourier transform infrared (FTIR) were used to analyze the synthesized. Pa-ZnO NPs were crystalline in nature, spherical like and have hexagonal wurtzite structure with a mean particle size of 34.16 nm.

Key words: Biosynthesis, *Phyllanthus acidus*, Pa-ZnO NPs, Characterization

1 Introduction

Metal nanoparticles are gaining more attention in recent years among researchers to fabricate nanoparticles from various metals through different fabrication processes such as physical, chemical, and biological methods. Zinc oxide nanoparticles have a substantial degree of positive influence on biological applications compared to other noble metals such as silver, zirconium, cadmium, lead, copper, cobalt, aluminum, and gold [1, 2]. Since zinc is one of the essential trace elements required for essential metabolic activity and regular cell functions, its notable essential roles are catalytic, structural, and regulatory ions, and it contributes significantly to the immune system, apoptosis, homeostasis, and oxidative stress [3, 4]. The metallothioneins are a group of zinc-binding specialized proteins, and they protect the cells from stress and toxic conditions induced by toxic metals. During aging and degenerative disease conditions, these zinc elements rectify the immune defects, minimize infection relapse, and inhibit aging [5]. Hence, in this study, the oxide form of zinc nanoparticles has been focused on due to the excellent reactivity of zinc nanoparticles. Conventional physical and chemical methods can synthesize these nanoparticles. Nevertheless, these approaches require a more sophisticated laboratory setup, not an ecofriendly, complicated process that includes a separate capping and stabilization process. Hence, the biological process overcomes these issues and yields well-capped and stabilized nanoparticles. Plant biomass, microbes, and biologicals have been identified as suitable source materials for the environmentally friendly synthesis of nanoparticles [6]. The plant biomass contained various biomolecules such as proteins, coenzymes, phenolic compounds, vitamins, flavonoids, and so on; these biomolecules contain several functional groups such as hydroxyl, amines, and carbonyls, which interact with metal ions and reduce them as nanoparticles. These biomolecules also possess a significant role in the capping and stabilizing of synthesized nanoparticles [7]. Hence, in this study a pharmaceutically well-recognized *Phyllanthus acidus* plant has been used, especially the leaf extract of this plant has been focused.

2 Preparation of Pa-ZnO Nanoparticles

Freshly collected *Phyllanthus acidus* leaves were washed using distilled water to eliminate any dust, and after that, they were dried at room temperature. 10 g of dried, finely cut leaves of the species were ground using a mortar and pestle, and the extract of the leaf species

was transported into 100 ml of deionized water under stirring. The subsequent mixture was poured into 0.05 M Zinc nitrate solution under continuous stirring on a magnetic hot plate at 90°C for several hours. The precipitate was continually washed in methanol and distilled water before being dried at 80°C. Finally, at 400°C, the product was calcined for 2 hours in a muffle furnace.

3 XRD Analysis

Phase and structural analysis of Pa-ZnO NPs prepared using *Phyllanthus acidus* is carried out by XRD analysis and shown in Figure 1. All marked diffraction peak positions in Figure 3 are well matched with the standard JCPDS Card: 36-1451. The corresponding X-ray diffraction peaks at observed planes (100), (002), (101), (102), (110), (103), (200), (112), (201), and (004) confirm the formation of hexagonal wurtzite structure of ZnO. The diffraction peaks' observed line broadening is proof that the produced Pa-ZnO NPs are in the nanoscale range. Major peaks' increasing full width at half maxima (FWHM) supports the decline in crystallite size. Using the Scherrer formula, the average crystallite size of Pa-ZnO NPs is determined from the X-ray line broadening.

$$D = \frac{0.9\,\lambda}{\beta \cos\theta}$$

D and λ represent the crystallite size and radiation's wavelength (1.5406 for Cu $k\alpha$), β is the peak intensity width at half maximum and θ is the peak position. The synthesized Pa-ZnO NPs have an average crystallite size of 34.16 nm.

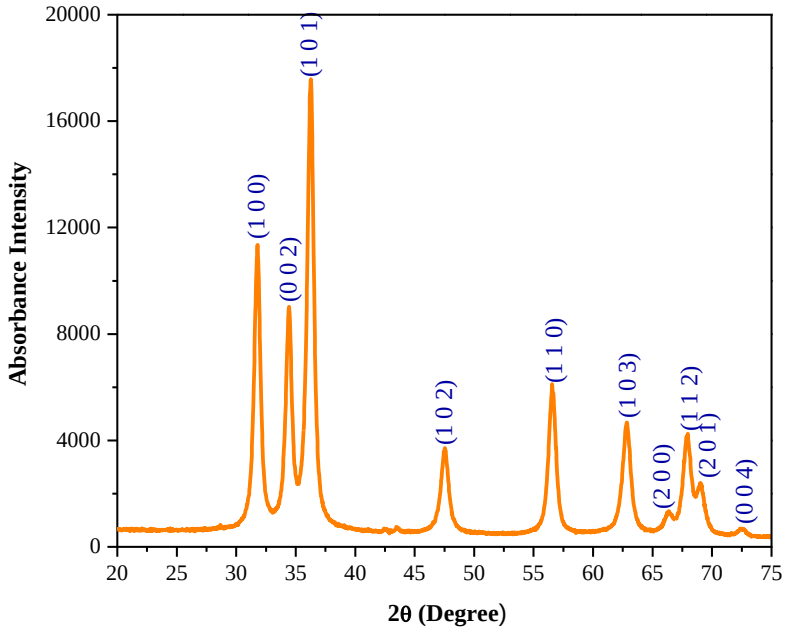

Figure 1. XRD Spectrum of Pa-ZnO NPs

4 SEM Analysis

The morphological features of the synthesized material were investigated through SEM. The obtained images of the ZnO sample showed spherical shape with significant particle aggregation, as shown in Figure 2. Pa-ZnO NPs are comparatively homogeneous due to the regular dispersal of Zn cations within a three-dimensional structure. The cluster (agglomeration) in the sample is a result of increased density carried on by the small gap between the particles, while it may also be related to the rapid grain development and nucleation at higher temperatures.

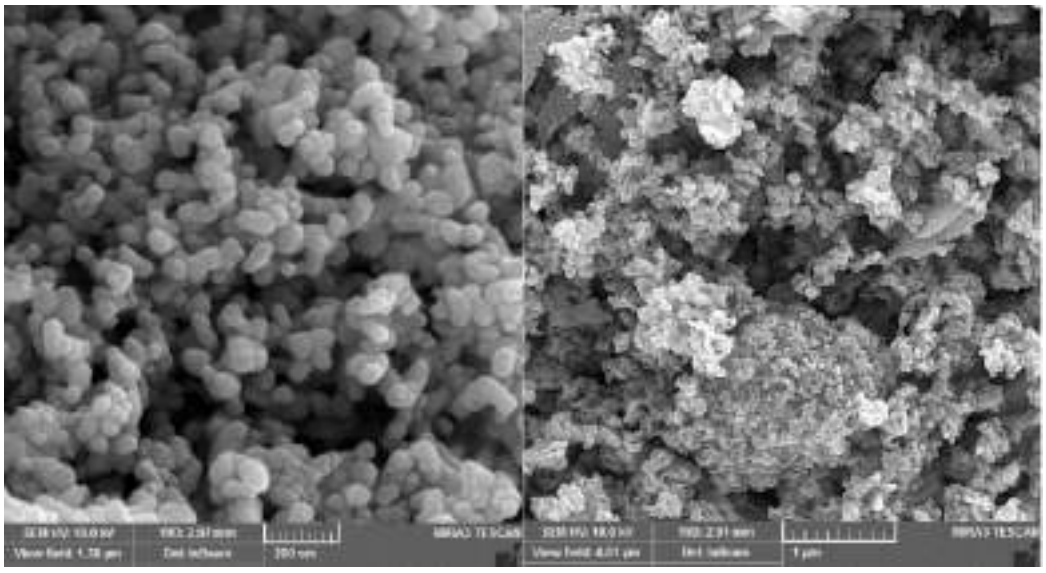

Figure 2. SEM images of Pa-ZnO NPs

5 FTIR Analysis

FTIR spectra of Pa-ZnO NPs produced using the green method was captured in the 400–4000 cm^{-1} range, as shown in Figure 3. The strong broad peak in higher region at 3412.13 cm^{-1} is due to the stretching vibration of hydroxyl (OH) groups. The peak around 1639.39 cm^{-1} is due to the C=O group. The C–O stretching vibration band arises at 1057.39 cm^{-1}. The =C–H bending vibration band arises at 907.19 cm^{-1}. The 538.36 cm^{-1} is attributed to the stretching vibration of Zn–O bonds and confirms the formation of product. FTIR analysis was done to identify the possible biomolecules responsible for the bio reduction of zinc oxide nanoparticles.

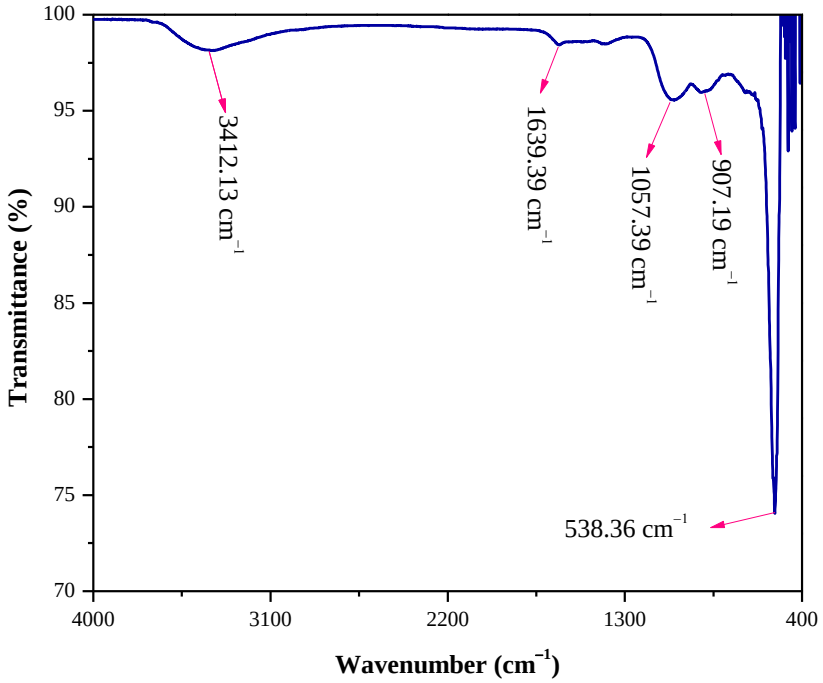

Figure 3. FTIR Spectrum of Pa-ZnO NPs

6 Conclusion

Green leaf extract from the *Phyllanthus acidus* plant was used to successfully prepare Ps-ZnO-NPs, which demonstrates its efficiency as an environmentally friendly, nontoxic, and cost-effective technique to synthesize nanomaterials. The *Phyllanthus acidus* extracts employed in the production of nanoparticles act as capping and reducing agents. The green synthesized Pa-ZnO NPs ranged in the size of 34.16 nm and had a spherical shape. Peaks in the FTIR analysis

revealed the functional groups involved in the synthesis of these ZnO Pa-NPs. They represented the number of functional groups that were found in various bioactive molecules. The present study concludes that Pa-ZnO NPs can be rapidly green synthesized using *Phyllanthus acidus* leaf extract and are inexpensive, non-toxic, ecofriendly.

References

1. K. Brindhadevi, M. S. Samuel, T. N. Verma et al., "Zinc oxide nanoparticles (ZnONPs)-induced antioxidants and photocatalytic degradation activity from hybrid grape pulp extract (HGPE)," *Biocatalysis and Agricultural Biotechnology*, vol. 28, Article ID 101730, 2020.
2. A. Pugazhendhi, T. N. J. I. Edison, I. Karuppusamy, and B. Kathirvel, "Inorganic nanoparticles a potential cancer therapy for human welfare," *International Journal of Pharmaceutics*, vol. 539, no. 1-2, pp. 104–111, 2018.
3. M. Narayanan and Y. Ma, "Influences of biochar on bioremediation/phytoremediation potential of metal-contaminated soils," *Frontiers in Microbiology*, vol. 13, Article ID 929730, 2022.
4. V. M. Mani, S. Nivetha, S. Sabarathinam et al., "Multifunctionalities of mycosynthesized zinc oxide nanoparticles (ZnONPs) from Cladosporium tenuissimum FCBGr: antimicrobial additives for paints coating, functionalized fabrics and biomedical properties," *Progress in Organic Coatings*, vol. 163, Article ID 106650, 2022.
5. M. J. Story, "Essential sufficiency of zinc, ω-3 polyunsaturated fatty acids, vitamin D and magnesium for prevention and treatment of COVID-19, diabetes, cardiovascular diseases, lung diseases and cancer," *Biochimie*, vol. 187, pp. 94–109, 2021.
6. S. Mishra, L. Cheng, and A. Maiti, "The utilization of agro-biomass/byproducts for effective bio-removal of dyes from dyeing wastewater: a comprehensive review," *Journal of Environmental Chemical Engineering*, vol. 9, no. 1, Article ID 104901, 2021.
7. A. Pugazhendhi, S. Vasantharaj, S. Sathiyavimal et al., "Organic and inorganic nanomaterial coatings for the prevention of microbial growth and infections on biotic and abiotic surfaces," *Surface and Coatings Technology*, vol. 425, Article ID 127739, 2021.

CP-115

DESIGNING OF VISIBLE LIGHT ACTIVE G-C_3N_4/Ni-ZnO PHOTOCATALYST NANOCOMPOSITE FOR THE REMOVAL OF INDIGO CARMINE

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Highlights

- A novel g-C_3N_4/ZnO heterostructure photocatalyst was synthesized by facile hydrothermal method.
- The composite material exhibit higher photocatalytic performance than the bare materials.
- The heterostructure could prevent the recombination effect.
- The heterostructure proved to be an efficient photocatalyst for anionic and cationic dye degradation

Abstract

Composite of g-C_3N_4/ZnO heterostructure were synthesized by facile hydrothermal method. The obtained photocatalysts with different ratios were characterized using X-ray diffraction (XRD), Scanning electron microscope (SEM), Fourier transform infrared spectrophotometer (FTIR), UV–Visible Diffuse reflectance spectroscopy (UV–Vis DRS) and X ray photoelectron spectroscopy (XPS). Among all composites 1:1 g-C3N4/ZnO exhibited best photodegradation performance than pure g-C3N4 and ZnO for Methylene blue and Indigo carmine dyes degradation. It showed 90% degradation for Indigo carmine dye. The scavenging studies showed that among the oxidants formed during photocatalysis, hole played a major role in methylene blue degradation.

CP-116

DIELECTRIC AND IMPEDANCE CHARACTERISTICS OF $CaCu_3Ti_4O_{12}$ CERAMIC PREPARED BY A FACILE SOL-GEL TECHNIQUE

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Abstract

Colossal dielectric materials play an essential role in microelectronic devices including ultracapacitors in hybrid –electric vehicles, pulsed systems and memory devices.These microelectronic devices mainly required a dielectric material with huge dielectric strength,low leakage current,low loss tangent,and good thermal stability relating to changes in the frequency and temperature. The perovskite-type of materials belong to the family of $ACu3Ti_4O_{12}$ (where A=Ca,Pb,Sr,..,) was possible candidates in the field of microelectronics owing to their excellent performance and larger dielectric permittivity.the CCTO ceramics were prepared by the facile sol-gel method. The prepared sample was characterized by Powder XRD,SEM.EDAX and Dielectric studies.Powder X-ray diffraction method was used to analyze the crystalline structure and phase formation.SEM micrograph shows the dense microstructure of the ceramics and EDX analysis illustrates the elemental composition of the products.the dielectric behavior of ceramics was studied as a function of frequency(1Hz-1MHz). The electrical properties were investigated by impedance analysis and the results of various studies of ceramics were discussed.

Keywords: Pure CCTO ceramics, facile sol-gel method, powder X-ray diffraction SEM .EDAX and Dielectric studies.

CP-117

TIGHT FOCUSING PROPERTIES OF CIRCULARLY POLARIZED LORENTZ GAUSSIAN BEAM

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Abstract

We investigate the focusing properties of circularly polarized Lorentz Gaussian Beam by high numerical aperture (NA) lens based on vector diffraction theory. We observed that in the presence of annular obstruction, the change in Lorential parameter has little effect on the focal structure. We also studied the effect of annular obstruction in the presence of primary aberration such as spherical aberration ,coma and astigmatism on the tight focusing properties of circularly polarized Lorentz Gaussian beam focusing properties of this kind of Lorentz beams may be used to construct tunable optical traps, which may pave the way for application of laser diode in tweezers technique.

Keywords: Circularly Polarized Lorentz–Gaussian beam, Vectorial Debye theory, Optical vortex.

CP-118

GREEN SYNTHESIS OF COPPER NANOPARTICLES USING RICINUS COMMUNIS LEAF EXTRACT AND STUDY CHARACTERIZATION AND ITS ANTIBACTERIAL ACTIVITY

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Abstract

The green synthesis of Copper nanoparticles using Ricinus Communis leaf extract as a capping agent. The preparation of Copper nanoparticles (CUO) by using Ricinus communis extract has desired quality with green synthesis method. The Ricinus communis leaf extract was mixed with Copper sulphate pentahydrate salt solution by heating to a temperature of 60^0C -70^0 C and the reduction reaction was studied by observing color change. After the solution is converted to the powder form in muffle furnace to heating of 400^0 C. The resulting Copper nanoparticles were characterized by X-Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscope (SEM). X-Ray Difraction analysis shows that the particles are FCC crystalline structure in nature. The FTIR spectrum analysis has confirmed the presence of functional groups of stabilizer Ricinus Communis in capping the copper nanoparticles. The SEM displays the formation of CUO nanoparticles with an average size of 99 nm- 189 nm. The antibacterial activity of Copper nanoparticles was studied against disease causing three bacterial pathogens like Pseudomonas species , Staphylococcus aureus and E- coli.

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