*PROCEEDINGS OF*

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# 2nd NATIONAL CONFERENCE ON EMERGING TRENDS IN MATERIALS SCIENCE (NCETMS - 2019)

## 26th & 27th September - 2019

ORGANISED BY

**PG & RESEARCH DEPARTMENTS OF PHYSICS & CHEMISTRY**

**GOVERNMENT ARTS COLLEGE**

Tiruvannamalai – 606 603, Tamilnadu

*Cheif Editors*

**Dr. R. RAVISANKAR**
Convener, NCETMS - 2019
Assistant Professor of Physics

**Dr. A. RAVI**
Convener, NCETMS - 2019
Assistant Professor of Chemistry

*Sponsored by*

*Tamilnadu State Council for Higher Education (TNSCHE)*

*Tamilnadu State Council for Science and Technology (TNSCST)*

*... In Association With ...*

Indian Association For Radiation Protection, Kalpakkam chapter

Indian Spectrophysics Association

Association of Chemistry Teachers

# 2nd NATIONAL CONFERENCE ON EMERGING TRENDS IN MATERIALS SCIENCE

**(NCETMS - 2019)**

26th – 27th September 2019

**Organized by**

**PG & Research Departments of Physics & Chemistry**
**Government Arts College, Tiruvannamalai – 606 603**

**Sponsored by**

**Tamil Nadu State Council for Higher Education** **&** **Tamil Nadu State Council for Science and Technology**

**In Association with**

**Indian Association for Radiation Protection, Kalpakkam Chapter**

**Indian Spectrophysics Association**

**Association of Chemistry Teachers**

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**Dr. A. Arun**

*Associate Professor & Head, Department of Chemistry*

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**Dr. M. Yogapriya., M.Sc.**

## FOREWORD

It gives pleasure to organize the second **National Conference on Emerging Trends in Material Science (NCETMS – 2019).** The conference is jointly being organized by Post Graduate Departments of Physics and Chemistry on **26th & 27th, September 2019** at Government Arts College, Tiruvannamalai. This conference is a forum for all stakeholders to discuss the on the different areas of research related to material science, technology and applications.

The conference particularly is aimed at encouraging the interaction of research students and developing academicians with most established academic community. Their contributions will certainly help in making this conference as grand success. The papers received contribute to greatly to the scientific knowledge in the field of Medical Physics, Crystal Growth, Thin Films, Nano Materials, Characterization and Applications, Green Energy, Functional Materials, and Advance Materials.

The participants will get an opportunity to interact with eminent persons who are working in the field of Material synthesis, Characterization tools and techniques in material science. The research area is kept open for the scientific community to promote the research and development in the field of material science and technology. The scientific deliberations will be in the form of Invited talks, Oral and Poster presentations.

NCETMS-19 has received an overwhelming response, with nearly 194 abstracts, which is the record in this series. The organizers are thankful to the members of the **National Advisory committee, Principal, Head of the Departments of Physics and Chemistry, Organizing team and local Organizing committee** and all those who have directly or indirectly helped in successfully organizing this conference. The editors of the proceedings are grateful to the reviewers for spending their valuable time to bring this proceeding in time and in good form. The scientific committee thanks all the Invited

speakers, Session speakers, Chair persons, Panel members and Contributing Authors to make this event successful.

We specially thank **Tamil Nadu State Council for Higher Education (TNSCHE), Tamil Nadu State Council for Science and Technology (TNSCST) and Department of Higher Education, Government of Tamil Nadu** for catalyzing and supporting this conference. We are very much thankful to **Indian Spectrophysics Association (ISPA) Chennai, Indian Association for Radiation Protection (IARP), Kalpakkam Chapter and Association of Chemistry Teachers (ACT)** for their financial support to organize this conference.

NCETMS-19 is grateful for the support received from **Dr. S. Gunasekaran**, the Founder President of Indian Spectrophysics Association (ISPA), Chennai and **Dr.M.Swaminathan,** Emeritus Professor, Nanomaterials Laboratory, Kalasalingam Academy of Research and Education are greatly acknowledged. As the conveners of the conference, we extremely grateful to **Dr.B.Venkatraman** Director, Health, Safety and Environmental Group, Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam for his constant support and encouragement.We once again thank all persons and organizations associated with this conference**.**

**Dr. R. Ravisankar & Dr. A. Ravi**

*( Conveners )*

# GOVERNMENT ARTS COLLEGE

*(Affiliated to Thiruvalluvar University, Vellore-15)*
Accredited by NAAC with 'B' Grade
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Date: 20/09/2019


**Dr. M. SUBRAMANI**
**Principal**


## MESSAGE

I am happy to learn that the Post Graduate & Research Department of physics and chemistry jointly organize National Conference Emerging trend in Material science (NCETMS– 19) during 26th & 27th September 2019 in the College premises. The topic chosen is ideal for the motivation of young minds to study and undertake research in the field of material science and technology.

This conference covers fascinating area of on crystal growth, thin film, polymer, nano science and technology, functional material, novel organic and inorganic materials, composite material, energy material and environmental and green material. I am sure those students' immense benches by such interaction. I hope that more than 300 delegates from various parts of the country will participate in NCETMS – 19. Our staff and students will be greatly benefited from the interactions with such Eminent Scientists, Experts and Academicians put on reword our material science.

I am glad to know that proceedings containing scientific abstract is being released during this conference. I congratulate and extend my best wishes to the Chair persons **Prof.R. Arunchunai Annadurai** and **Dr.A.Arun** and Conference conveners **Dr. R. Ravisankar** and **Dr.A.Ravi,** the Organizing secretaries **Dr.M.Balakrishnan** and **Dr.K.Rajathi** and their entire team involved in organizing conference.

I anticipate that the deliberations in the conference will arouse interest in the minds of scholars to understand the basic research in the field of material science and its applications.

It is my duty to thank the sponsoring agency Tamilnadu State Council for Higher Education (TNSCHE) and supported by Indian Spectrophysics Association (ISPA), Chennai, Indian Association For Radiation Protection (IARP), Kalpakkam Chapter and Association of Chemistry Teachers (ACT) for conducting this event in the college. I welcome all the national participants from various parts of India to this conference. I wish the conference great a success.

PRINCIPAL
GOVERNMENT ARTS COLLEGE
TIRUVANNAMALAI.

**K.S. KANDASAMY,** I.A.S.,
Collector and District Magistrate,
Tiruvannamalai - 606 604.

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# FOREWORD

I am glad to perceive that Post Graduate and Research Department of Physics and Chemistry is organizing National Conference on Emerging Trends in Material Science (NCETMS-2019) on 26th & 27th September 2019 at Government Arts College, Tiruvannamalai. The Conference is likely to cover broad range of topics on Material Science, Technology and its Application. This conference is expected to provide an excellent platform for exchange of latest information and technology in material science.

This conference will very much enrich and motivate the knowledge of young buds and students community who are pursuing science in their carrier. The scientific deliberations and interactions from academics, scientist and field experts will attract students from all walks of life especially the rural students to pursue research in new dimension

The faculty members and students of Government Arts College will be greatly benefited from the interactions with eminent persons and filed experts in material science during the conference. It is heartening to note that more than 300 delegates as participants in this august NCETMS-2019.

I am happy to know that proceedings of scientific abstract are being released during this event. I appreciate the conference conveners and their team for making good effort to conduct this event successfully in Tiruvannamalai.

I extend a hearty welcome to the delegates and wish the conference a grand success.

K.S.KANDASAMY, I.A.S.,

திருவள்ளுவர் பல்கலைக்கழகம்
THIRUVALLUVAR UNIVERSITY
(State University - Accredited by NAAC)
SERKKADU, VELLORE - 632 115, TAMIL NADU, INDIA.

**Prof. Dr. S. THAMARAI SELVI**
Vice Chancellor

19th September 2019

## MESSAGE

I am glad to know that Post Graduate and Research Department of Physics and Chemistry, Government Arts College, Tiruvannamalai is organizing National Conference on Emerging Trends in Material Science (NCETMS-2019) during 26th & 27th September 2019. The material research and technology is a promising area for the young scientific minds and it is believed that material science and technology will have greater impact in the industrial revolution. It becomes essential to have constant interaction among the researchers, academics, scientist, technologists and industrialist and this kind of conference would provide a platform for future directions.

The theme of the conference addresses Energy materials, nano materials, polymer based materials, smart materials, novel organic and inorganic materials, laser materials, energy conversion materials and nuclear science materials. I anticipate the event will provide a good plat form for academics, Scientist, Technologists and Industrialist a good opportunity for their research in the field or material science.

I appreciate the coordinated effort of the conveners **Dr. R. Ravisankar** and **Dr. A. Ravi** and Organsing secretaries **Dr. M. Balakrishnan** and **Dr. K. Rajathi** in organizing NCETMS 2019. This conference as a multi-disciplinary approach and provide the platform for the students, scholars, teachers and scientist to be have united participations under the umbrella of Government Arts College, Tiruvannamalai for research activities. I am happy to see the participation of event experts in the field of material science.

I wish the delegates and organization every success.

With the Best Wishes

19/9/19

**(Prof. Dr. S. THAMARAI SELVI)**

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**Dr. S. Gunasekaran, M.Sc.,Ph.D.,D.Sc.**
**TANSA Awardee**
**Dean, Research & Development**
**St. Peter's Institute of Higher Education & Research**
**Avadi, Chennai – 600 054. Tamil Nadu, India.**
**E-mail: deanresearchspu@gmail.com**
**Founder President, Indian Spectrophysics Association (ISPA)**
**Former Registrar, Periyar University, Salem**
**Former Head, Department of Physics, Pachaiyappa's College, Chennai.**

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# MESSAGE

**Dr. S. Gunasekaran**
**Dean, Research & Development**

Francis Bacon said "Reading maketh a full man; conference a ready man; and writing an exact man". Conferences bring together people of varied experiences and provide an opportunity to everyone to share their thoughts. The conferences have to be organized at various levels to offer a platform to various levels of researchers. The conferences are necessary to bring in culture of information exchange and feedback on developing trends in technologies. Mutual participation and high quality deliberations create inspiring learning environment resulting into innovative ideas. Today's industry expects such inputs to bring home new innovations and inventions. I am delighted to note that the Departments of Physics & Chemistry are organizing the National Conference entitled "National Conference on Emerging Trends in Materials Science (NCETMS 2019) "on 26$^{th}$ & 27$^{th}$ September 2019. This conference shall provide a forum to all researchers to exchange the information on research and innovations and enhance the quality of research. Certainly, this type of conference not only brings all the researchers and scholars at one platform, but it also inculcates the research culture among the entire fraternity of Education in the country, thereby, contributing to the development of nation. I hope that this conference would certainly induce innovative ideas among the participants paving way for new inventions and technologies various fields of research.

I, on behalf of ISPA congratulate, Dr. V. Nedunchezhiyan, Principal, Prof. R. Arunchunai Annadurai, HOD, Department of Physics, Dr. A. Arun, HOD, Department of Chemistry, Convenors Dr. Dr. K. Ravishankar, Department of Physics and Dr. A. Ravi, Department of Chemistry, Dr. M. Balakrishnan, Associate Professor, Department of Physics, Government Arts College, Thiruvannamalai and their team for initiating the conduction of such a conference in the esteemed College.

I wish the conference a grand success.

06/09/19

Dr. S. Gunasekaran

**Dr. M. Swaminathan, M.Sc., Ph.D.**
**Emeritus Professor, Nanomaterials Laboratory,**
**International Research Centre** **Kalasalingam University**
**Department of Chemistry,** **Krishnankoil-626126**
**E-mail:chemsam50@gmail.com,m.swaminathan@klu.ac.in** **Tamil Nadu, India.**

**16-09-2019**

## Message

I am extremely happy that " NATIONAL CONFERENCE ON EMERGING TRENDS IN MATERIALS SCIENCE" is jointly organized by Physics and chemistry department of Government Arts College, Tiruvannamalai in association with Indian Association for Radiation Protection, Association of Chemistry Teachers and Indian SpectroPhysics Association. Material Science is a multidisciplinary subject and the current trend is to develop smart materials for different applications. On this occasion, this National conference brings the delegates all over India to discuss the emerging trends in materials science. I appreciate the organisers for providing a wonderful platform to exchange advancements and innovations with each other in this research area. I take this opportunity to warmly welcome all the participants and congratulate the organisers for this initiative. I wish the conference a grand success.

M.SWAMINATHAN

**Dr. B. Venkatraman** HFISNT
**Outstanding Scientist**

सत्यमेव जयते

भारत सरकार
परमाणु ऊर्जा विभाग
इन्दिरा गाँधी परमाणु अनुसंधान केन्द्र
कल्पाक्कम 603 102, तमिलनाडु, भारत

GOVERNMENT OF INDIA
DEPARTMENT OF ATOMIC ENERGY
INDIRA GANDHI CENTRE FOR ATOMIC RESEARCH
KALPAKKAM 603 102, TAMIL NADU, INDIA

19th September, 2019

## MESSAGE

I am delighted to know that the Post Graduate and Research Department of Physics and Chemistry, Government Arts College, Thiruvannamalai, are organizing a National Conference on Emerging Trends in Material Science (NCETMS-2019) from 26th to 27th, September 2019.

Going into the genesis of materials science, it can be observed from history that it practically appeared as an independent branch of science in the end of 1950s. Today, materials science is an interdisciplinary area, combining many pure science disciplines such as solid-state physics, chemistry, mathematics, biology with engineering such as mechanical, electronics and computer science. In fact it can be stated that materials science and engineering has played and will continue to play a key role in ensuring better quality of life on mother earth.

I am happy to note that the Conference has special thematic sessions focusing in the areas of crystal growth, thin films, nano materials, polymers, functional materials, ultrasonic, novel materials and nuclear materials. I am sure that this National Conference would provide an excellent opportunity for fruitful interactions and exchange of ideas among academicians, Scientists, Technologists and Industrialists to share their research findings and brain storm new concepts in the field for future research. I am sure that the students, faculty and researchers attending the conference would also immensely benefit from such interactions. As, President of Indian Association for Radiation Protection (IARP), I am happy to note that IARP Kalpakkam is supporting this event. Ionizing radiations find wide applications in material science and engineering.

I appreciate the efforts of the conference conveners **Dr. R. Ravisankar** and **Dr. A. Ravi** and also the Organizing secretaries **Dr. M. Balakrishnan** and **Dr. K. Rajathi** of NCETMS – 19. I complement the organizers for choosing a highly important and a relevant topic for conference.

I wish NCETMS team and event all success.

(B. VENKATRAMAN)

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Dr.K.PANDIAN, M.Sc., Ph.D.
Controller of Examinations
University of Madras, Chennai-600005
Professor in Inorganic Chemistry

I am happy to know that the PG & Research Departments Physics and Chemistry, Government Arts College, Thiruvannamalai-606 603,TN is organising a two days National level Conference on **"Emerging Trends in Materials Science"** on 26th and 27th September 2019 to commemorate the *international year of Periodic Table 2019.*

I am sure that the conference will provide opportunity for the teachers, research scholars and students by sharing their knowledge and experience by interaction with eminent scholars. No doubt this conference will focus on recent trends and advancement of chemistry research. It is my privilege that I am a part of this conference.

On this occasion, I congratulate the organiser of this conference and all the participants a great success.

With regards,

Dr.K.PANDIAN

# Indian Science and Technology Association

**Elavenil**

**(Regd.110/2015)**

163/69, Secretariat colony, Kilpauk , Chennai-600 010, India

Email: istaindia18@gmail.com


**Prof. R. Jayavel**

**President**

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## MESSAGE

I am delighted to note that the Departments of Physics and Chemistry, Government Arts College, Tiruvannamalai are jointly organizing "National Conference on Emerging Trends in Materials Science (NCETMS 2019)" during 26-27 September 2019 in association with Indian Association for Radiation Protection, Indian Spectrophysics Association and Association of Chemistry Teachers. Materials Science is a multi-disciplinary field of research in modern science and technology, which plays an important role in various fields like Electronics, Medicine, Nanotechnology, Biotechnology, Energy, Spectroscopy, Information and Communication Technology.

I am very much impressed with the focus of the Conference on wide range of topics including Crystal Growth, Nano Science and Technology, Energy Materials, Functional Materials, Composite Materials, Solar Cell, Polymer based Materials, Environmental and Green materials, Smart Materials, Novel Organic and Inorganic Materials, Laser Materials, Energy Conversion and Storage Materials, Nuclear Science and various Materials Characterization techniques. This kind of conference will provide a platform for knowledge dissemination and knowledge sharing. I hope the participants would be very much benefited out of this event by getting the details of recent developments in the diversified field of Materials Science.

I congratulate the conveners **Dr. R. Ravisankar and Dr. A. Ravi** for their meticulous planning and dedication to organize the conference. Also I would like to appreciate the Principal and members of the Faculty, Government Arts College, Tiruvannamalai, for their motivation and cooperation in organizing the conference in a grand manner.

R. Jayavel

**Prof. R. Jayavel**

# UNIVERSITY OF MADRAS

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Dr.E.MURUGAN, M.Sc., M.Phil., Ph.D.,FRSC.,
PROFESSOR & HEAD

MEMBER - SYNDICATE
DIRECTOR- GUINDY CAMPUS


## Professor Dr. E. Murugan's Message

I am very happy to learn that an National Conference on Emerging Trends in Materials Science (NCTMS-2019) is being organised on 26th and 27th Sept-2019, by the P.G & Research Departments of Physics and Chemistry, Government Arts College, Tiruvannamalai-606 603, under the Convenorship of Dr. R. Ravisankaran, Department of Physics and Dr. A. Ravi Department of Chemistry. I am proud to mention here that in general the growth of Science and Technology has been steadily increased in India and more particular at Tamil Nadu. Research on Information Technology, Nano-technology, Bio-Technology, Stem Cell Technology and Cloud Technology has created remarkable impact on common man life by providing luxury, comfort, enhancing the health and thereby life span has been enhanced sizably.

Tiruvannamalai is one of the prominent and holy place having historic record in promoting the peace and harmony among the peoples through religious worship and science education. Though the District is consider to be economically backward but it marching ahead towards higher education. I understand that Dr. R. Ravisankar and Dr. A. Ravi are vibrant Researcher in the area of material science. But to my surprise, they jointly took this herculean task with intention to provide greater opportunity for interaction of scientists working in rural background and allow them to share their knowledge in frontier area's of science & Technology with specific reference to "Emerging Trends in Materials Science".

On this auspicious occasion, I whole heartedly expressing my advance Greetings and Wishes to the Principal, Faculty Members of Government Arts college, Tiruvannamalai and more specifically to the young Conveners Dr. R. Ravisankar Department of Physics and Dr. A. Ravi, Department of Chemistry to conduct the conference with grant successes.

**All the Best**

Date : 21/09/2019
Place : Chennai-25

21/09/2019

**(Prof. Dr. E. Murugan)**

PG & Research Department of Chemistry
Pachaiyappa's college
Chennai 600 030

**Dr. R. NANTHINI, M.Sc., M. Phil., Ph.D.**
Associate Professor & Head

Date: 18. 09. 2019

## MESSAGE

I am delighted to know that, National Conference on Emerging Trends in Material Science (NCETMS-2019) is being organized by PG and Research Department of Physics & Chemistry, Government Arts College, Tiruvannamalai.

On this proud and happy occasion, I extend my warmest greetings to the Department of Physics & Chemistry, especially the Conveners and Organizing Secretary for their tremendous hard work in hosting this conference.

I am sure that the conference will provide an excellent platform to the young researchers, academicians and industrial professionals from all over India to present their innovative research findings and discuss the practical challenges and solutions which they experienced in their fields.

I congratulate and appreciate each and everyone who is part of NCETMS-2019 and wish them all the very best for the grand success of the conference.

# About Indian Association for Radiation Protection (IARP)

*(Kalpakkam Chapter)*

The Indian Association for Radiation Protection (IARP), a non-governmental organization (NGO) of radiation protection professional's in India, was registered in 1968 under the Public Trust Act, 1950. The association has a large membership comprising of specialists and users of natural and man-made radiation sources. The Association is an affiliate of the International Radiation Protection Association (IRPA) since May, 1970. The Association has six chapters in different regions of the country (Delhi, Kanpur, Hyderabad, Tarapur, Kaiga and Kalpakkam). The aims of IARP include brining about proper awareness of the benefits of ionizing radiations amongst their users in particular and the public in general. It encourages adoption of appropriate means/ procedures for avoiding or reducing radiation exposure in the applications of ionizing radiations and nuclear technology in the country, such as power generation, industry, medicine, agriculture, scientific research etc., thereby maximizing the benefits to the society. It provides a forum for communication and exchange of information amongst specialists in the field of radiation protection and related disciplines in the country and with their counterparts in other countries. It conducts training courses to cater to the requirement of trained manpower in the industrial applications of radioisotopes in industry and research. The IARP publishes an open access web-based quarterly journal "Radiation Protection and Environment" (RPE). IARP has been serving the national and international scientific community for the past 50 years by organizing national regional conferences and workshops in the field of Radiation Protection and Safety.

**Post Graduate and Research Departments of Physics and Chemistry**

**2ed National Conference on Emerging Trends in Materials Science (NCETMS-2019)**

**PROGRAMME SCHEDULE**

**DAY – I Thursday, 26th September - 2019**

| Time | Events |
|---|---|
| 9.00 am to 10.00 am | Registration |
| 10.00 am to 10.45 am | Inaugural Function |
| 10.45 am to 11.00 am | Tea Break |
| 11.00 am to 11.45 am | **Dr. S. Gunasekaran,**<br>*Dean, Research & Development, St. Peter's Institute of Higher Education and Research, Avadi, Chennai*<br>"**Research Approach for Global Reach**" |
| 11.45 am to 12.30 pm | **Dr.M. Swaminathan**<br>*Emeritus Professor, Nanomaterials Laborotry, Department of Chemistry, Kalasalingam Academy of Research and Education , Krishnankoil*<br>**"Modified Semiconductor Oxide Nanomaterialsfor Energy And Environment"** |
| 12.30 pm to 1.15 pm. | **Dr.R. Jayavel,**<br>*Professor, Crystal Growth Centre, Anna University, Chennai*<br>**"Two Dimensional Hierarchical Nanostructures for Functional Devices"** |
| 1.15 pm to 2.00 pm | Lunch Break |
| 2.00 pm to 2.45 pm | **Dr.S. Peruncheralathan**<br>*School of Chemical Sciences, NISER Bhubaneswar*<br>**"Our Journey Towards Synthesis of Heterocycles: Materials to Biomedical"** |
| 2.45 pm to 3.30 pm | **Oral Presentation-I** |
| 3.30 pm to 3.45. pm | Tea Break |
| 3.45 pm to 4.30 pm | **Dr. Muthu Senthil Pandian**<br>*SSN Research Centre, SSN Institutions, Chennai*<br>**"Development of Device Quality 4-Nitrophenol Derivative Nonlinear Optical (NLO) Single Crystals And Fabrications of Type-I And Type-II SHG Elements"** |
| 4.30 pm to 5.15 pm | **Dr.V. Jaisankar**<br>*Post-Graduate & Research Department of Chemistry Presidency College (Autonomous), Chennai*<br>**"A Study on Solid Polymer Gel Electrolytes For Super capacitor Applications"** |
| 5.15 pm to 6.00 pm | **Oral Presentation-II / Post Presentation - I** |

**Post Graduate and Research Departments of Physics and Chemistry**

**2ed National Conference on Emerging Trends in Materials Science (NCETMS-2019)**

**PROGRAMME SCHEDULE**

**DAY – II Friday, 27th September - 2019**

| Time | Events |
|---|---|
| 9.30 am to 10.15 am | **Dr.S. Jayakumar,**<br>*Associate Professor in Physics,*<br>*RKM Vivekananda College, Mylapore, Chennai*<br>**"Smart Materials"** |
| 10.15 am to 11.00 am | **Dr.S.P. Rajasingh,**<br>*Assistant Professor of Chemistry,*<br>*Chikkanna Government Arts College, Tiruppur – 641 002,*<br>**"Perylene Diimide: A versatile Non-Fullerene Electron Acceptor Material"** |
| 11.00 am to 11.15 am | Tea Break |
| 11.15 am to 12.15 pm | **Oral Presentation – III** |
| 12.15 pm to 1.00 pm | **Dr. M. Selvapandiyan,**<br>*Associate Professor in Physics,*<br>*Periyar University PG Extension Centre, Dharmapuri*<br>"**Role of NaCl on the properties of Sulphamic Acid single crystals**" |
| 1.00 pm to 1.45 pm | Lunch Break |
| 1.45 pm to 2.30 pm | **Dr. K. Ganesan,**<br>*Assistant Professor of Chemistry,*<br>*Presidency College (Autonomous), Chennai*<br>**"Synthesis of Some Novel Ionic Liquids Under Conventional And Solid Phase Approach And Its Applications"** |
| 2.30 pm to 3.30 pm | **Oral Presentations – IV / Poster Presentations – II** |
| 3.30 pm to 4.15 pm | **Dr.K. Senthilkannan,**<br>*Dean and Director Research,*<br>*EGS Pillay Arts & Science College Nagapattinam*<br>**"Synthesis, Growth And Characterizations of LAF Crystal"** |
| 4.15 pm to 4.30 pm | High Tea |
| 4.30 pm to 5.00 pm | Valedictory Function |

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# Invited Talks

**Dr. S. Gunasekaran, M.Sc.,Ph.D.,D.Sc.**
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**Former Registrar: Periyar University**

**Former Head: Department of Physics, Pachaiyappa's College, Chennai.**

**Founder President: Indian Spectrophysics Association (ISPA), Chennai, India.**

## Research Approach for Global Reach

Research unveils the complexity of the universe and leads to the betterment of humankind. Quality of any research work and researcher is not just confined to their findings. Research publications of researchers play vital role in evaluating the contributions of researchers, institutions/organizations and the country where they belong to. Based on the citations received by the researchers for their publications, journal metrics are measured. These measurement criteria fortify the saying, "Ink of Scientists is holier than the blood of the soldiers", for the development of the country.

Research output arises out of publication of research articles in a reputed high impact factor journal and the citation indices remains significant in judging the standard of any higher education institution. To do a quality research, publications of research paper in a journal is very important. Journal of high impact factor must be considered while publishing our paper in the journal. Impact factor is one of the journal metrics deployed to evaluate the quality of the journal, based on the average number of citations received per paper published in that journal during the two preceding years. Impact factor was devised by Eugene Garfield in the year 1975. New Journals, which are indexed from their first published issue, will receive an IF after two years of indexing. Thomson Reuters assigns an impact factor to new journals with less than two years of indexing, based on partial citation data. Many counterfeit journals are also available with fake impact factor, by consulting list of scopus indexed journals and Scimago journal rank, researchers may ignore fraudsters. University Grants Commission (UGC) has also notified list of journals for the purpose of computation of Academic Purpose Indicator (API). In this way, journal metrics must be considered before publishing the research papers.

The next parameter h-index is an index to quantify an individual's scientific research output. The word h-index was coined by J. E. Hirsch in the year 2005. H-index is calculated by the number of papers with citation number greater than h. h – index is an author level metric, used to measure both productivity and citation impact of the publications of a scientist or scholar.

The index is based on the set of the scientist's most cited papers and the number of citations they have received in other publications. H-index is also called Hirsch index or Hirsch number. Seniority of a person is calculated by calculating the h-index of a person with his experience in years. For a person with h-index 20 have an experience of 20 years in his scientific activity is characterized as a successful scientist. Similarly, a person with h –index 40 in 20 years of his scientific activity is characterized as an outstanding scientist. A person with h-index 60 and have an experience of 20 years in research activity is characterized as truly unique individuals. For the advancement to tenure or promotion, h-index can be used as a criterion to avail promotion. If h-index is 12, the person can be promoted for Associate professor, if h-index is 18, the person can get promoted as a Professor, for h-index equal to 15 to 20, the person can enter the fellowship in the American Physical society. For a person with h-index equal to 45 can join the membership in the National Academy of Sciences of the USA. Mu-Hsuan Huang evaluated the scientific performance of an institution by extending the application of the h-index from the individual to Institutional level. For example, if the institution has 'h' individuals, each having an individual 'h' index equal to greater than 'h', then the h-index of an institution is h. A scientist is said to be truly unique individual, if the ratio of h-index to the years of research experience is 3, the scientist is said to be an outstanding scientist, if the ratio is 2. The scientist is called as successful scientist if the ratio is 1.

Google scholar introduced i10-index indicates the number of academic publications, an author has written that have at least ten citations from others. This index assists the h-index and gives more weight to the highly-cited papers.

Every research finding is considered as an intellectual property of a researcher, so it should not be copied by other research at any circumstances. Stealing others' intellectual property is known as plagiarism. It is the wrongful appropriation and stealing and publication of another author's language, thoughts, ideas or expressions and representing them as their own original work. Report on plagiarism arises due to the ignorance of citing the source which has been referred. Plagiarism can be avoided, by citing the sources. Although certain level of plagiarism is permissible by citing their source. Few software tools viz., iThenticate and URKUND are available to identify plagiarism. UGC recommends URKUND software to check the level of plagiarism.

Filing and getting Patents for the intellectual property of researchers is also important. This encourages every researcher to come up with new concepts and designs.

Aiming the good quantity of qualitative research publications raises the standard of the institution as well as the country. Researchers should be responsible for publishing their research work without compromising the quality of the journal for the sake of their own and the nation.

**INVT – 2**

## Modified Semiconductor oxide Nanomaterials for Energy and Environment

**Dr. M. Swaminathan**

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In recent years use of solar light in chemistry has aroused such a worldwide attention due to energy and environmental problems. The main goal of artificial photosynthesis is to utilize solar energy to produce different useful material or high - energy chemicals for energy production and for the photodegradation of pollutants. A great impetus to the development of photocatalysis, one of the processes of Artificial Photosynthesis, is derived from the growing demand to reduce the environmental pollution and energy shortages.Modified semiconductor oxide nanomaterials had been used for various applications in the field of photodegradation of pollutants, organic synthesis, fuel cells, hydrogen production from water and sterilization. Semiconductor oxides offer a green route for some organic transformations. Modified semiconductor oxides exhibit photoconductivity and electrocatalytic activity, which make them useful for solar cell and methanol fuel cell applications. We had developed a number of coupled and co-doped semiconductor oxides and characterized. This lecture will cover the characterization and multiple applications of some of these solar active advanced materials.

**INVT – 3**

## Two Dimensional Hierarchical Nanostructures for Functional Devices

**Dr. R. Jayavel**

*Crystal Growth Centre & Centre for Nanoscience and Technology*

*Anna University, Chennai-25*

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Two dimensional hierarchical nanostructures posses promising physic - chemical properties with multi - functionality for varios applications. Graphene - based nanocomposites are emerging as a new class of materials with excellent electrical, thermal, optical and mechanical properties, leading to their potential application in different areas, such as photovoltaics, sensors, batteries, photocatalyst and nanoelectronics. The study of decorating the graphene sheets with inorganic functional materials such as metals, metal oxides and metal sulfides is now becoming a promising and challenging area of research. In this study, flexible free standing reduced graphene oxide films have been synthesized by homogeneous evaporation induced self-assembly process. Multi-layered graphene oxide film structures were annealed under argon and nitrogen atmosphere to form the reduced graphene oxide films. The prepared reduced graphene oxide structure has been subjected to structural, optical, thermal and electrical property studies. Functional devices like, bimorphic electrical actuators, solid state supercapacitors, sensors and hole transport material free perovskite solar cells have been fabricated using the reduced graphene oxide films and the results will be discussed in detail.

**INVT – 4**

# Our Journey towards Synthesis of Heterocycles: Materials to Biomedical Applications

**Dr. S. Peruncheralathan**

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Heterocycles play an essential role in various fields ranging from biomedical to material sciences. Interestingly, heterocyclic compounds are present in 50% of the market drugs. In particular, medications like chloroquine, raloxifene, etc. are benzo fused heterocycles. Traditionally, benzoheterocycles are synthesized from either appropriate heteroatom substituted arenes or heteroarenes. Last few decades, the transition metal catalysis is playing a pivotal role in carbon – hetero bond-forming reactions. Several methods are developed and widely used in the industry. However, this approach is not well explored in heterocycle synthesis, especially 2 – aminobenzohetero cycles. Recently, we have demonstrated that α-functionalized arylacetonitriles as precursors for the synthesis of benzo fused heterocycles via selective C—X and C—H bond functionalization strategies. We employed suitable non-precious metal catalysts or organocatalysis for this purpose. Pyrazoles, a class of five-membered heterocyclic compounds,by virtue of their diverse applicationssuch as anti-inflammatory, anti-pyretic, anti-microbial, anti-viral, anti-depressant, agrochemical, cosmetic colourings, optical brighteners, UV stabilizers, photoinduced electron transfer systems, suitable to stabilize various metal ions, and utilized as ligands in cross-coupling reactions have attracted the attention of research workingin the area of material science, pharmaceutical, and medicinal chemistry, and synthetic organic chemistry. Further, the pyrazole polymeric analogues are particularly attractive due to their high thermal stability, the opportunity of using solution processing techniques for device fabrication.Our recent studies in this direction will be presented at this conference.

**INVT – 5**

## A Study on Solid Polymer Gel Electrolytes for Supercapacitor Applications

**Dr.V.Jaisankar**

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*Presidency College (Autonomous) Chennai 600 005, Tamil Nadu*

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The advances of portable electronics and the growing demand for miniaturised devices with high energy storage capacity becomes key interest of research. Many researchers are working in this direction to enhance the properties (storage capacity, life cycles) of power sources like battery, fuel cell and super capacitor. The electrochemical supercapacitors are one of the promising energy storage devices which provides low cost, high power density, high cycle life, large capacitance, high power delivery, fast charge-discharge characteristics and mechanical robustness. In recent years, extensive efforts have been devoted to explore new electrolyte materials to improve the overall performance of electrochemical supercapacitors (ESs). The major types of the solid-state electrolytes developed for ESs are based on polymer electrolytes, and only very limited work has been focused on inorganic solid materials (e.g., ceramic electrolyte. The polymer-based solid electrolytes for ESs can be further grouped into three types: the solid polymer electrolyte (SPEs, also known as dry polymer electrolytes), the gel polymer electrolyte (GPE) and the polyelectrolyte. Due to the presence of liquid phase in GPEs, some studies called them as quasi-solid-state electrolytes. The SPE is composed of a polymer (e.g., PEO) and a salt (e.g., LiCl), without any solvents (e.g. water). The ionic conductivity of SPE is provided by the transportation of salt ions through the polymer. On the contrary, the GPE consists of a polymer host (e.g., PVA) and an aqueous electrolyte (e.g., $H_2SO_4$) or a conducting salt dissolved in solvent. In this case, the polymer serves as a matrix, which can be swollen by the solvent, and the ions transport in the solvent instead of in the polymer phase, which is different from that of SPE.In the present study, we report on the preparation and characterisation of certain solid polymer gel electrolytes and the fabrication of supercapacitors.

# Development of device quality 4-Nitrophenol derivative nonlinear optical(NLO) Single crystals and fabrications of type-I and type-II SHG elements

**Dr. Muthu Senthil Pandian**

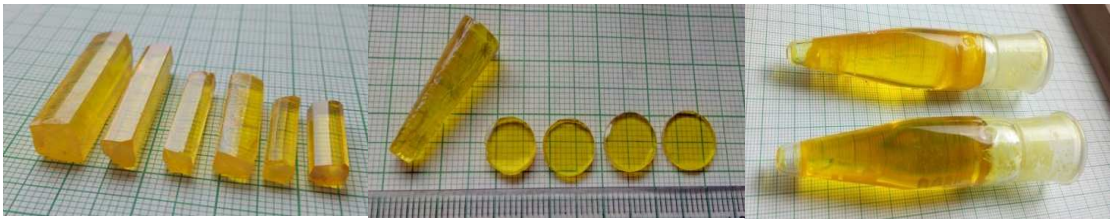
*SSN Research Centre, SSN Institutions, Chennai-603110, Tamil Nadu*

*E-mail: senthilpandianm@ssn.edu.in*

**Abstract**

Gravity driven concentration gradient is used in the uniaxially solution-crystallization method of Sankaranarayanan-Ramasamy (SR). TGS, GPI, KAP, SSDH, DGZCD, DGBCM, benzophenone and many more crystals have been successfully grown by SR method. Longest benzophenone crystal having dimension of 1350 mm length and 55 mm diameter was grown for the first time in solution growth by SR method. Starting with a thin plate as seed a large size crystal can be grown. The physical properties and crystalline perfection of the SR method grown crystal is normally superior to the conventional method grown crystals. The quality of the SR method grown crystals has been improved by several modifications made in SR method. The impurity segregation cannot be avoided in the existing SR method. So we planned to introduce the RSR method for growing good quality, unidirectional single crystals. The effect of rotation on unidirectional crystal growth method (Rotational Sankaranarayanan - Ramasamy (RSR)) has been proposed for the first time. The organic nonlinear optical 2-Aminopyridinium 4-nitrophenolate 4-nitrophenol (2APNP) crystals have been grown by (i) conventional slow evaporation, (ii) Sankaranarayanan-Ramasamy (SR) method and Rotational SR (RSR) method. The grown 2APNP crystals were subjected to various studies like HRXRD, laser damage threshold, chemical etching, Vickers microhardness, birefringence, UV-Vis NIR, dielectrics and piezoelectrics. The Rotational Sankaranarayanan-Ramasamy (RSR) method grown crystals show excellent optical, mechanical, dielectric and piezoelectric behavior and higher laser damage threshold capability compared to the conventional and normal SR method grown crystals. HRXRD and etching studies showed that the quality of the RSR method grown crystal is better than conventional and normal SR method grown crystal. The Rotational Sankaranarayanan-Ramasamy (RSR) method can be used to grow single crystals along a specific crystallographic direction such as the phase matching direction in nonlinear optical (NLO) crystals.

The unidirectional crystal growth method is ideally suited for crystal growth along this direction to obtain large size crystals required for obtaining SHG elements with minimum wastage. In addition, the unidirectional solution crystallization usually occurs at around room temperature; much lower thermal stress is expected in these crystals over those grown at high temperatures. Successful development of this unidirectional method will provide the technology to produce crystals at a yield close to 100% and easy scaling-up process.



**2AP4N crystals grown by (a) Conventional method, (b) SR method and (c) RSR method**

**References**

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[2] P. Karuppasamy, Muthu Senthil Pandian, P. Ramasamy, Sunil Verma, *Opt. Mater.* **2018**, 79, 152-171.

**INVT – 7**

## Smart Materials

**Dr. S. Jayakumar**

*Associate Professor in Physics, RKM Vivekananda College, Mylapore, Chennai – 4*

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There are Numerous Materials available and produced and useful for Research and Technology Development (Smart Materials).The recent trend of New Materials in Material Science subject is interesting, Everyday all over the world new material are synthesizedand used for various applications. Spectroscopic and Non-spectroscopic methods are available to characterize materials. The talk would highlight new materials such as 1) Organic material 2) Carbon – nanotube 3) Medicinal plant and 4) polymers itsproperties and how they are put to use and how they are helpful to society and mankind. The materials discussed are user friendly and the talk highlights various techniques used to obtain such new materials.

**INVT – 8**

# Perylene Diimide:
# A versatile Non-Fullerene Electron Acceptor Material

**Dr.S.P. Rajasingh**

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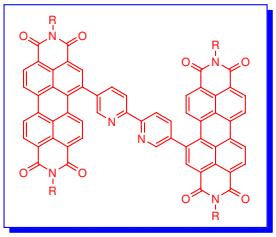
**Abstract**

Over more than 2 decades, fullerenes and their derivative have made high impact on chemistry and physics of electron transport materials, particularly in organic photovoltaic devices because of their electron accepting capability. Though the high electron affinity, efficient photo-generation, exciton dissociation and charge transport properties have made fullerene to be incorporated in the best performing devices, due to some disadvantages namely weak absorption in the visible region, limited opportunity of optical gap tuning, increased disorder upon functionalization and high cost, non-fullerene n-type materials are garnering increased attention.

Various types of non-fullerene acceptors have been synthesized and studied, among which perylene diimide (PDI) have received great attention due to its thermal, chemical and photochemical stability and outstanding electrochemical, photo-physical property and high electron mobility [3]. The large planar π-conjugated core has the ability to form strong π-π interactions which allows for efficient charge transport but limit the donor-acceptor interfacial area. The introduction of specific alkyl chains on imide position and modifying the bay region of PDI structure, aggregation of PDI can be minimized without compromising electron transport efficiency. One can do longitudinal extension through their imide and lateral expansion along their bay positions. Mostly bay region of Perylene diimides subjected for different functionalization through controlled bromination.



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[2] Rybtchinski, B, Rajasingh, P.; Shirman, E. US patent. **US 2015**/0152106A1.

# Role of Nacl on the Properties of Sulphamic Acid Single Crystals

**Dr. M. Selvapandiyan**

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*Dharmapuri – 636 705, Tamil Nadu,*

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## Abstract

Nonlinear optical (NLO) materials with enhanced third order nonlinear optical susceptibility $\chi^3$ have been used in wide range of applications such as laser technology, optical communication, optical storage technology, 3D optical memory, optical switching, optical modulating, and optical limiting etc. Pure sulphamic acid (SA) and NaCl doped sulphamic acid (SA) were grown by slow evaporation method at ambient temperature. The Z-scan technique was employed to determine the nonlinear refractive index, nonlinear optical absorption and third order nonlinear optical (TONLO) susceptibility of the grown crystals. The lattice parameters were determined by using single crystal and powder X- ray diffraction analyses. The presence of elements in the SA lattice was affirmed by EDAX analysis. The thermal stability of the grown crystals were analyzed by thermogravimetric and differential thermal analysis (TGA/DTA) and revealed that the grown crystals were thermally stable up to 331℃ and 334℃ for pure and NaCl doped SA. Vickers microhardness study reveals that the hardness of the crystals is increase with increasing load. The band gap energies were found to be 6.06 eV and 5.70 eV for pure and NaCl doped SA crystals respectively. From the PL specta the emission were observed at 335 and 424 nm for pure and 340 and 428 nm for doped SA crystal.

**INVT – 10**

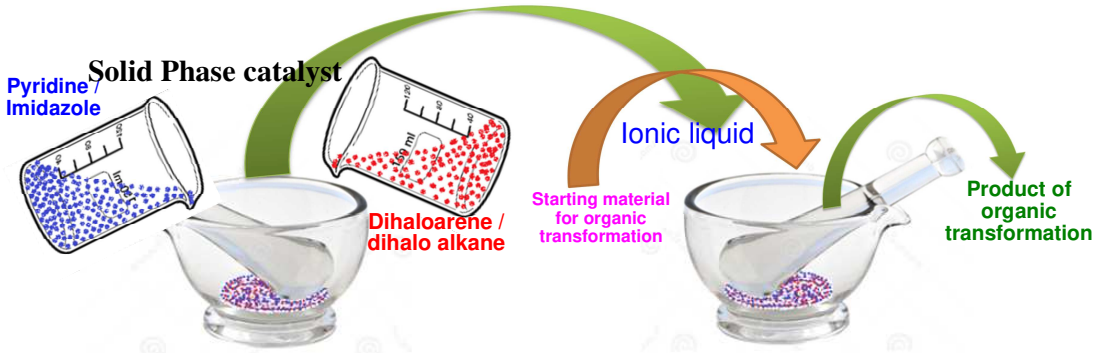
# Synthesis of some novel ionic liquids under conventional and Solid phase approach and its applications

**Dr. K. Ganesan**

*PG & Research Department of Chemistry, Presidency College (Autonomous), Chennai*

**Abstract**

Ionic liquid contains organic cation with simple / complex inorganic anions which shows higher thermal stability, ionic conductivity, high polar nature, non-toxic and non-volatility behaviors. Ionic liquids are exhibits number of biological, electrochemical, catalysis, separation science and chemical synthesis. Our recent research is focus towards the synthesis and characterization of some novel imidazole, pyridine type of ionic liquids. We totally avoided the toxic organic solvents for preparation of ionic liquids under solid phase solvent free approach. All the synthesized ionic liquids are showed excellent catalytic response compared to earlier literature reports for organic transformations.



# Synthesis, Growth and Characterisations (Dielectric, Photoconductivity And Ac/Dc Conductivity) of Laf Crystal

**Dr. K. Senthilkannan**

*Edayathangudy G S Pillay Arts & Science College Nagapattinam, 611002*

*Tamil Nadu*

*Email:* mscgoldmedalist@yahoo.in

**Abstract**

The single crystals of LAF are expediently grown by slow solvent evaporation technique. It is estimated from the X-ray diffraction studies that LAF crystals are of orthorhombic system, lattice parameter values are a as 5.778 Å, b as 6.032 Å and c as 12.334 Å. The frequency and temperature dependence of the dielectric constant / dielectric loss of LAF are properly investigated. The activation energy of the sample is computed by ac/dc conductivity studies. The photo conducting nature of LAF is studied by photoconductivity investigations.

**Keywords:** Dielectric, Photoconductivity, Ac/Dc conductivity, LAF crystal...

**INVT – 12**

## Environmental risk factor induced urinary stone disease

**Dr. R. Selvaraju**

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**Abstract**

Urolithiasis is serious debilitating problem through the world. All over the world 40% to 45 % of the population is suffering from urinary stone problem due to global warming, life style genetics, gender drug and dietary habits etc. The incidence of urolithiasis is very common in North India compare to southern states. People living in rock areas, where the climate is hot and dry seem to be more to urinary calculi disease. The inorganic organic chemical compound present in urinary stones .The present study carried out urinary stone composition by FTIR and XRD methods result are discussed.

**Key words:** Risk Factor, Urinary stones, FTIR and XRD.

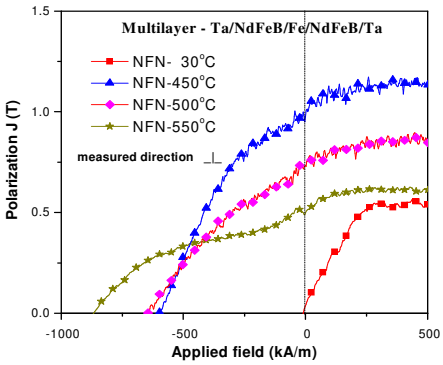
# Magnetic Behavior of RF Sputtered Nd-Fe-B / A-Fe Multilayer Thin Film

**S. Madeswaran**

*Department of Physics, School of Advanced Sciences, VIT, Vellore, India*

## Abstract

An enhanced remanence and a large maximum energy product are possible in a nanocomposite magnet with fully and perfectly exchange coupled grains of hard and soft magnetic phases. The soft and hard magnetic phases are having the advantages of the high remanence and the high magnetization, respectively, which would give such great possibility. Investigation on nanostructured exchange coupled magnets has been conducted since 1989. Bulk $Nd_2Fe_{14}B$ / α-Fe nanocomposite permanent magnets have brought much attention due to their high potential magnetic properties with advantages of good corrosion resistance, excellent fracture toughness, and low fabrication cast. A maximum energy product of as high as 440 $kJ/m^3$ can be achieved in a specially prepared bulk anisotropic $Nd_2Fe_{14}B$ / α-Fe nanocomposite. Although the maximum energy product has been improved in nanocomposite multilayer films, it is still lower than the bulk formation and theoretical calculation. Experimentally, high energy products require well textured and fine grained structure with high fraction of the soft phase with a high magnetization. As there are relatively large technical difficulties in thin films, not many investigations on textured soft/hard magnetic multilayer have been published. The foremost obstacle is that deposition of textured films at high temperature results into interdiffusion of the constituent elements, destroying the orientation and the formation of the appropriate hard phase. Hence, for this study, intermediate temperatures and subsequent annealing at high temperature were implemented and constituent elemental with the resulting magnetic properties were investigated. Multilayer consists of hard and soft magnetic structure of NdFeB (100nm)/ Fe (15nm) /NdFeB (100nm) thin films, grown by RF magnetron sputtering on Ta buffer layered Si(100) substrates. To fabricate Nd-rich magnetic target with a nominal composition of $Nd_{21}Fe_{64}B_{15}$, we use arc melting and subsequently plasma activated sintering.



After the film growth, Ta (20nm) cap layer was deposited to product the magnetic film from oxidation. The film depositions were carried out at high, intermediate and room temperature (550, 500, 450 and 30$^{o}$C). To study about interface and inter diffusion of constituent elements, we prepared additional set of multilayer by changing the position of α-Fe layer that is on top of the hard magnetic layer [NdFeB (200nm)/α-Fe(15nm)]. X-ray diffraction analysis and magnetic hysteresis loop (vibrating sample magnetometer) measurements were carried out. The magnetic behavior measured at room temperature with perpendicular to the films showed figures 1. Intermediate temperature, that is, 450$^{o}$C gives better properties compared with other films, Moreover the anisotropic nature of films are drastically varying by the deposition temperature and the degree of anisotropic constant were calculated by measuring hysteresis loop in parallel direction with respect to film. Significant changes in magnetic behavior can be observed while alter the film structure with same dimension. It can be seen that the remanence ratios, $J_{r\perp}$ / $J_{r\parallel}$, are in deference with preparation temperature and the trend is also desperately diverse from the films with inter layer of α-Fe.

# Crystal Growth Papers

**CYGP-1**

# Synthesis, Spectroscopic Characterization and Applications of Pure and Copper Doped L-Alanine Tartrate Single Crystals

**C.Surendra Dilip[1]*, J.Aarthy[2], M.Chitravel[3] and M.Adam Gani[4]**

[1]**Departmentof Chemistry, Government Arts College, Tiruchirappalli 620022*

[2]*Department of Physics, Cauvery College for Women, Tiruchirappalli 620018*

[3]*Department of Chemistry, TRP Engineering College, Tiruchirappalli 621105*

[4]*Department of Chemistry, M.I.E.T. Arts and Science College, Tiruchirappalli 620007*

**Abstract**

Single crystals of pure and Copper doped L-Alanine Tartrate were grown by slow evaporation method. The cell parameters were determined using single crystal X-ray diffraction method. To improve the physical properties of the LALTT crystal, Copper dopant was added by 2 mol%. ICP studies confirm the presence of Copper in the grown LALTT crystal. Transparency range of the crystal was determined using UV-VIS-NIR spectrophotometer. The functional groups of pure and doped LALTT crystals were analyzed by FT-IR spectroscopy. Using Vickers microhardness tester, mechanical strength of the material was found. Dielectric studies of pure and doped LALTT single crystals were carried out. The doped LALTT crystal is found to have efficiency higher than that of pure LALTT crystal.

**CYGP - 2**

# Growth and Characterisation [Mass Spectral, Beam Displacement, Influx, Photoluminesence] of Lapm Crystals

**R.Anitha[1], E. Karalmarks[1], S.Ezhilmathibhavadharani[1], K.Monisha[1], S.Anusiya[1],K.Suganya[1] andK.Senthilkannan[2]***

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*[2*]Department of R&D, Edayathangudy G.S Pillay Arts & Science College,*

*Nagapattinam-611002*

**Abstract**

The mass spectral data for LAPM is found to be 290 units the beam displacement is 1.289mm and 0.54mm for LW and SW. the influx is 2.9668 microns for NLO utility. PL is in the range of 398 nm is attributed to n-π* transition and the band gap is 3.1176eV. LAPM Crystals are of monoclinic in nature with a as 10.899Å, b as 7.912Å, c as 7.343Å, beta is 98o, space group is P21.

**Keywords:**Xrd, Mass Spectral, Beam Displacement, Influx, Photoluminesence, Lapm Crystal

**CYGP - 3**

# Luminescence Studies on Indium Doped RbBr Single Crystal

**P.Eswaran[1], S. Karthikeyan[2] and R. Ravisankar[3]**

*[1]Department of Physics, Saveetha Institute of Medical and Technical Sciences, Saveetha School of Engineering, Thandalam, Chennai-602105*

*[2]Department of Physics, Dr. Ambedkar Government Arts College, Chennai-600039*

*[3]Post Graduate and Research Department of Physics, Government Arts College, Tiruvannamalai-606603*

**Abstract**

Absorption, excitation and emission spectra of RbBr: In crystal have been investigated at room temperature. A broad absorption bands of A and C are composed of three sub bands, while the B band exhibits a doublet structure, which are ascribed to monomer and dimer center are observed. Absorption intensities of these bands decrease in the A and B bands being compensated by the increase in the C band.

**Keywords**: optical absorption, emission spectra, dimer center, monomer center.

**CYGP - 4**

# Growth and Characterization of Glycine Potassium Iodide Doped with Calcium Chloride (GPICC) Single Crystal

**D. Rajendiran[1], P. Jayaprakash[2], K.M. Freny Joy[3], K.Suresh[4] and R.Ravisankar[5]***

*[1]Post Graduate and Research Department of Physics, Shanmuga Industries Arts and Science College, Thiruvannamalai – 606603*

*[2]Department of Physics, St. Joseph's Institute of Technology, OMR, Chennai-600 119*

*[3]Department of Physics, Madras Christian College, Tambaram, Chennai – 600059*

*[4]Department of Physics, Annai Mira College of Engineering and Technology, Arapakkam, Vellore – 632517*

*[5*]Post Graduate and Research Department of Physics, Government Arts College, Thiruvannamalai – 606603*

**Abstract**

A single crystal of glycine potassium iodide doped calcium chloride (GPICC) has been grown by the slow evaporation technique at room temperature using solvent of deionized water. The single crystal X-ray diffraction study confirms that the unit cell parameters of GPICCcrystal.Functional groups present in the sample were identified by FTIR spectral analysis. The crystals were further characterized by UV-visible-NIR transmission spectrum in the range of 200nm to 1100nm. The measured SHG efficiency value for glycine potassium iodide doped with calcium chloride isvery closely to that of KDP. The photoconductivity study confirms the positive photo conducting nature of grown crystal.

**Keywords***:* Glycine Potassium Iodide, X-ray diffraction, FTIR, Photoconductivity.

**CYGP– 5**

# Crystal Growth and Characterizations of Organic Triphenylphosphine Oxide 4-Nitrophenol (TP4N) Single Crystals for Nonlinear Optical (NLO) Application

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**Abstract**

The optically good quality triphenylphosphine oxide 4-nitrophenol (TP4N) single crystals were successfully grown by slow evaporation solution technique (SEST) at room temperature. The cell dimensions of the grown TP4N single crystal were confirmed by single crystal X-ray diffraction (SXRD) measurement. Functional groups of TP4N crystal were confirmed by Fourier transform infrared (FTIR) spectral analysis. The optical transmittance of the grown crystal was determined by the UV-Vis NIR spectral analysis and it has good optical transparency in the entire visible region. The thermal stability of the TP4N crystal was investigated by thermogravimetric and differential thermal analysis (TG-DTA). Vickers microhardness analysis was carried out to identify the mechanical stability of the grown crystal. The work hardening co-efficient value was also calculated and it was found that the TP4N crystal belongs to the soft material category. Laser damage threshold (LDT) value was measured by using Nd:YAG laser (1064 nm). The Z-scan technique was carried out using solid state laser (640 nm) to analysis the nonlinear optical properties of the TP4N single crystal. It exhibits the self-defocusing and saturable absorbance effect occurs during analysis of closed and open aperture respectively. Several attempts have been made to grow the TP4N crystal by Sankaranarayanan-Ramasamy (SR) method. The results are discussed in detail.

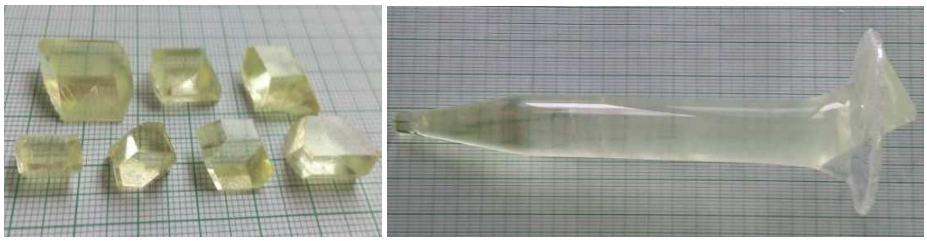

**Figure.1 (a) Conventional and (b) SR method grown TP4N single crystal**

**CYGP - 6**

## Pure and Benzoguanamine-Doped PVDF/KI/I2 Electrolytes for Dye Sensitized Solar Cell (DSSC) Applications

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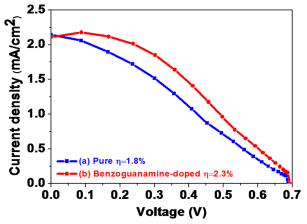
**Abstract**

Great attention is currently being paid to the dye sensitized solar cell (DSSC) due to its easy preparation, environment friendliness and high power conversion efficiency with low cost. The electrolyte plays a vital role in DSSC which is required for the continuous regeneration of the sensitizer. In 1991, Gratzel and O'Regan fabricated dye-sensitized solar cell (DSSC) with acetonitrile solvent, iodide/triiodide ($I^-/I_3^-$) redox couple contained liquid electrolyte and they achieved 7.9% efficiency.The intensive research works have been carried out in this area and iodide/triiodide redox couple based liquid electrolytes are found in maximum power conversion efficiency of 11.9%.The commercialization of DSSC is affected by the major drawbacks with liquid electrolyte such as short-term stability due to the evaporation of the solvent, corrosion of the counter electrode and sealing problems. The researchers are focusing on reducing the crystallinity of the polymer matrix, which improves the ionic conductivity of the polymer electrolyte.The polymer electrolyte has many advantages compared to liquid electrolyte such as good adherence to the electrode, flexible geometry, low volatility and high energy density. The pure and benzoguanamine-doped PVDF/KI/$I_2$ electrolytes were prepared by solution casting method.The synthesized polymer electrolyte films were characterized by powder X-ray diffraction (PXRD), Fourier transform infrared (FTIR) spectrum and AC-impedance analysis. The ionic conductivity of the pure and benzoguanamine-doped PVDF/KI/$I_2$ electrolyte films are $3.90\times10^{-6}Scm^{-1}$ and $1.21\times10^{-5}Scm^{-1}$ respectively. Powder X-ray diffraction studies revealed that the benzoguanamine-doped PVDF/KI/$I_2$ electrolyte has the higher amorphous nature compared to pure PVDF/KI/$I_2$ electrolyte. The dye sensitized solar cells (DSSCs) were fabricated using pure and benzoguanamine-doped PVDF/KI/$I_2$ electrolyte and the obtained power conversion efficiencies are 1.8% and 2.3% respectively under an illumination of 100 $mW/cm^2$.




**J-V curve measurements of (a) pure and (b) benzoguanamine-doped PVDF/KI/$I_2$ electrolyte**

**CYGP - 7**

# Growth of Organic Nonlinear Optical 2-Aminopyridinium 4-Nitrophenolate 4-Nitrophenol (2APNP) Single Crystals by Conventional, Unidirectional and Seed Rotation Technique for SHG Device Applications

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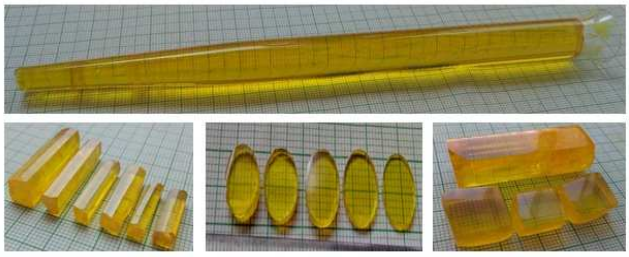
**Abstract**

The bulk size single crystal of 2-aminopyridinium 4-nitrophenolate 4-nitrophenol (2APNP) with the dimensions of 200 mm length and 10 mmdiameter was grown successfully along <001> direction by Sankaranarayanan–Ramasamy (SR) method within the period of 60 days. The average growth rate is 3 mm per day. Initially the 2APNP seed crystal was grown by slow evaporation solution technique (SEST). The grown crystal was subjected to single crystal X-ray diffraction (SXRD) measurement and the grown crystal belongs to Orthorhombiccrystal system with space group $Pna2_1$. The crystalline purity was confirmed by powder X-ray diffraction (PXRD) analysis and the obtained planes were indexed using FULLPROF software. The morphology of the grown crystal was indexed by WinXmorph software. The functional groups of 2APNPsingle crystal were confirmed by Fourier transform infrared (FTIR) spectrum analysis. The optical transmittance of the grown crystal was determined by UV-Vis NIR spectrum analysis and it has good optical transparency in the entire visible region. The optical band gap energy of the 2APNP was also calculated. The load dependent mechanical hardness of the grown crystal was analysed by Vickers microhardness test. The second harmonic efficiency (SHG) was analysed using Kurtz-Perry powder techniquewith different particle size and it confirms that the grown crystal has phase matchable.The same crystal was grown by the seed ration technique. The results are discussed in detail.



2APNP crystal grown by Conventional, Unidirectional and seed rotation technique

**CYGP - 8**

# Crystal Growth and Quantum Chemical Studies of 4-Nitrophenol 4-Aminobenzoic Acid Monohydrate (4NPABA) Single Crystal for Non-Linear Optical (NLO) Applications

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**Abstract**

The new organic crystal of 4-nitrophenol 4-aminobenzoic acid monohydrate (4NPABA) was successfully synthesized and grown by slow evaporation technique (SEST). The crystal structure of 4NPABA was confirmed by single crystal X-ray diffraction (SXRD) studies. The various functional groups were identified using Fourier transform infrared (FTIR) spectrum analysis. The optical transmittance of the grown crystal was analysed by using UV-Vis NIR spectral studies. The UV cut-off wavelength is obtained at 400 nm and it shows that the crystal has no absorption of light in the entire Visible and NIR region. The thermal stability of the title crystal has been investigated by TG-DTA studies. The molecular structure of 4NPABA was optimized and the structural parameters have been determined by density functional theory (DFT). The charge transfer characteristic of the title compound was studied by frontier molecular orbital (FMOs) analysis. The nonlinear optical (NLO) properties such as polarizability and hyperpolarizability were calculated. The polarizability and hyperpolarizability of the 4NPABA were calculated at the B3LYP/6-311++G (d,p) level using Gaussian 09W package. The calculated values of linear polarizability and hyperpolarizabilityare 2.683×10-23 e.s.u. and 11.865×10-30 e.s.u respectively. The charge delocalization of the present molecule was confirmed by NBO analysis.

**CYGP - 9**

# Growth and Characterisations(Chns, Ftir, Influx, Nlo, Hardness) of D32dmbc Crystals

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**Abstract**

NLO crystals are pre - dominate over non NLO crystals. D32 DMBC crystals are having huge opto electronic application, D32 DMBC are having formula C29 H24 Cl2 N2 O4, a system is monoclinic, space group is P21/c, the lattice para meters are 9.778 Å, 15.938 Å,17.583Å, beta is 101.94O. From CHNS analysis C is 65.01, H is 4.49, N is 5.25, Cl is not detected, O is 11.978, Mras534.11, FTIR assignments reveals the vibrations of functional group present at 3315, 3421, 3298, 1618, 1586, 1463, 1237, 1000, 750 & 705 cm-1, crystalline influx measurement specify 2.7668 microns for NLO utility.NLO property is the main criteria for optical application, D32 DMBC is 1.14 times than that of KDP and the hardness value is 3.433 for D32 DMBC organic crystals.

**Keywords:** Chns, Ftir, Influx, Nlo, Hardness, D32dmbc Crystals.

**CYGP– 10**

## Study of Optical and Thermal behaviour of Lithium Hydroxide and Cyanuric Chloride Single Crystal.

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**Abstract**

Lithium Hydroxide and Cyanuric Chloride (LHCC), one of the semiorganic crystals, was grown by slow evaporation technique at room temperature. The incorporation of lithium into the lattice site of cyanuric chloride was confirmed using single crystal XRD. The fundamental functional groups of LHCC were identified using FTIR spectral studies. Optical properties were analysed using UV-Vis Absorption studies. Thermal studies were carried out to discuss the thermal stability and various decomposition stages of the material.

**Keywords:** Crystal Growth, Spectral studies, UV-Vis-Absorption studies, Thermal studies.

**CYGP - 11**

# Piperazinium Hydrogen Phosphite Monohydrate NLO Single Crystal for Optical Limiting Applications

**R. Rajkumar[1], B. V. Vijayalakshmi[1], T. Kavitha[1], E. Chinnasamy[1] and P. Praveen Kumar[2]**

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[2] *Department of Physics, Presidency College, Chennai - 600 005*

**Abstract**

Organic charge transfer molecule of Piperazinium hydrogen phosphite monohydrate single crystal was crystallized by slow evaporation technique. The single crystal XRD was carried out to determine the cell parameter values. The FTIR and FT-Raman spectral studies were done to confirm the presence functional groups. UV-visible spectrum shows that the Piperaziniumhydrogen phosphite monohydrate crystal (PHPM) is transparent in the visible region.The third order nonlinear optical refractive index and nonlinear optical absorption co-efficient were calculated by Z scan technique. Optical limiting method is applied to find the limiting behavior of Piperazinium hydrogen phosphite monohydrate crystal.

**CYGP– 12**

## Synthesis, Growth and Characterization of Silver Bismuth Sulfide ($AgBiS_2$) Single Crystal by Vertical Bridgman Technique for Thermoelectric Applications

**K. Ramachandran, MuthuSenthil Pandian and P. Ramasamy**

*SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu*

**Abstract**

Thermoelectric materials can be used for direct conversion of waste heat into electrical energy. The I-V-$VI_2$ (I = Cu, Ag, Au or Alkali Metal; V = Bi, Sb, As and VI = S, Se, Te) groups of ternary chalcogenide semiconducting materials have received considerable interest because of their potential use in linear, nonlinear and especially in thermoelectric applications. High performance thermoelectric materials should possess large Seebeck coefficient, high electrical conductivity and low thermal conductivity. Several thermoelectric materials such as $Pb_{1-x}Mn_xTe$, $Bi_2Se_xTe_{3-x,}$ $AgBi_3S_5$, $AgSb_xBi_{3-x}S_{5,}$ $GaInSe_2$,$Ge_{1-x}Sn_xTe$, Te-doped InSb, $Mg_2Si$, $Bi_{2-x}$ $ln_xSe_{3,}$ $CoSb_{3,}$ $RhSb_3$have been grown by Vertical Bridgman technique, slow cooling method and zone melting technique. In the present work semiconducting silver bismuth sulfide ($AgBiS_2$) single crystal was successfully grown by Vertical Bridgman technique with steady ampoule rotation. The crystal structure and unit cell parameters of the grown $AgBiS_2$ single crystal were identified by single crystal X-ray diffraction (SXRD) analysis. Powder X-ray diffraction (PXRD) indicates single phase of $AgBiS_2$. Thermo gravimetric and differential thermal analysis (TG-DTA) was carried out to find out the melting and freezing point of the grown crystal. The optical transmission behaviour of $AgBiS_2$ single crystal was studied using UV-Vis NIR spectrum analysis. The temperature and frequency dependent dielectric permittivity and dielectric loss were analyzed using dielectric measurements. The load dependent mechanical stability of the $AgBiS_2$ single crystal was studied by Vickers microhardness analysis. The laser damage threshold value was measured using Nd:YAG laser. The electrical properties of $AgBiS_2$ single crystal were carried out using Hall measurements. The elemental composition of $AgBiS_2$ single crystal was analyzed by EDAX measurement.

**CYGP - 13**

# Synthesis, Crystal Growth, Optical, Thermal, Mechanical and Dielectric Properties of Mono (Bis(2-(4-butylphenyl)imino)methyl)phenoxy)zinc(II)dichloride (MBPMP) Single Crystal as a Nonlinear Optical (NLO) Material

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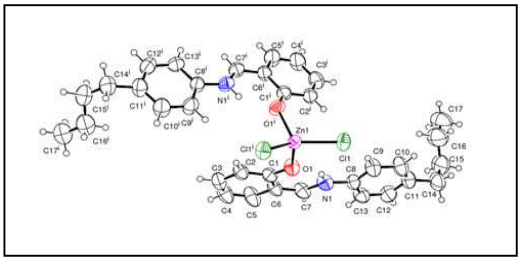
*[3]Thirumalai College of Engineering, Kanchipuram*

## Abstract

A new mono (Bis(2-(4-butylphenyl)imino)methyl)phenoxy) zinc(II) dichloride (MBPMP) single crystal was grown by slow evaporation technique in ethanol. Single crystal XRD studies confirm that the MBPMP crystal is mononuclear, with tetragonal coordination geometry and P41212 noncentrosymmetric space group. The FT-IR spectral analysis was used for identifying the functional groups and bonding nature present in the MBPMP crystal. The UV–Visible-NIR studies reveals that the MBPMP single crystal exhibits a very broad transparency window in the near infrared and visible regions between 220 to 1200 nm and the optical transparency of the MBPMP crystal is 99.49% with the lower cut-off wavelength of 220nm. The optical energy band gap evaluated from the transmission spectrum was found to be 5.63 eV. The Vickers microhardness number [1.8544 P/d2 kg/mm3] and the work hardening coefficient number (n = 2.326) indicates that the MBPMP single crystal is soft natured. The thermal property was analysed by TGA/DSC analysis. MBPMP single crystal exhibits lower dielectric constant and lower dielectric loss at higher frequencies indicating good quality optical crystal. The second harmonic generation efficiency of the MBPMP crystal was found to be 1.2 times greater than that of standard KDP crystal. The laser damage threshold value of the MBPMP single crystal was calculated to be 3.86 GW/cm2.



**Keywords**: Single crystal XRD, Optical studies, TGA/DSC, Microhardness analysis, Dielectric studies and SHG.

**CYGP - 14**

## Synthesis Growth Structural Spectroscopic and Optical Properties of L-Lysine Mono Hydrochloride Sodium Chloride Non Linear Optical Crystals

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**Abstract**

Semi-organic non linear optical material of L-Lysine monohydrochloride Sodium chloride in the ratio of 1:0.5 was grown by slow evaporation technique at room temperature. Single crystal XRD was carried out to examine the crystal system and unit cell parameters. Powder XRD patterns confirm the basic structure of materials and the functional groups are identified by using FTIR spectrum. TG/DTA analysis is confirms that the stability of grown crystals. The transparency of grown crystals was analysed by UV-VIS-NIR. The second harmonic generation (SHG) conversion efficiency has been estimated and the output power of the crystal was determined by using Kurtz powder technique.

**Keywords:** Crystal growth; Slow evaporation technique;L-Lysine monohydrochloride, Sodiumchloride.

**CYGP- 15**

# Growth and XRD, CHNSO and FTIRCharacterisations of LAPM Crystals

**M. Shahul Hameed[1], M. Mohamed Thowfik[1], S. Vijay Ganesh[1], G. Karthick[1], T. Sakthivel[1], K. Suganya[1] and K. Senthilkannan[2*]**

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*[2]Department of R&D, Edayathangudy G.S Pillay Arts & Science College, Nagapattinam-611002*

**Abstract**

LAPM CRYSTALS are having wide range of applications, it is monoclinic in nature with a is 10.899Å, b is 7.912Å, c is 7.343Å, beta is 98$^{o}$. the chemical formula is $C_6H_{19}N_4O_7P$ space group is $P2_1$, FTIR analysis specifies the vibrations at 1413, 3330, 3453, 879, 1577, 1693, 8777, 1289, 1332, 3004 & 1693 $cm^{-1}$. By CHNSO analysis C is 24.82, H is 6.55, N is 19.31, O is 38.62, S is not detected.

**Keywords:** XRD, CHNSO, FTIR, LAPM crystal

**CYGP - 16**

## Directional Growth, Physicochemical and Quantum Chemical Investigations on 2-Amino-5-Nitropyridinium Dihydrogen Phosphate (2A5NPDP) Single Crystal for Nonlinear Optical (NLO) Applications

**V. Sivasubramani, MuthuSenthil Pandian and P. Ramasamy**

*SSN Research Centre, SSN College of Engineering, Chennai-603110*

**Abstract**

Bulk size single crystals and its distinctive property play an important role in nonlinear optics (NLO), electronics and photonics. In the past decades, extensive efforts have been made to grow the crystal in bulk size with high quality for practical device applications. In this present work, an efficient organic nonlinear optical (NLO) 2-amino-5-nitropyridinium dihydrogen phosphate (2A5NPDP) single crystal was grown by modified Sankaranarayanan-Ramasamy (SR) method in the period of 60 days. The grown single crystal has the size of 80 mm length and 15 mm diameter. It is observed that the growth rate of the modified SR method grown 2A5NPDP crystal was found to be 10 times higher compared to the conventional method grown crystal. The unit cell parameters and morphology of the grown crystal were confirmed by Single crystal X-ray diffraction (SXRD) analysis. The molecular structure and the presence of functional groups were determined by NMR and FTIR spectrum analyses, respectively. The UV-VisNIR analysis shows that the grown crystal possesses good optical transparency (77%) in the visible and NIR region. The chemical etching study reveals that the grown crystal has less etch pit density (EPD). The title compound is thermally stable upto 175°C. Frequency dependent dielectric constant, dielectric loss and AC conductivity of the grown crystal were analyzed. The laser damage threshold measurement was performed using Nd:YAG laser (1064 nm). Photoluminescence (PL) spectral study evidences that the grown crystal has strong blue emission. The optical, chemical etching, dielectric and laser damage threshold studies clearly indicates that the crystal grown by SR method have low density of defects. The Kurtz-Perry powder second harmonic generation (SHG) test was carried out for 2A5NPDP crystal and it exhibits 3.5 times that of standard KDP material. Third-order nonlinear behavior was studied using Z-scan technique by employing Nd:YAG laser and it indicates that the grown 2A5NPDP crystal can serve as a promising candidate for NLO device applications. The theoretical calculations were performed by B3LYP/6-311++G (d,p) basis set.

The structural parameters of 2A5NPDP were studied using DFT method and the calculated results were compared with experimental values. The charge transfer characteristic of 2A5NPDP compound was studied by frontier molecular orbital (FMOs) analysis. The first-order hyperpolarizability of the present molecule was calculated and it was found to be $3.50\times10^{-31}$e.s.u, which is 108 times higher than the standard urea molecule. The hydrogen bonding of the title molecule was confirmed by Natural Bond Orbital (NBO) analysis. From the obtained results, it has been concluded that the grown 2A5NPDP crystal is a promising material for nonlinear optical (NLO) and optoelectronic device applications.

**CYGP- 17**

# Growth and Mass Spectral, UV, Thermal, Photo Conductivity of D32DMBC Crystals

**S.Subasri[1], R.Ranjani[1], M.Ponneeswari[1], R. Ranjitha[1], J.Santhiya[1], K.Suganya[1] andK.Senthilkannan[2*]**

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**Abstract**

NLO crystals are prevail over their counterparts by the SHG-NLO values, D32DMBC crystals are having enormous opto-electronic application, D32DMBC are having formula $C_{29}H_{24}C_{l2}N_2O_4$, a system is monoclinic, space group is $P2_1/c$, the lattice parameters are 9.778 Å, 15.938 Å, 17.583Å, beta is 101.94$^o$. Mass spectral data portrays that its molecular mass is 534 units, from the UV data the cutoff wave length is 340 nm and the corresponding band gap is 5.391eV, the thermal data reveals that the peak is 148$^o$C, the sharpness is due to good crystallinity. Photo conductivity study represents that D32DMBC is having negative photo conductivity.

**Keywords:** Mass Spectral, UV, Thermal, Photo Conductivity, D32DMBC Crystals

**CYGP - 18**

# Growth and Therapeutical and Spectral Characterisations of 4-Methoxyphenyl 2-Oxo-2h-Chromene-3-Carboxylate [4mp2o2hc3c] Crystals

**K. Suganya[1], R. Krishnaveni[2] andK.Senthilkannan[3*]**

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*[2]PG & Research Dept. of Microbiology, Idhaya College for Women, Kumbakonam*

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**Abstract**

A solution of dicyclohexylcarbodiimide (DCC) broke up in dried CH2Cl2 was added to an solution containing coumarin 3-carboxylic corrosive (1.0 mmol) and 4-methoxyphenol (1.0 mmol) and a synergist measure of N—N-Dimethylaminopyrimidine (NNDMAP) in anhydrous dichloromethane (CH2Cl2), under blending, After 25 hrs of mixing, dicyclohexylurea was sifted off and the arrangement was concentrated. The strong buildup was sanitized by section chromatography on silica gel utilizing chloroform (CHCl3) as an eluent. Dull crystals of the title compound - 4MP2O2HC3C were developed by moderate dissipation of an ethanol arrangement at room temperature. The synthetic recipe is C17H12O5. The mass spectral data for 4MP2O2HC3C is found to be 296 units the beam displacement is 1.279 mm and 0.52 mm for LW and SW. The influx is 2.9886 microns for NLO utility. PL is in the range of 396 nm is attributed to n-π* transition and the band gap is 3.1333eV. 4MP2O2HC3C Crystals are of Orthorhombic in nature with a = 6.264 Å, b = 10.436 Å,c = 20.622Å, volume is 1348.08 Å3 and space group is P212121. The 2-oxo-2H-chromene is a helpful commencement material for the development of heterocyclic mixes with a wide range of natural exercises. Particularly the 3-substituted subordinates shows pharmacological impacts, for example, pain relieving, hostile to joint pain, mitigating, against pyretic, hostile to viral, hostile to malignant growth and anticoagulant properties. 2-oxo-2H-chromenes (coumarins) have been additionally utilized in the field of prescription, beauty care products and fluorescent colors.

**Keywords:**Xrd, Therapeutical, Mass Spectral, Beam Displacementy, Influx,Pl, 4mp2o2hc3c Crystal, Bio Applications.

**CYGP - 19**

# Growth and Characterization of Sulphanilic Acid Doped Zinc SulphateSemiorganic Crystal

**E. Vinoth[1],R. U. Mullai[1], R. Arul Jothi[1], T. Suresh[1], M.Kumar[1], S.Gopinath[1]and S. Vetrivel[1*]**

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**Abstract**

Sulphanilic acid zinc sulphate(SZS) crystal was grown successfully by slow evaporation solution growth technique at room temperature. Single crystal X-ray diffraction analysis confirms that the monoclinic crystal system. The Powder XRD spectrum shows the good crystalline nature. The optical behavior was examined by utilizing UV-visible spectrum the cut-off wavelength was found to be 250 nm from the UV-visble spectrum. A presence of functional groups in title compound was identified by FT-IR analysis. SHG efficiency of SZS was found to be 0.9 times greater than that of known KDP. The surface micrographs of crystal surface and the surface smooth are appearing in the crystal surface of SZS are identified by FESEM analysis. The photoluminescence study shows that the spectrum of SZS belongs to green light emission. The thermal behavior of the grown crystal was studies by using TGA analysis shows that the crystal stable upto $245^0$C. The surface microscopic image of SZS crystal was identified by FESEM analysis.

**CYGP - 20**

# Synthesis, Growth and Characterization of Semiorganic Crystal 2-Aminopyridine Potassium Hydrogen Phthalate Potassium Nitrate (2APKHPK)

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**Abstract**

The growth of 2-aminopyridine potassium hydrogen phthalate potassium nitrate (2APKHPK)crystal and its optical properties are discussed in this chapter. The single crystal of 2APKHPK was grown by slow evaporation method.Single crystal X-ray diffraction analysis of grown crystal were recorded. The grown crystal was characterized by Powder X-Ray Diffraction (PXRD) which confirms that the grown crystal has good crystalline nature. The FTIR analysis is used effectively for identifying the chemical bonding and information about molecular structure of the synthesized compound. A well polished, defect free good transparent crystal was subjected to linear optical study. It is observed that the grown 2APKHPK crystal has good transparency in the entire visible region. The non-linear optical efficiency was measured and the result is compared with reference material KDP. Thermal analysis of 2APKHPK crystal was carried out using TGA and DTA. Laser Damage Threshold value was found for the grown crystal 2APKHPK using LDT study. Hardness values of the grown crystal were estimated by Vickers'smicrohardness test.

**Keywords:** Solution growth method; XRD; SHG; Hardness.

**CYGP - 21**

## Synthesis, Growth and Characterization of Zinc Borate Single Crystal

**A.Dilli Rani[1], S. Sudha[1], P. Jayaprakash[3], G.Mani[1], andM.Lydia Caroline[1, 2*]**

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**Abstract**

The Zinc borate crystal was synthesized and grown by the technique of slow evaporation. The monoclinic structure, $P_{21}/n$ space group and crystallinity of Zinc borate have been ascertained employing the analysis of single crystal X-ray diffraction studies. The functional groups were identified by FT-IR studies. The UV- visible and photoluminescence spectrum discloses the optical and electronic properties respectively for the grown crystal. Several optical properties specifically extinction co-efficient, reflectance, linear refractive index, electrical and optical conductivity were also determined. The second harmonic generation of the grown crystal was measured by Kurtz and perry powder techniques.

**Key words:** Single Crystal XRD; UV visible; Microhardness

**CYGP - 22**

## Growth and characterization of a 4 -Nitrophenol L-Citrulline NLO Single Crystal

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**Abstract**

Single crystals of 4-Nitrophenol and L-Citrulline(4NPLC) have been grown by the slow evaporation technique at room temperature using aqueous solution. The single crystal XRD study confirms monoclinic system for the grown crystal. The functional groups present in the grown crystal have been identified by FTIR spectral studies. Lower cut-off and optical band gap were determined from the UV-vis spectral studies using solid crystal sample. Further, the thermal resistance was observed by using TG/DSC analysis. The photoluminescence spectrum of 4NPLCwas recorded. In order to determine mechanical strength of 4NPLCcrystal for various loads using Vickers micro hardness tester. The Dielectric behaviour of the crystal has been determined in the frequency range from50 Hz to 5 MHz at various temperatures.

**Keywords:** Optical materials, Crystal growth, X-ray diffraction, Optical properties.

**CYGP- 23**

# Investigation on Growth and Characterization of Amino Acid Based Semiorganic Complex Crystal L-Threonine Tartaric Acid (LTA)

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**Abstract**

A good quality L-threonine tartaric acid (LTA) crystal of optimum size 7 mm x 3 mm x 2 mm was obtained within a period of 40 to 45 days. The grown L-threonine tartaric acid (LTA) crystals have been subjected to single crystal X- raydiffraction studies to determine the unit cell dimensions and cell parameters. It is observedfrom the single crystal XRD studies that LTA crystal belongs to orthorhombic crystal system. The crystalline nature of the grown crystal was determined by the Powder X-Ray Diffraction (PXRD) studies. Infrared spectra are an important record, which provide more information about the structure of a compound. A polished and suitable size of L-threonine tartaric acid (LTA) crystal was subjected to optical transmission study. The SHG efficiency of LTA crystal was found to be about 2 times greater than that of KDP. A thermal property of the material was studied by Thermogravimetric (TGA) and Differential Thermal Analysis (DTA). Vickers hardness number of as grown LTA crystal is found to be increase with the applied load. The dielectric study of LTA crystal was carried out as a function of frequency at different temperature.

**Keywords:** XRD; FT-IR; UV-vis-NIR; SHG.

**CYGP - 24**

# Spectroscopic and thermal studies of glycine crystal grown from Zinc Chloride (GZC) for optoelectronic applications

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**Abstract**

Good optical quality single crystals of Glycine Zinc Chloride (GZC) were grown from aqueous solution in 1:1 molar ratio at room temperature by slow evaporation technique. The grown crystals were characterized by various studies like FT-IR, single XRD, UV-Vis-NIR and SHG and the obtained results are discussed. The thermal behavior of the crystals has been investigated by TG/DTA analyses. The above characterization and the nonlinear optical properties confirm that the grown crystal is suitable for the fabrication of various optoelectronic devices.

**Keywords**: Glycine Zinc Chloride, Characterization studies, Nonlinear optics

**CYGP - 25**

## Materials synthesis, crystal growth and nonlinear optical properties of Semiorganic crystal: 4-dimethylaminopyridine lithium nitrate

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**Abstract**

Optically good quality semiorganicnlo crystal 4-dimethylaminopyridine lithium nitrate was grown by slow evaporation techniques at ambient temperature using water as a solvent. Powder xrd study confirmed as good crystalline nature of the 4-dmapln sample. Orthorhombic crystal system was identified by single crystal xrd study with cell volume v = 894 $å^3$. Fourier transform infrared spectroscopy identifies the presence of vibrational assignments of functional groups available in the 4-dmapln sample. Uv-vis-nir absorbance spectrum shows the lower cut-off wavelength at 280 nm with optical band gap value eg= 4.3ev. Dielectric studies show the polarization mechanism in the 4-dmapln crystal. Vickers micro hardness study reveals the mechanical behaviors of the crystal and calculated work hardening co-efficient is n = 1.3. Second harmonic generation (shg) efficiency of the grown 4-dmapln sample was found to be 1.17 times higher than reference kdp.

**Keywords**: crystal growth; nlo crystal; band gap; electrical properties; mechanical properties.

**CYGP - 26**

# Zinc selenide (ZnSe) is a useful semiconductor for homojunction or heterojunction

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**Abstract**

A representative rather than exhaustive review has been given on the solidification behaviour of organic nonlinear optical crystals. Many of the developments reported here represent quick experimental responses to the rapid theoretical advances made in the field of nonlinear optics. The article is divided into four parts. The first part deals with the characteristics of the organic nonlinear materials and need for large single crystals. The second and third parts are devoted to the thermophysical properties and experimental studies on crystallization processes. Here, recent work by authors is reviewed on the purification of source material, solidification behaviour and crystal growth. Various interactions between morphology, microsegregation, defects, growth velocity and temperature gradient are discussed. Specific examples of substituted anilines are presented. In the fourth section a stronger interaction is suggested between optical physicists and crystal growers to understand the problems of inhomogeneity, stress, damage threshold and doping in the organic crystals.

**CYGP - 27**

# Crystal Growth of Quaternary and Pentanary Chalcopyrite Alloy Single Crystals for Solar Cell Applications

**A. Christopher [1*], V. Neela[1] and P. Rajeswari[2]**

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**Abstract**

The growth of $CuInSe_{2(1-y)}Te_{2y}$, $CuGaSe_{2(1-y)}Te_{2y}$ and $CuIn_{1-x}Ga_xSe_{2(1-y)}Te_{2y}$ single crystals by chemical vapor transport technique in a closed tube, using iodine as a transport agent, is reported. Stringfellow's a-priori method is used in order to determine the interaction coefficients and the upper critical temperatures of pseudoternary chalcopyrite solid solutions. Resistivity and carrier mobility were determined by resistivity and Hall effect measurements using Van der Pauw method: all samples present p-type conductivity; the materials considered here have a large spread in the resistivity values.

**CYGP– 28**

# Red photoluminescence spectrum of CuAlS2: Mn

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## Abstract

The electrical and photoelectronic properties of the layered phase with $ZnIn_2S_4$ (III) structure, of the $Zn_xCd_{1-x}In_2S_4$ compounds ($0.65<x</1$) are investigated on single crystals, grown by chemical vapour deposition, whose structure and composition have been previously tested. The anisotropy of the electrical conductivity is reduced by the increase of the Cadmium concentration in the alloys and at the solubility limit ($x\cong0.7$) the electronic mobilities ratio $\mu\perp/\mu\parallel$ tends to unity. The energy gap, the photoluminescence emission band and the photoconductivity excitation peaks linearly shift to lower energies for increasing Cadmium content in the alloys. All the photoelectronic properties can be interpreted in the light of the well known models for the photogeneration and recombination processes in $ZnIn_2S_4$. Therefore, the disorder introduced in the system by the alloying process does not seem to modify significantly the high density of localized centres, whose presence is a typical characteristic of the $AB_2X_4$ systems.

**CYGP- 29**

## Growth and Dissolution studies on Copper Magnesium phosphate

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**Abstract**

Gallbladder and kidney are the vital organs in human body. The body it maintains proper balance of water and minerals as well as filtration and excretion of waste product. Due to chemical in balance in body the gallbladder and kidney are deposited hard mineral induced stone formation of kidney, urinary bladder, urinary tract and gallbladder. The prevention treatments of kidney stone and gallstone. The in vitro calcium magnesium phosphate incubatory potential of medicinal plant extracts using by Chow-Chow (*Sechiumedule)* and Ridge gourd *(Luffa acutangul).* The study revealed that grown and possible incubatory effect and crystal nucleation and growth result are disused.

**Keyword**: Gallbladder, Kidney stone, Dissolution, Medicinal plant

**CYGP - 30**

# Crystal growth, structural, optical, thermal, dielectric, mechanical and non linear optical studies of L-Tyrosine Zinc Carbonate single crystals

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[3]*Department of Physics, Vooress College Vellore.Tiruvalluvar University*

**Abstract**

L-Tyrosine Zinc Carbonate(LTZC) a semi-organic nonlinear optical single crystal has been grown by slow evaporation solution growth technique. The lattice parameters of the grown crystals are found out by single crystals X- ray diffraction technique and it is confirmed using powder X-ray diffraction. The modes of vibrations of different functional groups present were identified by using Fourier Transform Infrared (FTIR) analysis. The UV-Visible optical absorption spectrum shows that the crystal has high transmission with lowest UV cutoff wavelength of 230 nm. The calculated band gap of LTZC crystal was found to be 5.13eV. Dielectric constant and dielectric loss for various frequencies and temperatures were performed on LTZC crystal and the results were discussed in detail. The frequency dependence of ac conductivity for different temperatures was studied. The photoconductivity studies confirm that the crystal LTZC has negative photo conducting nature. The mechanical and thermal properties of the grown crystals have been studied. Surface morphological changes are observed in the grown LTZC crystal. The Non-linear optical second harmonic generation conversion efficiency of LTZC was determined using Q-switched Nd: YAG laser. The second harmonic generation conversion efficiency of LTZC is 2.12 times that of KDP.

**CYGP - 31**

## Process Development and Characterization of Semiorganic Nonlinear Optical Crystal 2-Aminopyridine Sodium Nitrate (2apsn)

**D. Sivavishnu[1], R. Srineevasan[1*] and J. Johnson[1]**

*[1]Post Graduate & Research Department of Physics, Government Arts College, Thiruvannamalai -606 603, Tamil Nadu, India.*

**Abstract**

2-aminopyridine sodium nitrate (2APSN), a nonlinear optical semiorganic crystal was grown successfully by slow evaporation solution growth technique at ambient temperature. Single crystal XRD analysis shows that the 2APSN crystal belongs to orthorhombic system and powder X-ray diffraction analysis confirms the crystalline nature of the grown 2APSN crystal. FTIR analysis of the grown sample 2APSN identifies the presence of various functional groups. Various proton ($^{1}H$) and carbon ($^{13}C$) environment are confirming the formation of title compound 2APSN. Further EDAX analysis is used to record the metal (sodium) in the synthesized compound 2APSN. In linear optical study UV cut off wavelength was found to be 397 nm from the grown sample and also transparent in the entire visible region is recorded. The work-hardening coefficient value n=2.36 by using Vickers microhardness test confirms the grown crystal belongs to soft category. The dielectric study revealed that the grown crystal posses low dielectric constant and low dielectric loss in the higher frequency region attributes that the 2APSN crystal is best suitable for NLO applications. In thermo gravimetric (TG) and differential thermal analysis (DTA), the thermal stability of the grown 2APSN crystal was found to be 382 ℃. Powder SHG efficiency study of 2APSN crystal shows 0.99 times more than that of standard KDP. Photoconductivity study of 2APSN crystal shows negative photoconductivity nature.

**Keywords:** Slow evaporation; XRD; UV; PL; Thermal; SHG; Photoconductivity.

**CYGP - 32**

# Synthesis, Growth and Characterization of 2-Aminopyridine Lithium Sulphate (2apls) Crystal

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**Abstract**

2-aminopyridine lithium sulphate (2APLS) crystal was grown successfully by slow evaporation solution growth technique at room temperature. Unit cell parameters were calculated using single crystal X-ray diffraction analysis, which confirm that grown 2APLS crystal belongs to triclinic crystal system. In the powder XRD pattern well defined Bragg's peaks are observed which reveals that the grown crystal has highly crystalline nature. Presence of various functional groups in the grown 2APLS crystal was identified by FT-IR analysis. The UV cut-off wavelength of 2APLS crystal was found to be 234 nm. The powder SHG efficiency of 2-aminopyridine lithium sulphate (2APLS) was found to be 1.25 times greater than that of standard KDP. The dielectric constant and dielectric loss of the grown crystal were observed for different temperatures. The mechanical behavior shows that as grown 2APLS crystal belongs to soft category.

**Keywords:** Slow evaporation; XRD; SHG; Dielectric.

**CYGP - 33**

# Growth and Characterization of Tartaric Acid Doped Potassium Hydrogen Phthalate (Tkhp) Crystal for Nlo Application

**R. Arul Jothi[1], E. Mythily[1], R.U. Mullai[1], E.Vinoth, T. Suresh, S. Gopinath[1] and S. Vetrivel[1*]**

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**Abstract**

A semiorganic nonlinear optical, tartaric acid doped potassium dihydrogen phthalate (TKHP) crystal was grown successfully by slow evaporation technique at room temperature. Powder X-ray diffraction analysis was carried out to confirm the crystalline nature of the grown sample. A crystal system and unit cell lattice parameter values of TKHP crystal are calculated using Single crystal X-ray diffraction analysis. UV cut-off wavelength and optical transmittance of grown crystal was identified by using UV-vis-NIR spectrophotometer. A powder sample of TKHP crystal was subjected to Kurtz-Perry powder technique to calculate the second order nonlinear optical property. Thermal stability and decomposition point of TKHP crystal was identified by TG/DTA analysis. Mechanical behaviour of TKHP crystal was analyzed using Vicker'smicrohardness test. Dielectric constant and dielectric loss were studied to find the polarization of TKHP crystal. Surface micrograph of TKHP crystal was observed using Scanning Electron Microscope (SEM).

**Keyword:** Slow evaporation; XRD; UV; Thermal analysis; NLO.

**CYGP - 34**

# Third Order Nonlinear Optical Properties of Piperazine Zirconium oxy Chloride (PZC) Crystal to Enhance the Optical Device Applications

**R. U. Mullai[1], R. Arul Jothi[1], E. Vinoth, T. Suresh, S. Gopinath[1] and S. Vetrivel[1*]**

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*Tiruvannamalai 606 603, Tamil Nadu*

**Abstract**

Optical quality crystal, piperazine Zirconium oxy chloride (PZC), was synthesized and grown successfully by slow evaporation solution growth technique at room temperature. Well defined Bragg's peak in powder X-ray diffraction analysis confirms the crystalline nature of the grown sample PZC. Unit cell parameters values were calculated using single crystal X-ray diffraction analysis confirms that the crystal belongs to Tetragonal crystal system. The wave number band assignments of the synthesized material are identified by using Fourier Transform Infrared spectroscopy (FT-IR). Linear optical study shows that the UV cut-off wavelength was found to be 260 nm and also the optical energy band gap was calculated using UV data. Maximum emission spectra of wavelength 477 nm evident the emission of blue laser from the Florescence (PL) spectra. As grown PZC crystal was subjected to thermal analysis to find the weight-loss and decomposition point using TG-DTA. Work hardening coefficient of PZC crystal was 2.36, which evident that the crystal belongs to soft category material. Third order nonlinear optical property was analyzed using Z-scan technique, which shows that the crystal PZC obeys the third harmonic generation.

**Keyword:** Slow evaporation; XRD; PL; Thermal analysis; Z-scan.

**CYGP - 35**

# Synthesis, Optical, Thermal, and Mechanical Properties of Picolinic acid Phosphate, a Semiorganic Enhanced NLO Single Crystal

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**Abstract**

Single crystals of Picolinicacid phosphate ( PAP ) were grown by slow evaporation technique. The optical studies reveal the transparency of the crystal in the entire visible region. Grown crystal was subjected to single crystal XRD diffraction technique. Thermal studies of LSP confirm the thermal stability of the crystal and it is stable up to 210°C. The functional groups and optical behaviour of the crystal were identified from FT-IR and UV-Vis analysis. The crystals were also characterized by microhardness and photoconductivity to determine the mechanical strength and the optical conductivity. Laser damage threshold and nonlinear optical activity of the grown crystal were confirmed by Q-switched Nd : YAG laser beam.

# Environment Science Papers

**EVSP - 1**

## Heavy metal Assessment in Beach Sands of East Coast of Tamilnadu

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**Abstract**

The elemental concentrations in the beach sand samples collected from East coast of Tamilnadu were studied using Energy-dispersive X-ray spectroscopy (EDXRF) technique. The selected elements Mg, Al, Si, K, Ca, Ti, Fe, Cr, Mn, Co, Ni, Cu, Zn, Pb, Cd, Zr, Sr has been determined in the beach sand samples. The elements occurred in abundance as is in the order of Si > Ca > Fe > Al > Mg > K > Ti > Mn > Zr > Sr > Zn > Pb > Ni > Cd > Cu > Co. The assessment of heavy metal enrichment and degree of contamination status is attempted using pollution indices. The mean concentration level of these metals in the beach sand was compared to those of the Earth Crust, Sandstone, Ultrabasic Rock to determine their anomalies. The results of this study would provide a useful aid for sustainable marine management in the region.

**Keywords:** Beach sand, Heavy metals, Pollution Analysis

**EVSP – 2**

# Spatial distribution of magnetic susceptibility and heavy metal assessment in Coastal sediment of South East Coast of Tamilnadu

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*[5*]Post Graduate and Research Department of Physics, Government Arts College, Tiruvannamalai - 606603*

**Abstract**

Magnetic methods have been successfully applied in environmental studies of soils and sediments for pollution analysis. In this work, the elemental composition in and magnetic susceptibility in coastal sediment collected from Poombuhar to Karaikal Tamilnadu coast were determined by EDXRF and dual frequency susceptibility meter The elements such as Mg, K, Ca, Ni, As Ba, V, Cr, Mn, Co, Zn, La, Pb, Ti, Al are reported. The heavy metals enrichment and contamination status is discussed with the pollution parameters. The Spatial distribution patterns of the heavy metals are discussed. The magnetic susceptibility measurement for low (0.465 kHz) and high (4.65 kHz) frequencies is carried out and values are reported. The spatial distribution of magnetic susceptibility in sediments is studied by contour maps.

**Keywords:** Sediments, Heavy metals, magnetic susceptibility, Statistical methods, spatial analyses

**EVSP - 3**

# Thermal Behaviour of Unfired and Fired Clay Bricks from DifferenT Environmental Area of Cavery Riverbed, Salem District

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**Abstract**

The objective of this paper is to determine the mechanical and thermal properties of fired clay soil bricks made from mixture clay soil. In this study, Bricks are extensively used building material all over the world owing to their low price, frequent availability, and ease of handling. However, as a matter of fact, they also consume a huge quantity of good quality clay. The purpose of the research presented in this paper was to determine the thermal properties of unfired and fired clay bricks. In this study, the mineralogical characteristics of raw materials were measured. The strength of clay brick was primarily influenced by a number of factors such as pre/post environmental condition. The x-ray diffraction studies were carried out on seven different samples of clay bricks (unfired and fired) collected from different locations of cavery riverbed areas of Salem District of Tamilnadu, India. The elemental characterization of the raw materials which were commonly expressed upto ppm level. using ICP-AES spectrometer. The results obtained in this study demonstrate that clay brick (fired) at TMB is the optimal mixture for both unfired and fired bricks.

**Keywords:** Cauvery riverbed, Clay bricks, Fired bricks, thermal properties, ICP-AES

**EVSP - 4**

# Mineralogical analysis of sediment samples of Ennore creek using spectroscopic technique

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*[3]Post Graduate and Research Department of Physics, Shanmuga Industries Arts and Science College, Thiruvannamalai – 606 603*

**Abstract**

In the present work, FT-IR Spectroscopic technique is used to find out the constituents of the minerals in the sediment samples of Ennore Creek of Tamilnadu. The major and minor minerals in the samples were identified from the band position or location of the peaks from the prominent i.r absorption peaks when compared with the available literature. The minerals such as quartz, orthoclase, microcline, albite, kaolinite, montmorlinite, calcite, aragonite and organic carbon are identified.\The identified minerals from the FT-IR study are further confirmed by PXRD technique. The identification of minerals is carried out by comparing the JCPD file manually with the XRD data of the samples. The combined techniques provide useful information about the mineralogical composition of the sediments and hence these methods are very much suitable for the mineral analysis of coastal sediments.

**Keywords:** Sediment, Mineral Analysis, FT-IR, XRD

**EVSP - 5**

# Estimation of acoustic constants of different clay brick specimens Through sound speed measurements

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**Abstract**

Bricks are extensively used building material all over the world owing to their low price, frequent availability, and ease of handling. However, as a matter of fact, they also consume a huge quantity of good quality clay and the evaluation of durability is important for proper selection of the brick. In the research of Nondestructive testing would reduce the time and cost of evaluation. Therefore, this study was undertaken to investigate the feasibility of using nondestructive testing methods for evaluating the properties of bricks and thereby possibly their durability. The acoustic constant method was chosen for the present study based on the acoustical properties and other related parameter were calculated using sound speed measurements is used to identify the durable and nondurable bricks. These findings may facilitate the use of classification of bricks and for the estimation of strength properties of various clay brick specimens.

**Keywords:** Acoustic constant, specific acoustic Impedance, Clay brick Specimens.

**EVSP - 6**

# Assessment of heavy metal contamination of sediments along South East Coast of Tamilnadu

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**Abstract**

The coastal sediment samples collected from the Poombuhar to Karaikal along the East Coast of Tamilnadu to assess the contamination and metal enrichment status. The sediments samples were analysis for heavy metal contaminants such as Fe, Cu, Mn, Cr, Co, Zn, As Zr, Cd, Ni and Pb using ICP-MS technique Sediments were classified as non-polluted or polluted by counting the enrichment factor (*EF*), Contamination factor (CF), geo-accumulation index (*Igeo*) and Pollution load index (PLI) based on the elemental background level of the analyzed elements in the literature. The ecotoxicological sense of heavy metal contamination is determined using Sediment Quality Guidelines (*SQGs*). The results in this paper will establish an initial view of sediment pollution in the South East coast of Tamilnadu.

**Keywords**: Sediment; Pollution, Heavy metal analysis, SQGS

**EVSP - 7**

# Determination of natural radioactivity levels of $^{226}Ra$, $^{232}Th$ & $^{40}K$ in Sediments of Chenab River, Pakistan

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**Abstract**

Unstable radioisotopes on the earth are cause of emitting radiations. In the present research work the natural radionuclides $Ra^{226}$, $Th^{232}$ & $^{40}K$ are determined in the sediments of the samples collected from River Chenab. Sodium iodide detector was used to measure the radioactivity in sediment samples. The detecting instrument is available at nuclear institute of agriculture and biology (NIAB) in Faisalabad for the measurement of natural radionuclide concentration. Standard values were compared with spectrum. The compiled results and calculation were conducted statistically.

**Keywords**: Natural Radioactivity, Sediment, Gamma ray spectrometry

**EVSP - 8**

# Magnetic properties as indicators of heavy metals pollution in the coastal sediment samples of South East Coast of Tamilnadu Using multivariate statistical analysis

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**Abstract**

The heavy metal concentration in coastal sediments from Thazhankuda to Kodiyakkarai along the East Coast of Tamilnadu, India was carried out using Energy dispersive X-ray fluorescence (EDXRF) technique. The magnetic susceptibility ($\chi$LF, $\chi$HF, $\chi$FD) measurement in the sediment was carried using dual frequency susceptibility meter. The relationship between magnetic susceptibility and heavy metal concentrations were investigated by Pearson correlation analysis, factor and cluster analysis to identify the sources of heavy metal pollution in sediments. The results indicated that a magnetic measurement is very useful methods to identify heavy metal pollution in sediments.

**Keywords**: Coastal sediment, Heavy metal, Magnetic susceptibility, Pollution analysis, Statistical Methods

# A heuristic study of soil texture from the district of Tiruvannamalai, Tamil Nadu using traditional hand feel method

**[1]Durai Ganesh, M. Tholkappian[2], K. Thillaivelavan[3] and R. Ravisankar[*1]**

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## Abstract

The texture of soil refers to the roughness or smoothness and it gives a better insight into the proportion of sand, silt, and clay in the soil. Sand is the largest particle (2 to 0.05 mm in diameter), it is gritty and cannot hold water. A sand particle that is smaller (0.05 to 0.002 mm in diameter) is classified as Silt. It is somewhat sticky and can hold water moderately. The smallest soil particle falls into the category of clay (less than 0.002 mm in diameter). It is very fine, sticky and can hold enough water in it. The study of soil texture provides environmentalists with first-hand knowledge of the transfer mechanism of the contaminants in different regions. In this study, the entire district of Tiruvannamalai in Tamil Nadu consisting of 18 blocks has been chosen. The total land cover of the district was divided into grids (Figure 1) and sample from each grid was collected as a representative of the corresponding region. The sampling location was identified using a handheld GPS device and the same was marked on the map using an open-source mapping software - QGIS.

The soil samples collected from 63 locations were carefully sieved and categorized into different types using the traditional hand feel method and the soil texture triangle (Figure 2).

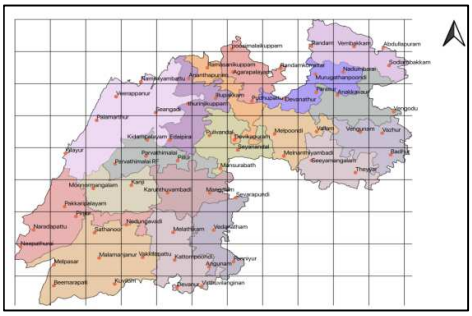

Figure 1

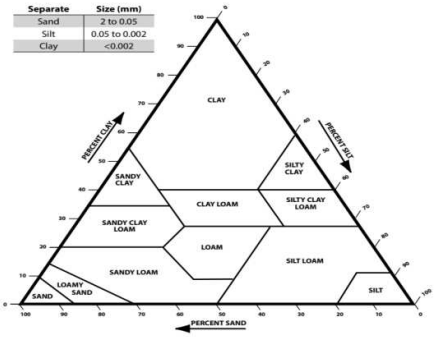


Figure 2

**Keywords:** Sand, Slit, Clay, Hand feel Method, Texture.

**EVSP - 10**

## Magnetic, Mössbauer and Micro-analyses of Archaeological Pottery Sample Excavated from Manaveli Village, Puducherry, India

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**Abstract**

The magnetic properties of archaeological pottery specimen combined with Mössbauer study can provide useful results for their characterization. The main objectives of the present investigation are to determine the technological factors applied for the pottery manufacturing (temperature, heating conditions, and duration of heating of the pottery). In order to do these findings, the pottery clay samples collected from the archaeological site Manaveli, Puducherry, India are analyzed. Different analytical methods such as Mössbauer, scanning electron microscopy coupled with energy dispersive spectrometer and vibrating sample magnetometer have been utilized to evaluate the firing temperature and firing conditions of the samples during their production.

**Keywords:** Archaeological pottery sample, Mössbauer study, Micro structural and chemical analysis, vibrating sample magnetometric study.

# Materials Papers

# Ultrasound HF Wavelength, Velocity, Compressibility, Impedance Studies of LAF Semi Organic Materials with Dissimilar Solvents at Different Concentrations (10%, 20%, 30% And 40%)

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**Abstract**

Many of Semi-organic materials have been preferred due to their NLO belongings and promptreaction to optical consequences compared to their inorganic counter parts [1-5]. Ultrasonic effects of LAF with solvents (Hot water (100$^{o}$C) - 958.3 kg/m$^{3}$) and (1,4-Dioxan - 1033 kg/m$^{3}$) are discussed here at different concentrations (10, 20, 30 and 40 mol%) and also wavelength, velocity, compressibility, acoustic impedance are measured at these different concentrations and found that wavelength increases if mol% increases, Velocity, impedance also same line with wavelength. conversely compressibility well decreases with proper increase in mol%.

**Keywords**: LAF, Ultrasonics, wavelength, velocity, compressibility, impedance...

**MATS – 2**

# Optical and structural Properties of Praseodymium containing (Sr-Ca) $2CeO_4$ through Solid State Reaction Method

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[2]*Advanced Materials Centre, Research Institute of Physical Sciences, Hyderabad*

**Abstract**

Strontium cerium oxide (Sr-Ca) $2CeO_4$ doped Pr3+ phosphor was synthesized by solid state reaction method at temperature 1443 K for 5h. The powder samples were characterized by X-ray diffraction (XRD), Raman spectra, Fourier Transform infrared spectra (FTIR), Scanning Electron microscope (ESM), Energy dispersive spectra (EDS), and photoluminescence. The X-Ray diffraction pattern reveals the crystallite size and the structure is orthorhombic. Photoluminescence excitation and emission spectra of are recorded at room temperature. The color co-ordinates were x =0 .6532 and y = 0.3297. This phosphor has to be studied for its potential commercial applications.

**Keywords:** Strontium cerium oxide, Charactersation techniques

# Synthesis and Characterization of novel Bioactive Glass - In Vitro Studies

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**Abstract**

Melt quench experimental method was used to prepare a new B2O3 based bioactive glasses with low lithium bromide and low lithium fluoride content. The aim of this work is to investigate the bioactivity nature of prepared glass samples with composition Na2O-LiBr-CdO-B2O3-P2O5 and Na2O-LiF-CdO-B2O3-P2O5.The melt derived glass ceramics were characterized by using X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS). For In vitro studies, the bone bonding ability is evaluated by examining the formation of hydroxyl apatite layer (HCA) on its surface when treated in Simulated Body Fluid (SBF) for few days. SEM and EDS analysis were used for surface morphology of the glass ceramics as well as to detect the presence of crystalline phase hydroxyl carbonate apatite (HCA) formation onto the surface of glass ceramics. SEM and EDS confirms the in vitro bioactivity of glass ceramics.

**Keywords**: Bioactivity, Bone bonding, Hydroxyl carbonate apatite, In Vitro studies, SBF

**MATS – 4**

## Integrability Aspects of Two-Coupled Hirota Equations

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**Abstract**

The integrability aspects of two-coupled Hirota equations which include the higher order effects such as third order dispersion (TOD) and self-steepening (SS), is analyzed using the Painlevé test. The soliton solutions for the system under study are obtained using Hirota bilinearization technique. Hence, the theoretical investigation on the system establishes the possibility of the simultaneous propagation of optical pulses through nonlinear fibers using wavelength division multiplexing.

**MATS – 5**

# Pomogranate Additives in Lipf$_6$ Electrolyte Material for Battery Applications

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**Abstract**

The lithium ion battery widely used in electric vehicles, laptops, smart phone. Pomegranate added in $LiPF_6$ electrolyte was prepared by sol gel method at 80 $^{o}$ C. The prepared materials were analyzed by PXRD, SEM, CV analysis. Crystal system and crystallite size of the material was recorded by PXRD studies. The morphology of the material was investigated by SEM. Electrochemical properties of the material was investigated by CV instrument.

**Keywords:** EC, DEC, DMC, Pomogranate additives, Electyrolyte; LiPF6

**MATS – 6**

## Lithium Hexafluoro Phosphate [$Lipf_6$] Electrolyte Interface for Li Ion Battery Application

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**Abstract**

Lithium ion battery used in different devices such as, electronic high energy storage devices, electric vehicles, and military communication in equipment, voting machines, and etc, Lithium hexafluorophosphate [$LipF_6$] is the most used electrolyte salt in commercial Li-ion batteries [LIB]. Electrolyte components in a standard solvent mixture of ethylene carbonate [EC], diethyl carbonate [DEC], and dimethyl carbonate [DMC]. Lithium ion battery has high performance one, excellent stability, cycle life time, better energy density, high columbic efficiency. The Aloe vera mixed $LiPF_6$ was prepared at $80^0$ C. The prepared materials were subjected to various studies such as powder XRD analysis, functional group analysis and the electrochemical impedance spectroscopy [EIS] analysis. The cycle life, cycle stability, and cycle cell performance were studied by cycle voltammetry spectroscopy [CV]. The scanning electron microscopy [SEM] analyzed the structural morphology of the sample.

# γ-ray radiation shielding parameters for $Pb(No_3)_2$ loaded Clay bricks, an efficient shilding building material

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**Abstract**

The γ-ray radiation shielding parameters, such as Linear attenuation coefficients, Mass attenuation coefficients, Mean free path, HVL and TVL were calculated, for different $Pb(No_3)_2$ loaded clay bricks were measured using trans mission method in a good geometry set up. The experimental calculations were measured at 1173 to 1333 keV radiation of $^{22}Na$ and $^{60}Co$ point isotropic γ-ray sources. The γ-rays were counted by $2^{"}\times2^{"}$NaI (Tl) detector which is connected to 8K Multi-Channel Analyzer (MCA) and gamma spectrometer. The experimental and theoretical calculations were compared. These theoretical calculations were estimated by using X-COM. There is a good agreement between experimental and theoretical calculations.These results suggest that, among all, the light weight clay brick is not suitable for radiation shielding. Comparatively light weight clay, the natural and lake clay bricks, attenuates more radiation, but the lake clay brick with $7^{th}$ concentration is a good shielding materials.

**Key words:** Shielding parameters, Gamma ray attenuation coefficient, $Pb(No_3)_2$ concentration clay bricks, point isotropic γ-ray sources, good geometry setup.

**MATS – 8**

## RG-TZO hybrid photo anode with enhanced Photo current efficiency for dye sensitized solar cells

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[2]*Centre for Nanoscience and technology, Anna University, Chennai- 600025,*

**Abstract**

$Ti_xZn_{1-x}O$ and RGO-$Ti_xZn_{1-x}O$ nanocomposite were successfully synthesized by the simple Coprecipitation technique using source materials of zinc acetate and Titanium chloride. Their photo voltaic performance was investigated in an effort to enhance the light to current conversion for dye sensitized solar cells. In studying the photo electric properties of $Ti_xZn_{1-x}O$ and RGO- $Ti_xZn_{1-x}O$ porous films sensitized by the ruthenium(II) *cis*-bis- complex. The highest short circuit current was measured among them, which was proved to be related to the fast electrons transferred in the hybrid electrodes. ZnO semiconductor has high band gap energy and conduction band of p- state orbitals are more advantageous than those of s-orbitals in attaining the desired IPCE. Due to fast electron transport and durability of electrons in ZnO semiconductors, it is speculated that the recombination of electrons are partially prohibited with triiodide in the electrolyte. Graphene, which offers an excellent electron transport property and possesses an extremely high specific surface area, is highly desirable for use as a two-dimensional catalyst support. In addition, the highest transient photocurrent was obtained for the RGO-$Ti_xZn_{1-x}O$ sample. It is because graphene is an excellent electron-acceptor with superior conductivity due to its two dimensional π-conjugation structure; in the RGO-$Ti_xZn_{1-x}O$ system, the excited electrons of $Ti_xZn_{1-x}O$ can transfer from the CB of $Ti_xZn_{1-x}O$ to RGO. Thus, in the RGO-$Ti_xZn_{1-x}O$ anode, RGO serves as an electron collector and transporter which effectively suppress the charge recombination, leaving more charge carriers to form reactive species which in turn results in the highest photocurrent response. Here, we report the high photo current production activity over the noble metal-free reduced graphene oxide RGO-$Ti_xZn_{1-x}O$ nanocomposite photo conversion/ catalytic under simulated solar irradiation. The results exhibit significantly improved photo conversion by 5.4 compared with that of the pristine $Ti_xZn_{1-x}O$, and are better than that of the optimized $TiO_2$ under the same reaction conditions.

Furthermore, the apparent quantum efficiency (QE) of 20% at 11μm film was obtained for the optimized RGO-$Ti_xZn_{1-x}O$ nanocomposite, owing to the remarkable redox property and oxygen storage capacity. The PCE of the $Ti_xZn_{1-x}O$ anode cell was conspicuously improved by loading the RGO and the maximum PCE was 5.4. The overall solar to electric energy conversion efficiency was about 20% for RGO-$Ti_xZn_{1-x}O$ (AM-1.5,100 mW/$cm^2$) compared with pristine anode.

**Keywords:** $Ti_xZn_{1-x}O$ nanocomposite, Reduced Graphene oxide, Photocurrent, impedance, electron life time, DSSCs.

**MATS – 9**

# Predicted Lifespan with the Laboratory Mock Test Sample and the Real Time Experimental Investigations Onp91 Vs SS 347 Dissimilar Metal Weld Joint For High Pressure Steam Pipeline in the Methanol Plant

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**Abstract**

The dissimilar weld joints that the combination of low alloy ferritic with austenitic steels are commonly used in many process plants. In methanol process plant, the reformer conzon outlet header is playing a vital role to determine the plant efficiency as well as high pressure steam system (HPS). The superior corrosion resistance and creep strength of more expansive austenitic alloys are advisable for the similar applications but designed with the combination of P91 low alloy ferritic steel with SS347 austenitic steel generally, due to the availability and economy.These combinations are widely used in the high temperature regions and utilised more than thousandsin a single plant. Many of the DMWs demonstrated premature failure at in services with unacceptable time frame below the expected creep life of either base metal to HAZ and well below the design life of the plant. The failures can generally be attributed to large differences in chemical composition, coefficient of thermal expansion and creep strength between these two alloys. Premature failure can result in forced plant outages that can cost the methanol production and lost revenue. It has serious impact on plant efficiency as well as production availability. In the present investigations clearly evidenced that the years of observations for the real time failure on the combination of P91 Vs SS347 DMW with correlation of predicted life span by the laboratory mock test specimen.

**Keywords:** DMW, dissimilar metal weld joint failure, P91VsSS341, Ferritc and Austenitic weld joint, Remaining Life Estimation, P91 Failure Root Cause, etc.,

# Molecular Geometry, Nlo, Mep, Homo-Lumo and Mulliken Charges of 3ecl, 3mcl, 3dmcl Compounds By Using Density Functional Theory

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**Abstract**

The quantum chemical calculations of organic compounds such as (E)-1-(2,6-bis(4- chlorophenyl)-3–ethylpiperidine-4–ylidene)-2-phenylhydrazine (3ECl), (E)-1-(2,6-bis(4-chlorophenyl) –3–methylpiperidine–4–ylidene)–2–phenylhydrazine (3MCl) and (E)-1-(2,6–bis(4-chlorophenyl)-3-dimethylpiperidine-4-ylidene)-2-phenylhydrazine (3DMCl) have been performed by Density Functional theory (DFT) using B3LYP method with 6-311G (d, p) basis set. The electronic properties such as frontier orbital and band gap energies have been calculated using DFT. Global reactivity descriptor has been computed to predict chemical stability and reactivity of the molecule. The chemical reactivity sites of compounds were predicted by mapping MEP surface over optimized geometries and comparing these with MEP map generated over crystal structures. The charge distribution of molecules predict by using Mulliken atomic charges. The Non-linear optical property was predicted and interpreted the Dipole moment (μ), Polarizability (α) and Hyperpolarizability (β) by using density functional theory.

**Keywords:** Mulliken charges, MEP, HOMO-LUMO, NLO, Molecular Geometry.

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**MATS – 11**

# A Facile Hydrothermal Induced a Novel Mno2/G-C3N4 Hetrostructure for Efficient UV Light Photocatalyst for Pollutants Degradation

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[3]*Department of Physics, Government Arts College, Dharmapuri-637401*

**Abstract**

Herein, a heterostructure based on MnO2 and g-C3N4 was constructed by simple hydrothermal technique combined with annealing process. The hybrid nanomaterial was characterized by a variety of techniques to study its structural, morphological, optical and elemental composition by suing XRD, TEM, Raman, UV, PL, BET and EDAX analysis. XRD and FESEM results that α-phase MnO2 structure and individual spherical shaped morphology with average diameter of around 25-50 nm was observed. The optical band gap and specific surface area of the MnO2/g-C3N4 composites were in the range of 2.60–2.78 eV and 65.23–100.21 m2/g, which is confirmed through UV-vis DRS and N2 nitrogen absorption –desorption analysis. The photocatalytic activity of the photocatalysts was evaluated by degradation of methyl orange and toxic phenol pollutants. The results demonstrate that the MnO2/g-C3N4 hybrid catalyst showed outstanding degradation of about 98% and high stability (only loss 3%) towards methylene blue. This can be attributed to the separation of photogenerated electron-hole pairs, suppresses the recombination of free charges. The possible photocatalytic mechanism was also discussed.

**Keywords:** MnO2, g-C3N4; Hydrothermal; UV light; Electron-hole separation; methylene blue.

**MATS – 12**

# A Study of Superionic Conduction in the Mixed System $CdJ_2 – 2Ag_20 – V_2O_5$

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**Abstract**

Polycrystalline samples of the mixed system $(CdI_2)_a$ $[(2Ag_2O)$ $(V_2O_5)]_{100-d}$ $(20 \leq d \leq 80)$ containing 20, 30, 35, 40, 45, 50, 55, 60, 70 and 80 mole% $Cdi_2$ respectively were prepared by solid state reactions. The transport number measurements were made on powder specimens of the various compounds by e.m.f. method. It was found that typical compositions having 40, 45, 50, 55, and 60 mole % $CdI_2$ would exhibit silver ionic transport number values of 0.95, 0.97, 0.97, 0.99, and 0.98 respectively

**Keywords**: $CdI_2 – 2Ag_2O$ - $V_2O_5$, Characterisation

**MATS – 13**

## Computational Studies on Different Π-Bridge Configuration in D-((Π) N-A)2 Based Organic Sensitizers for Dye Sensitized Solar Cell (DSSC) Application

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**Abstract**

Dye sensitized solar cells (DSSCs) represent a promising alternative to conventional silicon based photovoltaic technology, providing high photon-to-current conversion efficiency with possibly reduced fabrication cost. Metal free organic sensitizers have been designed for dye sensitized solar cell (DSSC) application. The dyes with D-$((\pi)_n$-$A)_2$ of 14 different structures are analyzed by density functional theory (DFT) and time dependent density functional theory (TD-DFT). The ground state geometries of the sensitizers have been optimized in both the gas phase and chloroform phase using Gaussian 09W [1] package, with Becke's three-parameter hybrid functional combined with the correlation functional of Lee, Yang and Parr (B3LYP) with 6-311G(d,p) basis set. Triphenylamine as donor and cyanoacrylicacid as acceptor in D-$((\pi)_n$-$A)_2$ dyes were studied. The effect of thiophene and cyanoacrylic π-bridge in the D-$(\pi$-$A)_2$ dyes by varying the Bi-bridge configuration were studied by the DFT and TD-DFT methods. The various parameters of designed dyes such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), light harvesting efficiency (LHE) and electronic absorption spectrum were analyzed. The obtained results show that the designed TH-14 dye molecule maybe more efficient sensitizer for DSSC applications compared to other dye molecules. The results will be discussed in detail.

# Synthesis and Characterization of N-Phenyl-P-Phenylenediamine Derivatives

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**Abstract**

Although p-phenylenediamine (PPD) and related compounds have been used in oxidation hair dye. One new N-phenyl-p-phenylenediamine derivative containing electron acceptor unit have been prepared. They present sensitizing properties and have been associated with contact dermatitis, so it is important to examine the product to prevent the occurrence of contact dermatitis in patients. In this study we developed a new crystal which can be used as safe hair dye. The prepared compound has been characterized morphologically using X-Ray diffraction. The XRD pattern also exhibits a sharp peak at around 2θ=260 suggesting the compositions comprising multi-walled simple nano tubes that have either been chemically functionalized or physically modified to increase their affinity for hair. The IR spectrum of composite gives the peaks at 1515 and 1492 cm-1, reveals the benzenoid ring stretching of the secondary and primary amines of PPDA derivative. The thermal stability and melting point of the material were identified by TG/DTA analysis. Optical properties were studied through UV-Visible and photoluminescence studies. The two phenyl rings of PPDA are straightly conjugated with each other due to a disruption of the bridge secondary amine and the λmax is about 450 nm, corresponding to the π to π* transition of neat PPDA. The variation of the conjugation length of PPDA derivative can be well monitored by UV-Vis; studies. On the other hand, a desirable magnification of the non-linear optical (NLO) properties was found for the new material as the derivative crystallize in non-centrosymmetric space groups, a necessary condition for NLO responses.

**Keywords:** N-Phenyl-p-phenylenediamine, Zinc nitrate hexahydrate, nonlinear optics

**MATS – 15**

## Characterisation of Structures Grown by Movpe Using X-Ray Diffraction

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**Abstract**

This paper describes the double and triple axis diffractometers available for characterising heteroepitaxial layer structures in the laboratory environment. The relative merits of the techniques are described. To demonstrate the materials information available from the diffractometer data (usually referred to as rocking curves) examples are given of the analysis of layer thickness and lattice parameter values for single heteroepitaxial layers, two layer structures and multiquantum well structures. For layers with a defect density of less than $10^5$ per $cm^2$ detailed analysis of rocking curve data is carried out by comparing experimental results with simulated data. X-ray diffraction also offers a non-destructive means of fully characterising the state of relaxation of strained layer systems.

**Keywords:** heteroepitaxial layer**,** Characterisation, XRD

# Bridgman growth of $Cd_xHg_{1-x}Te$

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## Abstract

Recent developments in the bulk Bridgman growth method for $Cd_xHg_{1-x}Te$ are reviewed. Both melt mixing and heat flow control techniques have been applied in attempts to produce more uniform material in terms of composition. In the U.K. work has concentrated on application of the Accelerated Crucible Rotation Technique (ACRT) to achieve the required uniformity improvements. Elsewhere, various means to control isotherm shape have been used with the same aim. The ultimate use of the material is in infra-red detectors and Bridgman grown $Cd_xHg_{1-x}Te$ has produced these successfully for both photoconductive and photovoltaic applications.

**MATS – 17**

# The Co-Existence of Multi-Component Liquid and Solid Intermediate Phases before the Hetero-LPE of III–V Solid Solutions

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**Abstract**

Liquid phase epitaxial growth of III–V solid solutions invariably involves contact between the multi-component saturated or undersaturated liquid and solid phases which are not in thermodynamic equilibrium because either the number of components is different or the composition of the layer to be grown differs from the composition of the underlying layer. The non-equilibrium system must relax to the final equilibrium state through some intermediate ones.The main point of the present review is to show that all non-equilibrium systems encounted in hetero-LPE come through the following stages of relaxation. Partial dissolution of the solid with simultaneous formation of a thin diffusive dividing layer (0.5–3 nm thick) (DDL) at the solid/liquid interface (in the subsurface region of the solid). The layer contains all the components of the given system and in some cases the quasi-equilibrium between the saturaed multi-component liquid and the solid diffusive dividing layer can be observed experimentally. If the DDL is mismatched to the substrate the former must be strained. So, the Gibbs potential of the solid increased additionally and the liquid must become supersaturated by additionally dissolving the substrate.The nucleation and the growth of centres of a new phase at some points on the solid/liquid interface with the simultaneous dissolution of the solid at other areas of the same interface (mechanism of “etch-back and regrowth”.

# Preparation and thermal conductivity of doped semiconductors

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**Abstract**

Semiconductor material to which has been added carefully controlled amounts of impurities (dopant) is the basis of modern electronics. A parameter which has to be taken into account when assessing the suitability of a semiconductor for a particular application is its thermal conductivity. This article has been written with the view to providing a convenient collective source of information on the preparation of doped semiconductors, the various techniques employed in the measurement of thermal conductivity and an update on the thernal conductivity behaviour of most of the established semiconductors.A brief coverage of the main methods employed in the preparation of semiconductors and of doping techniques is presented in Section 1, while a comprehensive coverage of the measurement of thermal conductivity is given in Section 2. In Sections 3 and 4 are reported the thermal conductivity data on elemental and alloy semiconductors and on compound semiconductors

**MATS – 19**

## Optically detected insulator-metal transition in $CuFeS_2$

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**Abstract**

Optical reflectivity spectra of $CuFeS_2$ have been studied at high pressures up to 140 kbar by using a diamond anvil cell. An abrupt change of spectral shape occurs at a critical pressure $P_C \approx 60$ kbar. This value agrees with the pressure at which electrical resistivity versus pressure curve shows an abrupt decrease, which has been interpreted in terms of a pressure induced electronic and structural instabilities. Dielectric function and optical absorption spectra obtained by Kramers-Kronig analysis from the reflectivity spectra indicate that precursory phenomena take place prior to the insulator-metal transition.

# Electrical Properties of Doped and Undoped Mn0.05Cd0.95Se

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## Abstract

Electrical conductivity and Hall Effect of $Mn_{0.05}$ $Cd_{0.95}Se$ have been measured from 40 K to 300 K. The crystals were subjected to different annealings and doping processes. The fitting of the Hall coefficient data to the model based upon a parabolic conduction band and a single ionized donor level yielded the value of the density-of-state mass of the conduction band. A variational calculation of the electron mobility was performed considering the following limiting scattering mechanisms: optical-phonon scattering, acoustic-phonon scattering, piezo-electric scattering and scattering by charge carriers. The results of the calculations are in good agreement with the experiment for Cd-annealed and doped samples. The results of different annealings indicate that the native point defects play an important role in determining electrical properties of $Mn_{0.05}Cd_{0.95}Se$.

**MATS – 21**

# Phase Diagram, Growth and Properties of Quarternary Diamond-Like Alloys in the Cuinse$_2$-Cdse System

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**Abstract**

The results of a systematic investigation on diamond-like semiconducting alloys in the quaternary system Cu-Cd-In-Se are reported. The analysis of the $(CuInSe_2)_{1-x}$-$(2CdSe)_x$ pseudo-binary phase diagram, obtained by microstructural, DTA and X-ray examinations, shows the existence of of three homostructural regions: the tetragonal chalcopyrite (α-phase), the cubic zincblende ( β -phase) and the hexagonal wurtzite ( γ -phase) structures, stable, at room temperature, in the composition ranges $0 \leq x \leq 0.05$ ( α -phase), $0.33 \leq x 0.70$ ( β -phase), $0.70 \leq x \leq 1$ ( γ -phase). Single crystals of the $\boldsymbol{x} = 0.05$, $\boldsymbol{x} = 0.50$ and $\boldsymbol{x} = 0.70$ compositions, belonging to the α, β and γ regions respectively, have been grown by using $CdI_2$ as flux material under the following conditions: molar ratio 14:1 of flux to solute and cooling rate, starting from 970 K, of 3 deg·hr$^{-1}$ The main transport properties of some compositions of the diagram are presented and discussed.

# X-Ray Crystal Structure of the Quaternary Semiconductor Compound: $Aggasnse_4$

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**Abstract**

This is the first diffractometric X-ray structural study of a quaternary semiconductor compound. Crystals of $AgGaSn()Se_4$ are tetragonal with space group I42d and cell dimensions: a = 5.853(2)Å, c=10.820(4)Å, V=370.7Å$^3$, $\boldsymbol{Z}$=2, $\boldsymbol{Dx}$ = 5.419 $\boldsymbol{g/cm^3}$. The structure was refined by full matrix anisotropic-isotropic least-squares technique using data taken at room temperature with $MoK_\alpha$ radiation, λ = 0.71069Å ($\boldsymbol{\mu}$ = 281.1 $\boldsymbol{cm^{-1}}$, $\boldsymbol{F}$(000) = 528). Final value of $\boldsymbol{R}$ = 0.0455, $\boldsymbol{Rw}$ = 0.0396 for 185 unique reflections with I #62; 3σ(I). The structure determination has shown that Se atom occupies the general position (0.2530 0.2749 0.1398) with an occupation factor of 0.5; Ag and () share the position (0 0 0) and Ga and Sn the (0 0 12).The crystalline structure of the studied quaternary compound presents disordered tetrahedral (Ag)(Ga)Se(Sn)() units with bond distances (Sn,Ga)-Se = 2.471 (2)Å; Ag-Se = 2.659 (2)Å and ()-Se = 2.314(2)Å. The fundamental difference between this structure and the chalcopyrite one is the anions position: e vs d (Wyckoff notation) respectively. The structure can also be described as I42d coming from an I4 structure comprised of distorted tetrahedral (Ag)(Ga)Se(Sn)() units disordered in such a way that a 2 (z=18) is generated.

**MATS – 23**

# Insight Mechanism of the Selective Lanosterol Synthase Inhibitor: Molecular Modeling, Docking and Density Functional Theory Approaches

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**Abstract**

Cholesterol is an important biological molecule that plays major roles in membrane structure. It is a precursor for the synthesis of the steroid hormones, the bile acids, and vitamin D.Lanosterol synthase (Oxidosqualene cyclase) is an enzyme, plays a central role in cholesterol and sterols biosynthesis. Lanosterol synthase drugs used to lower the level of cholesterol in the blood and treat wide variety of diseases like atherosclerosis, coronary heart diseases etc. It becomes one of the most promising targets for the discovery of effective anticholesteraemic drugs. Molecular modeling techniques and density functional theory (DFT) approaches is employed to reveal structural and chemical features essential for the development of small molecules as lanosterol synthase agonists. The best pharmacophore model consists of two hydrogen-bond acceptor (HBA) and three hydrophobic (HY) features. It has exhibited high correlation coefficient of 0.9549, cost difference of 73.79 bits, and low RMS value of 0.9624. The best model was validated through different validation method. The best validated model was used as 3D query in the chemical database to retrieve lead compounds against the lanosterol synthase. Molecular docking was performed in order to identify the possible protein ligand interactions. Further electronic characteristics, such as HOMO and LUMO energies, energy gap and density of state spectrum were investigated. The results obtained from molecular modeling and DFT studies were very helpful to design the novel selective inhibitors of lanosterol synthase with desired biological activity.

**Keywords:** Lanosterol Synthase; Pharmacophore modeling; Virtual screening; Molecular docking; DFT; Density of State spectrum.

**MATS – 24**

# Screening the Bioactive Constituents of Solanum Nigrum Using FTIR-ATR, UV-Vis & GC-MS Techniques and Confirming the Antihistamic Activity Using Molecular Docking Studies

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**Abstract**

The present study has been carried out to characterise the bioactive constituents present in the Ethanolic extract of Solanum nigrum leaves (Solanaceae) using FTIR – ATR and UV- Vis Spectroscopic techniques. This plant is a traditional medicinal plant used to treat various ailments in mankind. The bioactive constituents of the plant Solanum nigrum are Flavonoids, Tannins, Terpenoids, Saponins and Alkaloids. The Ethanolic extract of Solanum nigrum leaves contains Flavonoids and Tannins. FTIR – ATR spectroscopy is an established time saving method to characterise and identify the functional groups present in the extract. The occurrence of bands for Phenols and polyphenolic compounds confirmed the presence of Flavonoids and Tannins. The presence of bioactive constituents of Solanum nigrum has also been identified by observing the bands corresponding to electronic transitions observed in UV spectrum. GC-MS studies have been carried out to separate the various bioactive components based on their volatility . Separated each component has the capability of curing various ailments such as antibacterial , anti-inflammatory, antioxidant , antihistamic , anticancer activities etc . In the present study the antihistamic activity is considered and this has been confirmed using the molecular docking studies.

**MATS – 25**

## Surfactant and Metal -Assisted Hydrothermal Synthesis of Hydroxyapatite Powder

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**Abstract**

Hydroxyapatite [HAP] chemically represented as $Ca_{10}(PO_4)_6(OH)_2$ is one of the well-known bioceramic material for the regeneration of bone tissue because of its excellent biocompatibility, bioactivity and also osteoconductive properties. Its chemically and crystallographic similarity to the main inorganic component of natural bone. Especially this material is employed in dental and orthopaedic applications. In the present work, the hydroxyapatite powder was produced by doping with metal and polyoxyethylene lauryl ether (Brij-35) as a surfactant through hydrothermal method. The Ca/P ratio is very nearest to the stoichiometric value (1:67). The phase purity, particle size and morphology of the powder samples were characterised by techniques such as X-ray diffraction analysis, scanning electron microscopy and FTIR. This work report that synthesized hydroxyapatite powder using templates through hydrothermal method offered an efficient and economical route to achieve high quality nano-sized products with suitable size and high level of crystallinity after calcination. The as synthesised powder is to be tested further for its biocompatibility.

**Keywords**: Hydroxyapatite, Metal, Biomaterials, Hydrothermal method, POELE.

**MATS – 26**

# Optical and structural Properties of Praseodymium containing (Sr-Ca) 2CeO4 through Solid State Reaction Method

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**Abstract**

Strontium cerium oxide (Sr-Ca) 2CeO4 doped Pr3+ phosphor was synthesized by solid state reaction method at temperature 1443 K for 5h. The powder samples were characterized by X-ray diffraction (XRD), Raman spectra, Fourier Transform infrared spectra (FTIR), Scanning Electron microscope (ESM), Energy dispersive spectra (EDS), and photoluminescence. The X-Ray diffraction pattern reveals the crystallite size and the structure is orthorhombic. Photoluminescence excitation and emission spectra of are recorded at room temperature. The color co-ordinates were x =0 .6532 and y = 0.3297. This phosphor has to be studied for its potential commercial applications.

**Keywords**: Strontium cerium oxide, Charactersation techniques

**MATS – 27**

# A Novel composite of YSZ-BCP/Chitosan coated on surgical grade 316L SS for biomedical application

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**Abstract**

Calcium Deficient Biphasic Calcium Phosphate has gained in biomedical applications in recent years due to their biocompatible features of the living bone. In particularly biphasic calcium phosphate, consisting of hydroxyapatite (Hap, $Ca_{10}(PO_4)_6(OH)_2$) and β-tricalcium phosphate (β-TCP) β-$Ca_3(PO_4)_2$), belong to the calcium phosphate family has received more attention because of its chemical elements similarity matches to the natural human bone and dentistry. But low mechanical strength of CDBCP limited its applications in load bearing. In order to improve the mechanical strength of CDBCP, YSZ was added. In this present work, composited bio-ceramic materials (YSZ-BCP/CS) were coating on surgical grade 316L SS through electrophoretic deposition. The developed bioceramics materials coated 316L SS were studied with suitable analytical techniques. Then the coated surgical grade 316L SS were studied corrosion resistant and tested *InVitro* analysis. These results conclude that the prepared material is suitable for biomedical application.

**MATS – 28**

# A suitability study of Niobium substituted bioactive glass for its potential application in hard tissue repair

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**Abstract**

Bioactive glasses are the most promising bioceramic material widely used in orthopedic and dental applications due to their superior bioactivity, and biocompatibility. To enhance their surface reactivity of bioactive glasses biologically relevant metallic ions can be substituted into inorganic glass matrix. The substitution of trace amount of Niobium ion into bioglass matrix has shown great potential to enhance the bone forming ability through the proliferation and differentiation of osteoblasts. Niobium ion also improves the calcification which helps to form a new bone tissue and can promote alkaline phosphatese activity of osteoblasts. Within this mind new composition of bioactive glasses have been synthesized and coating was made on 316L SS. Electrochemical investigations such as potentiodynamic polarisation and electrochemical impedance studies have been carried out to evaluate the corrosion resistance of the coated substrates. In vitro biocompatibility studies also been investigated and results revealed that the developed materials are promising candidate for hard tissue repair.

**Keywords:** Development of biomimmetic implants for hard tissue replacement.

**MATS – 29**

# Chemical Characterization and Physico Chemical Properties of Cashew Nut (Anacardium Occidentale) Oil And Cashew Nut Shell Liquid

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**Abstract**

"Proximate composition and mineral concentration of Cashew nut (Anarcadium occidentale) were investigated using standard analytical methods. The physicochemical characteristics of cashew nut shell liquid were also determined. The proximate composition (%) was as follows: moisture (7.2), ash (2.8), crude fat (49.1), crude protein (36.3), crude fibre (3.2) and carbohydrate (by difference) (1.4). The mineral composition (mg/100g) of cashew nut showed potassium (27.5 ± 0.4) to be the highest, calcium (21.5 ± 0.0), magnesium (19.3 ±0.1), sodium (8.2 ± 0.2) and phosphorous (14.0 ± 0.2). Zinc and iron concentrations were lower. The physicochemical properties of cashew nut oil were as follows: colour (yellow), refractive index (1.458), specific gravity (0.962), acid value (10.7mgKOH/g), saponification value (137mgKOH/g), iodine value (41.3mgiodine/100g) and free fatty acid (5.4mgKOH/g). This is an indication that the oil is non- drying, edible and may not be used for soap making. The CNSL extracted was dark brown in colour. Ash and moisture content (%) were: 1.2 and 3.9 (for IND species), and 1.3 and 6.7 (for AFR species). Specific gravity and refractive index were 0.941 and 1.693 (for IND variety), and 0.924 and 1.686 (for AFR variety). Saponification, acid, free fatty acid (mg KOH/g) and iodine (mg iodine/100g) values were (58.1, 12.1, 6.1, 215 respectively (for IND species) and 47.6, 15.4, 7.8, 235.(for AFR species). The investigation showed that CNSL is a drying oil and it is useful in industries for paints, varnishes and surface coatings."

**Keywords;** Nutritive value, Iodine, Protein, carbohydrate, Fat.

**Abbreviations:** CNSL, Cashew nut shell liquid;

# Medicinal Papers

**MEDP – 1**

# Effect of foliar application of Biostimulants and Estimation of Colchicine content by HPLC method in Glory lily

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**Abstract**

Glory lily is an important medicinal plant belongs to the family liliaceae. It is known for its alkaloids colchicine and gloriosine. Colchicine is used in the treatment of gout and rheumatism. Gloriosine is used to induce polyploidy in plants. To find out the suitable concentration of biostimulants, two level of each biostimulants was used for the experiment. With this background, the present investigation was carried out in Kachiperumal village, Jayankondam Taluk, Ariyalur District to study the effect of foliar application of bio-stimulants and estimation of colchicine content by HPLC method in glory lily. The experiment was laid out in Randomized Block Design with eleven treatment and three replications. The treatments consists of application of two levels of Panchagavya (2% and 4%), Humic acid (0.2 and 0.4%), Sea weed extract (0.3 and 0.6%), Vermiwash (1:5 and 1:10 dilution) and Effective microorganism (1:500 and 1:1000 dilution). Colchicine was estimated by HPLC method. The colchicine content was recorded the highest in the treatment which received the application of Humic acid @ 0.2%.Ther results were discussed.

**Key words:** Glory lily, biostimulants, colchicine and HPLC method

**MEDP – 2**

# Efficacy of (2s)-2-[4-[(2-Amino-4-Oxo-1H-Pteridin-6-Yl) Methylamino] Benzoyl] Amino] Pentanedioic Acid in Pregnancy Anemic Patients by FTIR-ATR Spectroscopy

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**Abstract**

Anemia is a commonest haematological disorder that occurs in pregnancy. According to the recent standard laid down by 'WHO' anemia is present when the Hemoglobin (Hb) concentration in the peripheral blood 10.5gm/dl or less. The most common cause of anemia in pregnancy is lack of iron. Less often, it is caused by folic acid deficiency. In some population, 80% of pregnant women are anemic. Those most at risk are woman from low Socio-economic groups and teenagers. Anemia is diagnosed by estimating the haemoglobin concentration and examining a peripheral blood smear for the characteristic red blood changes. As a result, the number of red blood cells that carries oxygen to the body and tissues is thus reduced. Iron and folate supplementation is indicated during pregnancy to prevent the complication. Since iron and folic acid in amounts necessary for the fetus are preferentially transported to the fetus, the mother is likely to develop iron deficiency anemia and folic acid deficiency anemia. The present study attempts to evaluate the spectral differences between healthy blood and pregnancy anemia diseased blood and also to find the efficacy of Folic acid (FOLIC), (2S)-2-[[4-[(2-amino-4-oxo-1H-pteridin-6-yl)methylamino]benzoyl]amino]pentanedioic acid using FTIR-ATR Spectroscopic method. Ten Pregnancy anemic women were enrolled in the study. FTIR-ATR blood spectra were recorded over the region 4000-450 $cm^{-1}$ on a Perkin Elmer Model Spectrum Two FTIR-ATR spectrometer. Pregnancy anemia is diagnosed by estimating the hemoglobin concentration and examining a peripheral blood smear for the characteristic red blood changes. In order to find the efficacy of Folic acid, it was observed that the values of Protein, Lipid and cholesterol bands are significantly different between pre and post treatment. Spectra were analyzed and the internal ratio parameters were calculated and hence the efficacy of Folic acid (FOLI) is estimated. The results are further validated with statistical analysis by applying the dependent t-test, which indicated that the spectral variations are statistically significant.

**MEDP – 3**

# A Structural and Spectral Characterization with Theoretical Studies on 2 Octadecanoic acid, 17-oxo-, methyl ester from Natural Plant of Aegle Marmelos Leaves

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**Abstract**

The Octadecanoic acid, 17-oxo-, methyl ester is isolated from methanolic extract of the leaves of Aeglemarmelos by using Gas Chromatogram-Mass spectrometry analysis were studied. The title compound is used for traditional medicine like anticancer activities of the isolated compound against colon cancer. Density functional theory (DFT) have performed by using B3LYP/6-31G (d,p) level is employed for obtaining the electronic, spectroscopic, inter-molecular interaction and Nbo properties of title compound. The experimental and predicted theoretical like FT-IR (4000–400 $cm^{-1}$) spectrum have excellent correlation . The UV–Vis spectroscopic studies along with highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) analysis were used to elucidate information regarding charge transfer within the molecule.Electron acceptor and donor region are show in the MESP and additionally conformed in mulliken charge. MEP analysis show reactive sites in the compound.

**Keywords:** FT-IR, HOMO-LUMO, DFT.

**MEDP – 4**

# Spectroscopic Molecular Characterization with DFT Theoretical Studieson 1, 1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester from AegleMarmelos Leaves

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**Abstract**

In this work the traditional medicinal plant aeglemarmelas leaves was extracted by methonal. A highly sensitive and accurate multiplex gas chromatography – mass spectrometry (GC-MS) technique is reported many compounds presented and the listed out of the first compound was study in DFT. The molecular structure of 1, 1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester compound was establishing using spectroscopy technique (FT-IR, UV-Vis). A suitable level of theory was developed, based on correlating the experimental and theoretical data. Quantum mechanical theoretical calculation study on, HOMO-LUMO,NBO analysis was executed to know the transfer of electrons within the molecule ,MEP, Mulliken's charge analysis of 1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester. In addition Molecular docking methods were employed with 1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester, molecules with the same set of receptors (proteins) to find the best of four molecules for drug identification.

**Keywords:** GCMS, FT-IR, UV-Vis, NBO, MEP, Docking study.

**MEDP – 5**

# Medicinal Uses of Usnic Acid

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**Abstract**

Lichens are the symbiotic association of algae and fungi. The spectral analysis was carried out to elucidate usnic acid. The medicinal properties carried out in this compound showed a wide range of uses to mankind. It showed greater interesting properties of antibiotic, anti inflammatory, analgesic etc., The usnic acid is widely used in healing of skin wounds as antiseptic. It possesses great anti tumour quality. Thus usnic acid is a great boon in the pharmacological, biochemistry fields.

**Keywords:** usnic acid, antibiotic, analgesic, antisepic, antitumour

**MEDP – 6**

## The quantum chemical calculationsof Phytolisolated from Omni neem

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**Abstract**

The present study reveals that the Phytol isolated from the methanol extracts of leaf of the plant Omni neem. The Phytol have been simulated using DFT/ B3LYP/6-31G(d,P) method and compared structural and spectroscopic properties with aid of spectroscopic(FT-IR,UV-Vis) tools. The complete assignments were performed on the basis of the PED of the vibrational modes, calculated using VEDA 4.0 program. The general agreement between the observed and calculated frequencies was established.The UV–Vis spectrum of the compound was recorded in the region 200–400nm in ethanol and electronic properties such as oscillator strength, excitation energies, and wavelength were calculated by TD-DFT/ B3LYP method. A study on the Mulliken atomic charges, molecular electrostatic potential (MEP) and HOMO, LUMO energy levels are also constructed. The stability of molecule has been analyzed by NBO analysis.

**MEDP – 7**

# Investigation of Hirschfeld surface analysis, Spectroscopic, Pharmacokinetics and Molecular Docking Studies on Anti-cholesterol drug

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**Abstract**

High blood cholesterol can affect anyone. It's a serious condition that increases the risk for heart disease, the number one killer of Americans—women and men. Cholesterol is a fat-like substance, found in the blood stream and also in bodily organs and nerve fibres. Cholesterol was defined as total serum cholesterol expressed in millimoles per litre of blood (mmol/l) a continuous variable with mean and standard deviation. High-density lipoprotein (HDL) cholesterol or good cholesterol it protects you against heart disease, Low-density lipoprotein (LDL) cholesterol or bad cholesterol it leads to a build-up of bad fat in the artery walls, which can lead to heart disease. Triglycerides are often present in people who have diabetes or alcoholism. Statin are drugs that can lower your cholesterol. They work by blocking a substance your body needs to make cholesterol. Statin may also help your body reabsorb cholesterol that has built up in plaques on your artery walls, preventing further blockage in your blood vessels and heart attacks. In the present investigation, the Intermolecular interaction of Statin drug was analyzed by Hirschfeld surface analysis. FT-IR spectrum confirms the presence of the functional groups in the title compound. Pharmacokinetics describes how the body affects a specific xenobiotic/chemical after administration through the mechanisms of absorption and distribution, as well as the metabolic changes of the substance in body. Molecular docking is one of the most frequently used methods in structure-based drug design, due to its ability to predict the binding-conformation of small molecule ligands to the appropriate target binding site.

**Keyword:** Cholesterol, Hirschfeld surface analysis, FT-IR, Statin, Pharmacokinetics

**MEDP – 8**

## Surface morphology of wound dressing material and analyses of its water absorption and degradability properties

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**Abstract**

A wound dressing material has been synthesized from goat fibrin, meat collagen and neem leaves extract. SEM /EDAX analysis confirmed the smooth surface, porous nature and each of the elements present in the biomaterial, corroborated the curative property of the biomaterial. Sustaining a moist-free environment around the injured surface is essential and water absorption study substantiated the good water absorption capacity of the biomaterial. Ash –test results showed 5.287±0.04% of the biomaterial. Further, water-soluble ash and acid -soluble ash were found to be 1.146±0.05 and 2.524±0.022 % of the biomaterial respectively, favoring a not detrimental environment.

**MEDP – 9**

# Synthesis and Characterization of Biodegradable pH-responsive sodium alginate based hydrogels for medical and environmental applications

**S. Sudarsan[1], D.S. Franklin[2], G. Chitra[3], M. Sakthivel[4], M.S. Selvi[5] and S. Guhanathan[6*]**

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**Abstract**

Biodegradable pH-responsive hydrogels are investigated extensively in medical fields for their tunable physicochemical properties but are degradation time duration causes appropriate biological responses. To introduce soil and PBS biodegradation methodologies to these hydrogels, we have developed a stimuli responsive hydrogel based on sodium alginate, diols and acrylic acid, which can be functionalized with large macromolecular polysaccharide hydrogels simply by mixing SA/DIOLS/AA in water with the appropriate biomolecules at room temperature. These stimuli responsive hydrogel macromers can spontaneously cross-link polymers such as SA/DIOLS/AA to produce rapidly cross-linking, highly swollen, cytocompatible, and hydrolytically degradable hydrogels suitable for all kind of medical and environmental applications. These stimuli properties, combined with SA/DIOLS/AA of functionalization, establish strong potential for its usage in recent applications.

**Key words:** Biodegradable, sodium alginate, diols, acrylic acid, pH-responsive, tunable properties

**MEDP –10**

## A biological approach for synthesis of copper oxide nano particles by fenugreek (Trigohella sp.L) leaf extract and its antibacterial activity

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**Abstract**

The present investigation, the development of copper oxide nano particles (CuO Nps) from leaf extract of fenugreek where copper oxide acts as the precursor. The X -ray diffractio (XRD) analysis shows that the crystalline structure, functional groups of the samples were identified by using Fourier Transmission Infrared (FT-IR) Spectroscopy. Their shape, structure and composition were assessed by Scanning Electron Microscopy (SEM) and energy dispersive spectroscopy ( EDX). The results indicated that synthesized CuO Nps were spherical shape with particles size 20 to 30 nm. The presence of flavonoids and their interaction with the CuO Nps were confirmed using FT-IR. Antibacterial activities of the CuO Nps were studied against pathogenic gram positive Staphylococcus (S. aureus) and gram negative Escherichia coli (E. coli).

**MEDP –11**

# FT- Raman spectral studies on medicinal plants from *ocimum* species

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## Abstract

Fourier Transform Raman (FT-Raman) spectroscopy is a time saving, nondestructive and highly informative technique based on molecular vibrations. Raman spectroscopy is currently becoming one of the most powerful method especially for detection of natural product distribution in plant tissues. This paper highlights identification of chemical composition of leaves, stems and seeds of two groups of *ocimum* species plants : *ocimum sanctum* and *ocimum kilimandcharicum.* A number of organic compounds and their functional groups are identified by the spectral pattern. O-H, C=C,C=O,C-H,C-C,C≡C, C-N and C-H are the major functional groups identified in the plants.

**Keywords:** FT – Raman, Ocimum sanctum, Octimum Kilimandcharicum, functional groups, Octumum species.

# Nano Technology Papers

**NANP – 1**

# Environmentally-Friendly Green Approach for the Production of Zinc Oxide Nanoparticles and Their Anti-bacterial Properties

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**Abstract**

Zinc oxide (ZnO) Nanoparticles has been extensively studied because of its importance for fundamental investigations and practical applications, such as gas sensors, magnetic storage media, solar energy transformation, lithium ion electrode materials, semiconductors and catalysis. The synthesis of Zinc oxide (ZnO) nanoparticles using $ZnSO_4$ $7H_2O$ by Green method using *Cat's Claw Flower* Extract. The obtained Zinc oxide (ZnO) nanoparticles were characterized by X-Ray diffraction (XRD), AFM, SEM, FT-IR spectroscopy and UV-Visible spectroscopy. The Zinc oxide (ZnO) Nanoparticles were subjected to Antimicrobial activity also. It showed the enhanced bacterial action of Nickel oxide nanoparticle (NiO) with higher mortality value against the E.coli.

**Keywords:** Copper (II) Precursors; XRD; FTIR; UV and Microbial activity.

# Facile Approach to Synthesize MgO Nanoparticles by Using Clitoria Ternatea - Characterization and In Vitro Antioxidant Studies

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**Abstract**

Facile approach to synthesize the metal oxide nanoparticles is getting an increased attention in various biomedical applications such as, to treat antibiotic resistant diseases. Magnesium oxide nanoparticles (MgONPs) were synthesized by using leaf as the stabilizer in a green synthesis approach. The preliminary screening of MgONPs in the presence of C. ternatea extract was observed by UV–visible spectrophotometer. X-ray diffraction (XRD) pattern have proved the crystalline nature of the MgONPs; Photoluminescence (PL) measurement studies are used to identify the quality and defects in the crystal structure. FE-SEM with EDS has showed the size of 50–400 nm with specific binding energies. FT-IR has revealed the functional groups present in the plant extract and the peak at 521 cm-1 indicated the characteristic absorption bands of MgONPs.

**Keywords:** Copper (II) Precursors; XRD; FTIR; UV and Microbial activity.

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# Eco Friendly Green Synthesized Cobalt Nanoparticle Chitosan with Ocimum Basilicum Leaves Aqueous Extract

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**Abstract**

Metallic nanoparticles stabilized using a biodegradable polymer such as chitosan can be used for the development of drug delivery systems because chitosan acts as an effective adjuvant owing to its efficient interaction with and permeation across the cellular membranes. Chitosan is widely used because of its low toxicity and high biocompatibility. The presence of a stabilizer such as chitosan in the synthesis of metallic nanoparticles can facilitate modification of the surface physical absorption, specific recognition, and electrostatic interaction and thus improve stability, which is important for determining the potential use of metallic nanoparticles as therapeutic agents. Chitosan is used as a stabilizer and as a reducing agent in the synthesis of Cobalt nanoparticles (CoNPs). The concentration of chitosan affects the size and stability of the prepared nanoparticles. **S**weet Basil (Ocimum basilicum) is unusual among the many culinary herbs in the mint family Lamiaceae in that it is thought to have its origins in India. This plant has been cultivated in India and the Middle East since ancient.

**Keywords:** Chitosan, NiO, UV –Visible, XRD, FT-IR and Antimicrobial activity.

# Viscosity and thermal conductivity of copper oxide nanofluid dispersed in poly vinylpyrrolidone

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## Abstract

Nanofluid is a novel heat transfer fluid prepared by dispersing nanometer-sized solid particles in traditional heat transfer fluid to increase thermal conductivity and heat transfer performance. Until now, there have been few researches on the characteristics of dispersion and rheological properties of nanofluids. Since nanofluids are expected to be used under flow conditions and the flow of suspension is sometimes drastically different from that of most common heat transfer fluids that have Newtonian characteristics, it is essential to have the rheological properties of nanofluid to use practically. Also, to understand the mechanism of heat transfer enhancement it is crucial to have the ideas on the fluid-particle and particle-particle interactions within the fluid. Since the rheological properties can provide us with the knowledge on the microstructure under both static and dynamic conditions, the study on the rheological properties of nanofluid may reveal the route to understand the mechanism of heat transfer enhancement, and hence the design of nano-particles for the maximum heat transfer enhancement.

In this research we have considered the rheological properties of nanofluids made of CuO particles of 30 nm in length and poly vinylpyrrolidone (PVP) in conjunction with the thermal conductivity enhancement. The surface properties of CuO-PVP nanofluids were investigated by ATR-FTIR, transmission electron microscopy, effects of the concentration ratio of CuO nanoparticles on the stability, viscosity and thermal conductivity of nanofluids were investigated experimentally. The measured thermal conductivity shows the effect of CuO nano particles on the increase in thermal conductivity of the nanofluids. The loading limit of nano particles were also determined using stability experiments.

**Keywords:** Polymers, Nanoparticles, Polymeric nanofluids, Rheology, thermal conductivity

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# Eco-Friently Synthesis And Characterization Of Zinc Nanoparticle Using Ocimum Basilicum-Lamiaceae ( Thiru Neetru Pathilai, Sweet Basil) Leaf Extract

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**Abstract**

The Eco-friendly synthesis of Zinc nanoparticles have been synthesized by leaf extract of *OcimumBasilicum-Lamiaceae (ThiruNeetruPathilai, Sweet Basil)*. This method is completely a green method, free from toxic and harmful solvent. The surface morphology is observed by Atomic Force Microscope (AFM). The formation of copper nanoparticles confirmed by UV-Visible spectrophotometer (UV-Vis), X-ray diffraction (XRD) and fourier transform infrared spectroscope (FTIR). Scanning electron microscope (SEM) with energy dispersive X-rayspectrometry (EDS) attached usually with HR-SEM gives the elementalcomposition of the catalyst (EDS).analysis, Transmission electron microscope (TEM), Copper nanoparticles fabricated by reducing agent lithium borohydrate. Structure analysis revealed the Body cantered cubic (BCC) crystal structure of Zinc nanoparticles. The FTIR measurement was carried out to identify possible biomolecule responsible for efficient stabilisation of Zinc nanoparticles.

**Keywords:** Nano technology, Characterisation techniques

# Green Synthesis Of Copper Nanoparticles Mediated By Ocimum Basilicum-Lamiaceae ( Thiru Neetru Pathilai, Sweet Basil)Leaf Extractand Chracterisation

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**Abstract**

The Green synthesis of Copper nanoparticles have been synthesized by *Ocimum Basilicum - Lamiaceae (ThiruNeetruPathilai,Sweet Basil)*. This method is completely a green method, free from toxic and harmful solvent. The surface morphology is observed by Atomic Force Microscope (AFM). The formation of copper nanoparticles confirmed by UV-Visible spectrophotometer (UV-Vis), X - ray diffraction (XRD) and Fourier transform infrared spectroscope (FTIR). Scanning electron microscope (SEM) withenergy dispersive X – rayspectrometry (EDS) analysis and Transmission electron microscope (TEM).Copper nanoparticles fabricated by reducing agent, sodium borohydrate. Structure analysis revealed that face centred cubic (fcc) crystal structure of copper nanoparticles. The FTIR measurement was carried out to identify possible biomolecule responsible for efficient stabilisation of copper nanoparticle.

**Keywords:** Nanoparticale, Green synthesis, Analytical techniques

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## Structural and Optical Properties of Zno and Ni Doped Zno Nanoparticles

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**Abstract**

Zinc Oxide (ZnO) is a good candidate for transparent conducting electrodes in solar cell applications because of its transparency in UV and Visible region. Here we report the synthesis and characterisation of ZnO and Nickel doped ZnO nanoparticle by hydrothermal method. Zinc acetate ($CH_3COO$) Zn.2H2O, Nickel nitrate Ni $(NO_3)_2.6H_2O$ and sodium hydroxide (NaOH) are used as starting materials. The obtained products are subjected to X-ray diffraction (XRD) to confirm its crystalline nature and to identify their crystal system. It is found that The average crystallite sizes of them are calculated using Scherer formula. The strain ($\varepsilon$) and dislocation density ($\delta$) of the materials are also calculated from XRD data. Different functional groups present in them are conformed by FTIR spectroscopic studies. The cut off wavelengths are determined at the edge of the absorption band using UV-VIS spectrometer and also the optical energy gaps are estimated by using Tauc relation. The morphological studies of ZnO and Ni-ZnO nanoparticles are analysed by SEM image in different micrometer range.

**Keywords:** Hydrothermal synthesis, autoclave, ZnO, Ni-ZnO, band gap.

# Influence of surfactants on the properties of CuO nanoparticles

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**Abstract**

Surfactants are used to ensure the size reduction of nanoparticles during synthesis. Herein, the influence of surfactants such as EDTA and ethylene glycol on the properties CuO nanoparticles has been studied. Copper oxide nanoparticles prepared in the presence of EDTA and ethylene glycol have been subjected to various characterizations such as XRD, SEM, UV-Vis and FTIR. From SEM analysis, the morphology of the nanoparticles has been obtained. The structure and crystallite size of the material were obtained using XRD analysis. FTIR studies reveal the presence of CuO bond vibrations. The band gap and optical properties of the material were investigated through UV-Visible spectroscopy.

**Keywords:** - Copper oxides, surfactants, SEM, XRD, FTIR, and UV-Visible

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## Nickel Vanadium Oxide Nanomaterials for Gas Sensors

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**Abstract**

The versatile redox property of vanadium oxide explores it in various applications like catalysis, electrochromism, electrochemistry, energystorage, sensors,microelectronic, batteries etc., In this presenwork, Nickel vanadium oxide nanocompites were prepared using ammonium meta vanadate and nickel nitrate as starting materials. The morphology and the structure of the sample were obtained from Scanning Electron Microscopic (SEM) and X-ray diffraction respectively. The SEM studies confirmed that the materials formed at the end of the reaction are in nanoscale. The XRD studies reveal the formation of nickel vanadium nanocomposites and the polycrystalline nature of the samples is evident through the appearance of multiple peaks in the XRD patterns. The optical properties and bond vibrations were analyzed from the UV-Visible and FTIR studies.

**Keywords:** - Nickel vanadium oxide, Nanocrystalline material, Nanoconmposites, XRD.

# Facile Hydrothermal Synthesis of Pure and V Doped Cerium Oxide ($Ceo_2$) Nanoparticles

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**Abstract**

Nanocrystalline pure and V doped cerium oxide (VCO) nanoparticles of about 15-20 nm in size have been synthesized by facile hydrothermal method. The prepared samples are subjected to different characterization studies like powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Transmission electron spectroscopy (TEM), UV-Vis absorption and Photoluminescence (PL) spectroscopy. The powder XRD pattern showed that the cubic fluorite structure of cerium oxide. A spherical like morphologies of the prepared pure and VCO nanoparticles are observed in the SEM and TEM studies. The PL mechanism of pure and VCO may be originated from the recombination of an electron and a photogenerated hole caused by surface defects and oxygen vacancies. Moreover, the prepared samples exhibit photocatalytic activity in the degradation of methyl orange dye, indicating that the ceria nanostructure is promising as a rare-earth metal oxide photocatalyst.

**Keywords:** Rare earth metal oxide; VCO; Nanoparticles; Hydrothermal process; Optical properties

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## Comparative Study of Structural and Optical Properties of Lead Ferrites

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**Abstract**

Lead ferrite nanomaterials have been successfully synthesized by sol-gel and hydrothermal method. From the XRD analysis, the calculated lattice parameters reveals that the crystal structure of synthesized lead Nanoferrites have cubic structure. From Debye-Scherrer formula the average crystalline sizes are found to be 33nm and 20nm respectively. The dislocation densities are calculated as $2.45549x1015m^{-2}$ & $2.33029x10^{15}m^{-2}$ and their strain values are calculated as 0.24409 and 0.14811 for lead Nanoferrites synthesized by sol gel and hydrothermal method respectively.

The different functional groups and molecular vibrations are conformed by using FTIR spectrograph, which shows the presence of the substituted metal ions. From UV-VIS spectroscopic studies, the cut-off wavelengths are found to be 211.2nm and 211.8nm respectively. The optical band gaps are calculated from the Tauc plot and the direct band gap energy is found to be 3.4eV and 4.6eV and the indirect band gap is found to be 4eV and 5eV.

The morphological studies are analyzed by SEM analysis with different micrometrical ranges at 1µm, 5µm and 10µm respectively. The SEM images of lead ferrite nanomaterials synthesized by Sol-gel method shows nanoflakes in the magnification range of 1µm, 5µm and 500nm and hydrothermal method shows nanoparticles in the magnification range of 5 µm, 10 µm and 20 µm respesctively. From VSM results, magnetic properties of synthesized nanomaterials are analyzed. It is clear that the Nanoferrites synthesized by hydrothermal route have zero Coercivity and finds applications in transformer and motor cores to minimize the energy dissipation and also in some electronic devices.From this work we found that the results obtained from all the characterization techniques the lead nanoferrite particles synthesized through hydrothermal have very good results leading to highly challenging nanomaterials of very low dimension. Further more from the VSM analysis the same material synthesized through hydrothermal method achieves super paramagnetic behaviour which is less pronounced in the material synthesized by sol-gel method.

**Keywords:** Sol-Gel, Hydrothermal synthesis

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# Eco- Friendly Synthesis of Copper Oxide nanoparticles using Calotropis Gigantea and its Anti- Microbial Assay

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**Abstract**

Nanotechnology is one of the thriving developments of Materials Science. The evolvement of environ permissive process for nanoparticle synthesis is the Paramount of Nanotechnology. The Unsafe methods for nanoparticle synthesis has triggered present day researchers to focus on Eco- Friendly ways which employ low toxicity and cost efficient particle fabrication. CuO nanoparticles are synthesised by reducing the copper ions in copper sulphate salt using shade dried flower extract of Calotropis Gigantea.

The light absorption characteristics were studied by observing electronic spectrum with electronic transitions. The functional groups, the reducing, stabilizing and capping agents were investigated from phytochemical studies and correlated with vibrational band analysis by using FTIR-ATR and FT-RAMAN spectroscopy. The fluorescence property of the nanoparticles was studied by Photoluminescence Spectroscopy. The Crystalline nature was examined by PXRD analysis. The hydrodynamic size of the nanoparticles was measured using DLS analysis. The surface morphology was investigated from SEM-EDAX and AFM structures. The incorporated nanoparticles were found to be good Anti-Microbial agents that make them suitable for many Medical Applications since they are less toxic and more effective.

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## Structural, Electrical and Magnetic Properties of Mgco Sr Nanoferrite

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**Abstract**

The present work focused on the synthesis of $Co^{2+}$ substituted $Mg_{0.8}Sr_{0.2}$ $Fe_2O_4$nanoferrite and studied their structural, electrical and magnetic properties. The structural properties were studied by X-ray diffraction (XRD) analysis, which confirms that all the samples exhibit single phase spinel structure and are in nanometer range. FT-IR results also support the formation of spinel structure ferrite. The microstructure natures of present ferrite compositions were identified as spherical shaped particles. The composition depended magnetic properties of synthesized ferrite compositions were carried out by vibrating sample magnetometer (VSM) and shows that all the nanoparticles exhibits ferrimagnetic nature at room temperature.The different electrical response of ferrite materials with different frequency range were observed in dielectric and impedance analysis.

**Key Words:** Nanoferrite, magnetic ferrite, co-precipitation, $(Mg_{0.8}Sr_{0.2-x}Co_x)Fe_2O_4$

# Synthesis, Structural Properties of Ag Doped Cobalt Oxide Nano Particles and its Antibacterial Activity

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## Abstract

This research article describes the effect of doping silver (Ag) on structural, optical and antibacterial activites of cobalt oxide nanoparticles.These nanoparticles were synthesized by microwave irradiation techniques. The various weight percentage of silver (5, 10, 15, and 20%) was doped in order to study its doping effect. The synthesized Ag doped $Co_3O_4$ nanoparticles characterized by Powder X-Ray Diffraction(XRD), Fourier transform infrared spectroscopy(FTIR), Scanning electron microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDX), Transmission electron microscopy (TEM). The XRD results show the Ag doped $Co_3O_4$ crystalline nature with cubic structure. TEM image shows the Ag doped $Co_3O_4$ nanoparticles are agglomerated particle with spherical morphology. The UV-Vis-NIR spectra shows Ag concentration increases the corresponding band gap shifted from $E_g$ =5.25 eV to 4.44 eV. Fluorescence spectra show the excitation peak at 569 nm depicted a strong red shift. The synthesized Ag doped $Co_3O_4$ nanoparticles possessed potent antibacterial activity against Gram-positive (Bacillus subtilis, Staphylococcus aureus) and Gram-negative (Escherichia coli, Pseudomonas aeruginosa) bacteria.

**Keyword:** Nanoparticles; Structural properties; TEM; Spherical shape; Antibacterial activity

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## Synthesis of Vanadium Ferrite Nanoparticles through Microwave Irradiation Assisted Method

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**Abstract**

Vanadium ferrite nanoparticles were synthesized successfully by microwave irradiation assisted method. The crystalline nature of the nanoparticles is evident from the presence of peaks in the X-Ray diffraction pattern. The synthesized material assumes the monoclinic system, matched with JCPDS file with the card no. 00-019-0641. The average crystallite size is found to be 9nm calculated using Debye-Scherer formula. The strain value is calculated as 0.99378 from Williamson – Hall plot. The dislocation density is found to be $1.16520X10^{14}$ $m^{-2}$. The different functional groups and molecular vibrations are conformed by Fourier transform Infra-red Spectroscopy. The cut off wavelength of sample is determined as 211.31nm by UV-VISIBLE spectroscopic studies. From Tauc plot it is found to be 4.28 eV for direct and 4.85 eV for indirect transition. From the graphs, the most linear response is observed for direct transition. This indicates that synthesized materials can be used for manufacturing Opto-electronic devices. The morphological survey of vanadium ferrite is done by using SEM at 500nm, 1μm and 2μm respectively. From the micrographs we can confirm the presence of nanoparticles and they are uniformly arranged. From VSM analysis, we calculated the saturation magnetization as 8.7480E-3 emu, coercivity as 358.48 g, and retentivity is 301.41 E-6 emu.

**Key words:** nano ferrites, Tauc plot, Microwave Irradiation Assisted Method

# Natural Product as an Organic Capping Agent: Synthesis and Characterization of CdS Quantum Dots (QDs)

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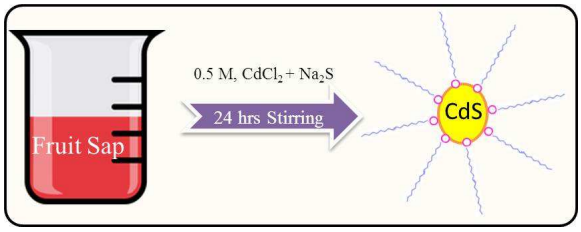
## Abstract

Synthesis of low-dimensional semiconductor quantum dots (QDs) has received great attention for potential use in sensor, catalytic, biomedical and device applications. They have unique properties such as optical sensing, photo-degradation and bio-sensing compared to their high dimensional (>10nm) nanoparticles (NPs). Synthesis of cadmium sulphide (CdS) QDs from green sources is most desirable and challenging one. An organic molecules act as a capping and stabilizing agent in a main role of size and shape controller in nano synthetic methodology. In literature, it is reported that*O. ficus-indica*fruit sap contains (94.4%) Water, (29%)Glucose, (24%) Fructose, (199 m/100g) of Potassium, huge number of phenolic, flavonoid, alkaloid compoundswhich can act as an organic capping and stabilizing agents. Here we report the synthesis of CdS Quantum Dot (QDs) in one step process from natural product source*O. ficus-indica*fruit sap,which act as a capping and stability agent. Synthesized CdS QDswere characterized using UV-visible spectrophotometer, Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray diffraction, High-resolution Transmission Microscopy with selected area electron diffraction pattern, Energy Dispersive X-Ray Analysis. From UV-Visible DRS report, we found the very low band gap energy. FT-IR indicated organic functional groups and CdS metal atoms. Raman scattering offers high specificity in molecular identification. XRD studies (JCPDS Card No. 10-0454) showed the formation of (111), (220) and (311) planes of cubic nature. HR-TEM followed by SAED analysis indicated the formation of spherical, crystalline, CdS of diameter ranging from 3-5 nm. EDAX analysis confirmed the presence of Cd and S in nanospher.

Keywords: CdS, quantum dots, Organic capping agent, one-pot



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# Fabrication and Characterization of Vinyl Ester / Nickel Oxide/Typha Angustifolia Nanocomposites

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**Abstract**

Unlike traditional composites like metal matrix and ceramic matrix composites, polymer matrix composites are lighter and also with comparable strength. The light weightiness is one of the important characteristics of composite materials for technological applications. In perspective of making lighter composites however with great strength, additionally endeavours were made to change the reinforcements in the vinyl ester network. Typha Angustifolia fibre, in addition to nano nickel oxide, was utilized as reinforcement in vinyl ester framework to prepare composites. They were characterized by Fourier Transform Infrared Spectroscopy, Scanning Electron Microscopy, and TGA-DTA. Measurement of mechanical properties like Tensile strength, impact strength, flexural Strength, hardness and physical properties like water absorption, density, specific gravity, etc. have been carried out. The effect of fibre characteristics, nano particle size, particle distribution on mechanical properties, thermal properties and physical properties has also been studied.

**Keywords:** Nano composites, vinyl ester, nickel oxide, mechanical properties, Typha Angustifolia

# Influence of Cu Doping On the Structural, Optical and Photocatalytic Properties of $Sns_2$ Nanoflakes

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**Abstract**

Cu-doped $SnS_2$ nanoflakes were successfully synthesized by solid state reaction at low temperature and characterized by Powder X-ray diffraction (XRD), FT-IR, FT-Raman, scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS), transmission electron microscopy (TEM), photoluminescence (PL) and UV-Vis spectra. X-ray diffraction pattern revealed the presence of hexagonal $SnS_2$ phase with preferential orientation along (011) direction. SEM and TEM observations revealed the formation of nanoflakes. The photocatalytic activity of Cu doped $SnS_2$ was tested with red reactive 120 (RR 120) dye and the results indicated that Cu doping enhanced the photocatalytic activity of $SnS_2$ (~75% within 90 min).

**Keywords:** Cu doped $SnS_2$; Solid state reaction; Energy bandgap; Photocatalytic degradation.

**NANP – 19**

# Rapid Green Synthesis and Characterization of Silver Nanoparticles Using Eclipta Prostrata Root Extract

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**Abstract**

Silver nanoparticles were successfully synthesized from silver nitrate through a rapid green synthesis method using Eclipta prostrata root extract as a reducing cum stabilizing agent. The experimental procedure was readily conducted at room temperature and pressure, and could be easily scaled up. The silver nanoparticles thus obtained were characterized using UV-Visible Spectroscopy (UV-VIS) which yielded an absorption peak at 417 nm. The biomolecules responsible for capping of the bio-reduced silver nanoparticles synthesized using plant extract were successfully identified through FTIR analysis. It was evinced through Scanning Electron Microscope (SEM), and X-ray diffraction (XRD) analysis thatthe silver nanoparticles were crystalline in nature and spherical in shape.The average size of the particles obtained using Scherrer's formula was 32 nm. The adopted technique for silver nanoparticle synthesis is suitable for large-scale production.

**Keywords:** Silver Nanoparticles, Green Synthesis, Characterization, Eclipta prostrata

# Chemical Compositional Analysis of Bismuth Oxide Nanoparticles using Spectroscopic Techniques

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**Abstract**

The bismuth oxide nanoparticles were synthesized using precipitation method by varying the precursor concentration of Bismuth. The synthesized samples were analyzed to find its composition and functional groups using spectroscopic techniques such as Fourier transform infrared spectroscopy (FTIR), and High Resolution Transmission electron microscopy (HR-TEM) and X-ray diffraction (XRD). The FT-IR spectrum confirmed the functional groups and the presence of Bi-O bonds. The formation of $Bi_2O_3$ nano crystals in the sample is confirmed by X-ray diffraction analysis and the diffraction pattern confirmed that $Bi_2O_3$ nanoparticles belong to α-phase with monoclinic structure. HR-TEM revealed the presence of spherical, cylindrical and some irregular shaped particle size of 50nm. Results are discussed and conclusion is drawn.

**Keywords:** $Bi_2O_3$, FTIR, XRD, HR-TEM

**NANP – 21**

## Preparation and properties of nano-ceramic conducting glasses

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**Abstract**

The nano-ceramic conducting glasses have possessed technological importance because of their simple composition and strong glass forming characteristics. Several effective approaches have been made to enhance the ionic conductivity and chemical durability of the alkali ion conducting binary phosphate glasses, which include the addition of another glass former, modifier oxide and alkali halides. The nano-ceramic glasses are synthesized by conventional quenching technique with nano ceramic as dopant materials. The nanodopants may improve the physical properties of conducting glass. All the molten samples were cast into a stainless steel plate in air and annealed at 573K to remove thermal stresses for 6 h and then very slowly cooled to room temperature. XRD patterns of the both alloy containing nano-composites and the base glass have anamorphous nature. The variation in electrical conductivity with temperature may be explained by change in the nano-particles (NPs) ions. The shifting of plasmon bands were explaind based on the spectroscopic studies.

**Key words:** Synthesis, Physical Properties, Nano-ceramics, conducting glass.

**NANP – 22**

# Green Synthesis of Platinum Nanoparticles using Mukiamaderaspatanaextract and its catalytic action in reduction of rhodamine-B dye

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**Abstract**

The bio-prospective field is dynamic area of research in the recent years. The present article reports a green synthetic route for the production of highly stable, bio-inspired platinum nanoparticles using dried *Mukiamaderaspatana* leaves. The method is facile, cost effective, simple and reproducible. The reduction of platinum ions and the formation of platinum nanoparticles has been monitored using UV-visible spectroscopy. The Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Spectroscopy(HRTEM), SAED and X-ray diffraction results reveal that the platinum nanoparticles are crystalline in nature.Fourier transmission infrared spectroscopy showed that nanoparticles were capped with plant secondary metabolites. X-ray diffraction showed that the particles were crystalline in nature with face centered cubic structure that the size range of the synthesized platinum nanoparticles was 14.30nm. Scanning Electron Microscopy confirmed by the presence of irregular spherical shaped platinum nanoparticles, Transmission Electron Microscope image illustrated platinum nanoparticles with oval irregular shaped and an average size of ~10-20nm. Also the size dependent catalytic activity of platinum nanoparticles in the reduction of cationic dye, rhodamine-B by $NaBH_4$ is studied by UV-visible spectroscopy. The efficiency of synthesized platinum nanoparticles as an excellent catalyst is proved by the reduction of rhodamine-B which is confirmed by the decrease in the absorbance with time and is attributed to electron relay effect.

**Keywords:** Platinum nanoparticles, Mukiamaderaspatana, Rhodamine-B, catalysis

**NANP – 23**

# Green Synthesis of Cuo Nanoparticles Using Ipomoea Pes- Caprae (Kudhirai Kulambu) Extract and their Optical Properties

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## Abstract

The investigation aim the synthesis of copper oxide nanoparticles (CuO) using I*pomoea Pes-caprae* plant extract at room temperature. Thesis method is completely a green method free from toxic and harmful solvent. The CuO NPS were synthesized by mixing copper nitrate and *ipomoea pes -caprae* leaf extract. The biosynthesized copper oxide nanoparticles were characterized by UV -Vis spectroscopy, Fourier -transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM).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 image brought out that the particles were spherical in shape, and the size was found to be ranging under 70nm. Further, the synthesized CuO NPs were tested for antibacterial activity by standard disc diffusion method. The optical properties and the results were discussed.

**Keywords:** Ipomoea pes-caprae leaves, CuO, Green synthesis, FTIR and optical properties.

# Facile synthesis of Mesoporous $TiO_2$ Nanospheres by Microwave-Assisted Hydrothermal method and its applications in Dye Sensitized Solar Cells (DSSC)

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## Abstract

The pioneering O'regan and Graetzel are invented a dye sensitized solar cells (DSSC) and it has tremendous breakthrough to convert the sunlight into electricity. Due to its low-cost, facile fabrication, relatively high efficiency and stability, it is gaining its unique attention to the photovoltaic cells. DSSC has four segments such as photoanode, dye, electrolyte and counter electrode. Among them $TiO_2$ nanocrystalline material (photoanode) plays a prominent role to improve the performs of DSSCs owing to its crystalline nature, different structure, high specific surface area for better dye loading, excellent light scattering for efficient light harvesting, phase structure, suitable pore size for enough electrolyte diffusion. Mesoporous $TiO_2$ nanospheres are one of the most potential nanomaterials for the above requirements. In the present work, mesoporous $TiO_2$ nanospheres were successfully synthesized by microwave-assisted hydrothermal method. The synthesized materials were characterized by powder X-ray diffraction (PXRD), $N_2$ adsorption and desorption isotherm, field emission scanning electron microscopy (FESEM) and high-resolution transmission electron microscopy (HRTEM). The powder X-ray diffraction pattern shows that the material has mixture of anatase and brookite phase. The nitrogen adsorption and desorption isotherm shows that the material has surface area of 87 $m^2$ $g^{-1}$. The average pore size distribution analysis shows that the material has pore size of 11.2 nm. The morphology studies show that the synthesized $TiO_2$ material has sphere morphology. The power conversion efficiency of $TiO_2$ nanosphere as a photoanode based DSSC has 7.2% and the commercial P25 material based DSSC has 4.1%. From the observed results it has been concluded that the mesoporous $TiO_2$ nanosphere structure are good candidate for the DSSC application.

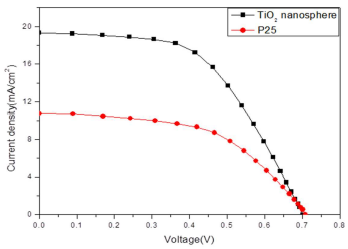


**Figure 1**. I-V curves of commercial P25 and mesoporous $TiO_2$ nanosphere based DSSC

**NANP – 25**

## Large Scale Synthesis and Characterization of Pure $La_2O_3$ and Doped Ce Nanostructures by Usng Sol Gel Chemical Methods

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**Abstract**

Pure $La_2O_3$ nanoparticles have been prepared by a sol gel method. The prepared sample has been calcined at 300°C, and 600°C to study the effect of calcinations temperature on the stability, phase and morphology of $La_2O_3$. XRD analysis reveals an interesting result of increase in phase stability. This may be accounted to the oxygen richness of the sample which has been confirmed through EDAX. An XRD result also reveals phase transformation. The morphologic analysis performed with FESEM reveals transformation from nanoparticles to nanorods. The formation of $La_2O_3$ is confirmed through the La-O vibrational peaks in FT Raman Spectroscopy and the band gap of the samples have been examined with UV-vis Spectrophotometer. The prepared samples with such high phase stability may be applied for photocatalytic application.

**Keywords** : $La_2O_3$, Photo Catalysts, Band Gap and Crystalline size.

# Synthesis of Copper nanoparticles using organic herbal (Annona Squamosa Leaves) extract

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## Abstract

The synthesis of nanoparticles (NPs) has progressively gained more attention due to its multiple applications in various fields. In recent years, a special emphasis was given worldwide to the biological synthesis approach using various organic herbal plants, to reduce metal salts into metal ions. In the current work, copper sulfate was reduced into copper nanoparticles using Annona Squamosa leaves extract. The formation of Cu NPs was confirmed by various spectroscopic and microscopic techniques. The crystallinity of the nanoparticles was observed by XRD patterns. Fourier Transform Infrared Spectroscopy analysis indicated that the synthesized nanoparticles contain carbonyl groups, phenolics, and other reducing agents which are the phytochemicals of leaves extract. The optical properties of the synthesized nanoparticles were studied using UV-visible-NIR spectroscopy and spectrofluorometry. The size distribution of synthesized nanoparticles was studied using DLS technique. The surface morphological study showed that the nanoparticles varied in size and shape which was strongly supported by the DLS study. In summary, we have highlighted that the Annona Squamosa leaf extract play a vital role in reducing the copper sulfate into copper nanoparticles. Moreover, in future, this green approach will be an effective and eco-friendly technique for the synthesis of copper nanoparticles suitable to use for multipurpose applications with reduced toxicity.

**NANP – 27**

# Synthesis and Characterization of Silver Nanoferrites through Hydrothermal Process

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## Abstract

Silver nanoferrites have been synthesized through hydrothermal method. The crystalline nature, lattice parameters hence the structures, particle size, strain and dislocation density is found from X-Ray diffractogram. From the lattice parameters we come to the conclusion that the silver nanoferrite assumes hexagonal structure. The mean crystallite size is found to be 10.472nm using Debye-Scherer formula. The dislocation density is calculated as $9.1188\times10^{15}cm^{-2}$ and the strain is found to be 0.6. The FTIR spectroscopy is used to deduce the molecular vibrations and to conform different functional groups. An absorbance spectrum is obtained by using UV-VIS spectrometer. From the UV-VISIBLE spectra the cut-off wavelength is determined to be, 374.52nm. Using this UV-VIS data the Tauc plot is drawn from which we calculated the direct energy band gap and indirect energy band gap value are 4.53eV and 5.16eV respectively. From SEM image we find that the synthesized materials have uniform nanoflakes throughout the surface. From the VSM analysis we found that our material exhibits a soft magnetic behaviour.

**Key words:** nano ferrites, VSM, hydrothermal method.

# Catalytic Reduction of 4-Nitrophenol Using Green Synthesized Ag@Cu Nanoparticles

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**Abstract**

In this report, a facile and green methodology was adopted for the preparation of bimetallic Ag@Cu nanostructures using carbon nanodots (CNDs), without the aid of any other toxic chemical or reducing reagents. First, CNDs was developed through one pot hydrothermal technique using natural product as a single carbon source. Afterwards, the prepared CNDs were exploited as reducing as well as stabilizing agents for the preparation of bimetallic Ag@Cu nanoparticles. The effects of concentration and pH were studied on the synthesis of bimetallic Ag@Cu nanoparticles. The formation of bimetallic Ag@Cu nanoparticles was analyzed by visual observation and UV-vis spectrophotometer. The morphological and structural features of synthesized CNDs and Ag@Cu nanoparticles were characterized by transmission electron microscopy (TEM) and X-ray diffraction techniques. It is revealed that mono dispersion of CNDs and Ag@Cu nanoparticles with average particle size of 3 and 10 nm were formed. X-ray diffraction studies confirmed that the prepared Ag@Cu nanoparticles were crystalline in nature. Furthermore, the as prepared nanostructures were exhibited excellent catalytic behavior toward 4-nitrophenol and methyl orange in the presence of sodium borohydride. The catalytic activity of bimetallic Ag@Cu nanoparticles was compared with bare Ag and Cu nanoparticles. The simple green strategy of developing bimetallic nanostructures using CNDs can be extended in the field of catalysis, energy and sensors. **Keywords:** Green synthesis, Nanoparticles, UV, XRD and TEM.

**NANP – 29**

# The Metal Sensing Behavior of Plant Derived Carbon Dots and Their Metal-Oxide Nanocomposite for Photocatalytic Applications

**Rajaiah Alexpandi[1], Arumugam[1] and Veera Ravi[1]***

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**Abstract**

In the present study, we prepared *Diplocyclos palmatus* leaf extract derived fluorescence carbon dots (CQD) and made an uncomplicated ON-OFF-ON sensor strip for the detection of $Cd^{2+}$ and $Fe^{3+}$ ions. Interestingly, the fluorescence (FL) emission of CQDs has quenched and enhanced while individually binds with $Cd^{2+}$ and $Fe^{3+}$, which denotes the metal sensing behavior of CQDs. Interestingly, CQDs are not showing any lethal effects like acute toxicity or cardiovascular toxicity in Zebrafish, which authenticates their biocompatibility. Therefore the positive biocompatibility,the prepared CQDs were suggested as submissive bio-imaging probe for biological studies. Subsequently, the CQDs were doped with $TiO_2$ using methanol extract of *D. palmatus* under hydrothermal condition. The obtained CQDs@$TiO_2$ nanocomposite have showed efficient photocatalytic activity under sunlight due to their narrowed band gap (2.0 eV). It exhibited photocatalytic deactivation of bacteria (*Vibrio harveyi*) as well as dyes (Malachite Green) under sunlight exposure. The CQDs@TiO2 nanocomposite effectively deactivated the Vibrio harveyi by inducing the ROS stress, and thereby, damaged the bacterial membrane and cellular components. Further, the first and foremost study was examined the toxicity level of photocatalyzed dye using Zebrafish as animal model. It was found that MG had caused severe acute-toxicity, cardiovascular toxicity and organ-toxicity thereby it induced the intracellular ROS as well as apoptosis; whereas PMG does not show any toxic effects, is reputable substantiation of the MG-dye degradation by CQDs@$TiO_2$ nanocomposite under sunlight.

**Keywords:** Diplocyclos palmatus, Carbon dots; metal-sensing; $TiO_2$ photocatalysis

**NANP – 30**

# Synthesis and Characterization of Bismuth Sulfide ($Bi_2S_3$) Nanoparticles By Microwave Assisted Chemical Route

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## Abstract

In the present work, $Bi_2S_3$ nanoparticles were successfully synthesized by microwave assisted chemical route using bismuth nitrate as bismuth source. Thiourea and Thioacetamide were used as two different sulfur sources and Ethylene Glycol was used as solvent. The synthesized samples were investigated by X-ray diffraction technique. The diffraction patterns indicate that the samples possess orthorhombic phase and the particle sizes were found to be 27 nm and 20 nm for the as prepared $Bi_2S_3$ samples (two kinds of sulfur source compounds- thiourea and thioacetamide). While the particle sizes were found to be 26 nm and 24 nm for the annealed samples (at 200 $^oC$ for one hour) of $Bi_2S_3$. The functional groups present in the synthesized samples were analyzed using FTIR spectroscopy. The strong peaks located at 755$cm^{-1}$, 583$cm^{-1}$ and 497$cm^{-1}$ were assigned to the Bi-S vibration. The optical properties of the $Bi_2S_3$ nanoparticles (annealed at 200 $^0C$) were studied using UV- Vis spectroscopy. The $Bi_2S_3$ nanoparticles show transparency above 600 nm. The optical bandgap ($E_g$) of the $Bi_2S_3$ nanoparticles were found to be 1.80 eV. The SEM images of the as-prepared $Bi_2S_3$ nanoparticles reveal that the synthesized products mainly consist of flower shape and the average particles sizes of the prepared samples were found to be 90 nm. When the prepared nanoparticles were annealed at 200 $^0C$ for 1 hour, the flower like shape changed into nanorods and the particle sizes were found to be 70 nm. The Energy Dispersive X-ray spectroscopy (EDX) studies confirmed that the nanoparticles were composed of Bi, S, and O with no other impurities indicating the complete disappearance of the surfactant during the growth and assembly process.

**Keywords:** Bismuth sulfide nanoparticles; XRD, FTIR, UV-Vis, SEM and EDX.

**NANP – 31**

# Wet Chemical Synthesis and Characterization of Zn Doped $V_2O_5$ Nanoparticles

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## Abstract

In the present work, wet chemical solution process was used to synthesize pure and Zn doped $V_2O_5$ nanorods with various concentration of Zn ranging from 5-15%. The structural analysis (XRD) revealed that the pure and Zn-doped samples annealed at 60 $^{O}$C exhibit the tetragonal phase. The samples calcined at 600 $^{O}$C were found to be in orthorhombic phase with a preferential orientation according to the direction (002) plane. SEM analysis revealed that the variation in size and shape of the grains in the $V^{5+}$ lattice by Zn-doping concentration. The SEM images of pure and doped $V_2O_5$ samples annealed at 600$^{O}$C for 1 h show that the particle size decreases with increase of $Zn^{2+}$ concentration from 5-15%. In the EDS spectra, the excepted peaks belonging to V, O and Zn elements were only observed, thereby confirming the purity of the prepared pure and Zn-doped $V_2O_5$ system. The substitution of Zn-leads to reduced Photoluminescence (PL) intensity owing to the increase of non-radiative recombination centers. Considering the simple, low cost method of synthesis, this synthetic route could also be easily extended to prepare other metal oxide nanostructure modified colloidal $V_2O_5$ nanorods for enhancing optoelectronic properties.

**Keywords**: Zn doped $V_2O_5$ nanorods; XRD, SEM, EDX, PL.

**NANP – 32**

# Pongamia pinnata leaf extract as a reducing agent in generating in-situ Silver (Ag) nanoparticles – Preparation and Characterization of Cellulose-agnp nanocomposites

**M.Kishanji[1], M.Bhavani[1], G.Mamatha[1], M.Veeraswamy[1], D.Madhuri[2], D. Suresh Kumar[3] and K.Madhukar[1]***

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*[3]Department of Physics, South Campus, Telangana University, Bhiknoor. Telangana.*

**Abstract**

The *Pongamia pinnata* leaf extract was used to generate silver nanoparticles (AgNPs) and to infuse into hand casted cellulose matric film to make Cellulose nanocomposite. These cellulose nanocomposite film were characterized by various experimental method to asses its capacity for the medical, food package applications. The results from Fourier transform infrared (FTIR) spectroscopic, energy dispersive X-ray analysis (EDX), scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques reveals that the nanocomposites films possessed good tensile properties, indicating *that* the reinforcing effect of AgNPs. The antibacterial studies showed good zone of inhibition, indicating good antibacterial activity against *Escherichia coli* bacteria.

**Keywords:** In situ generation; silver nanoparticles; cellulose nanocomposite films; antibacterial activity; packaging material.

**NANP – 33**

# Preparation and Analysis of Cellulose / Ag-Cunp Bimetallic Nanocomposite Films using Vitex Nedungo Plant Extract as Reducing Agent

**Mamatha Gouda[1], Bhavani Macha[1], Veeraswamy Maragani[1], Mohan Babu Nadru[2], Madhuri Dumpala[3] and Madhukar Katakam[1]***

[1] *Polymer Nanocomposites and Functional Materials Laboratory, Department of Physics, Osmania University, Hyderabad.*

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[3]*Department of Physics, Osmania University College for Women, Koti, Hyderabad.*

**Abstract**

We are reporting the preparation and characterization of cellulose nanocomposites with *in situ* generation of bimetallic nanoparticles (NP), such as Silver (Ag) and Copper (Cu), using *Vitex negundo* (Vavil) leaf extract as a reducing agent. The cellulose/Ag-CuNP composite films were prepared and characterized by FT-IR, XRD, SEM, TGA, and Antibacterial activity. The infrared spectra showed that involvement of OH groups in the reduction of salts in to their metal nanoparticles. The Scanning electron micrograms (SEM) reveals uniform distribution of nanoparticles in the cellulose matrix and they are in spherical in shape. The EDAX spectra confirmed the presence of metal nanoparticles. X-ray diffractograms displayed formation of Silver (Ag), Silver oxide (AgO), Copper (Cu) and Copper oxide (CuO) nanoparticles. Synergy effect of Silver and Copper nanoparticles showed improved thermal and antibacterial properties. The antibacterial activity of nanocomposites showed good Antibacterial activity for five different bacteria such as *E. coli, Pseudomonas, Bacillus, Klebshiella* and *staphylococcus*. This makes these systems are good candidature for the food, packing and medical applications.

**Keywords:** Bimetallic nanoparticles, Vitex negundo, *in situ* generation, cellulose nanocomposites, Green synthesis.

**NANP – 34**

# Tensile Properties of Thermoplastic Starch based Green Nanocomposites

**D. Suresh Kumar[1], N. Mohan Babu[2], N. Bikshamaiah[3], S. Ramesh[4] and K. Madhukar[4]**

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*[2]Department of Physics, South Campus, Telangana University, Bhiknoor.*

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*[4]Polymer Nanocomposites and Functional materials Laboratory, Department of Physics, Osmania University, Hyderabad.*

## Abstract

The outstanding properties of polymers and its composites are finding numerous applications in many fields. But synthetic polymers pose environmental problems such as degradation. So in order to find a solution for white pollution, research is going on in developing biodegradable composites, which are also known as green composites. In the present work we made an attempt to prepare thermo plastic starch based green composites. But due to limited mechanical strength of starch, these composites cannot be directly used for packing applications. Hence, in order to improve the properties of composites Graphene Oxide (GO) was used as reinforcement. In this study the green nanocomposites were prepared with increasing content of Graphene Oxide by melt mixing method and tensile properties of these composites were measured by Universal testing machine. The results showed that tensile properties are increased by incorporation of Graphene Oxide into thermoplastic starch matrix. However tensile properties are increased up to certain loading of Graphene Oxide and further increase in Graphene Oxide loading caused decrement in tensile properties. This is may be because of agglomeration of Graphene oxide at higher loadings in the composites.

**NANP – 35**

# Green Synthesis of Copper Oxide Nanoparticles from Betel Leaf Extract for Water Purifier and Antifungal Activity

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*[4]Department of Physics, Govt. Arts college for Women, Mayladudhurai*

**Abstract**

Bio - synthesis of CuO nanoparticles has been achieved using environmentally acceptable plant extract. It is observed that betel leaf extract can reduce Cu ions into CuO nanoparticles within 15 and 30 minutes of reaction time. Here the present study is carried out to establish the catalytic and antibacterial activity of synthesized CuO nanoparticles. The XRD data illustrated characteristic diffraction patterns of the elemental silver phases and the average size of the crystallites are estimated from the peak profiles by Scherrer method. FT-IR spectra of the leaf extract after the development of nanoparticles are determined to allow identification of possible functional groups responsible for the conversion of metal ions to metal nanoparticles. Catalytic activity of silver nanoparticles is analyzed using UV–Vis absorption spectra. The results were discussed.

**Keywords:** betel Leaf, XRD, antifungal activity

**NANP – 36**

# Bio Approach - Synthesis and Characterization of Metal Nanoparticles from Aromatic Medicinal Plants

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*Department of Engineering Physics, Annamalai University, Annamalainagar-608002*

**Abstract**

Bio - synthesis of metal nano particles has been achieved using environmentally acceptable medicinal plant extract. It is observed that different medicinal leaf extract can reduce metal ions into metal nanoparticles within various reaction time. Here the present study is carried out to establish the optical and antibacterial activity of synthesized metal nanoparticles. The XRD data illustrated characteristic diffraction patterns of the elemental metal phases and the average size of the crystallites are estimated from the peak profiles by Scherrer method. FT-IR spectra of the leaf extract after the development of nanoparticles are determined to allow identification of possible functional groups responsible for the conversion of metal ions to metal nanoparticles. An optical property of metal nanoparticles is analyzed using UV–Vis absorption spectra. Moreover, the antibacterial activity is screened against both gram-negative and gram positive microorganisms. Thus, this method can be used for rapid and eco-friendly green synthesis metal nanoparticles of size range 7-18 nm possessing antimicrobial activity suggesting their possible application in environmental remediation. The results were discussed.

**Keywords:** Medicina plants, XRD, metal nano particles

**NANP – 37**

# Nickel Molybdenum Selenide Composites as Efficient Trifunctional Electrocatalysts for Water Splitting Reactions

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**Abstract**

The visible light-responsive photo catalyst $BiVO_4$-$TiO_2$ was synthesized by hydrothermal method. The structural properties of the prepared Nano composite had been characterized using X-ray diffraction, scanning electron microscopy, transmission Electron microscopy, X-ray photo electron spectroscopy, photoluminescence spectroscopy. The experimental results of photocatalytic degradation also show that the novel composites exhibit remarkable visible-light photo catalytic activities for methylene blue dye degradation. The high visible photocatalytic performances are attributed to photo induced interfacial charge transfer in the heteronanostructure. This new composition is expected to show considerable potential applications in water purification.

# Synthesis of CdS-$TiO_2$ for Visible Photocatalytic Activity

**V.Thirupugazhmani, K.Thirumalai, S.Shameena, L. Ilavarasan, M.Ganapathi and A.Ravi***

*PG & Research Department of Chemistry, Government Arts College, Tiruvannamalai*

**Abstract**

The visible light-responsive photo catalyst CdS-$TiO_2$ was synthesized by hydrothermal method. The structural properties of the prepared Nano composite had been characterized using X-ray diffraction, scanning electron microscopy, transmission Electron microscopy, X-ray photo electron spectroscopy, photoluminescence spectroscopy. The experimental results of photocatalytic degradation also show that the novel composites exhibit remarkable visible-light photo catalytic activities for methylene blue dye degradation. The high visible photocatalytic performances are attributed to photo induced interfacial charge transfer in the heteronanostructure. This new composition is expected to show considerable potential applications in water purification.

**NANP – 39**

## Improvement of the properties of Ferrite by substitution of A- and B- sites in $CuFe_2O_4$

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**Abstract**

$Cu_{0.5}Ni_{0.5}$ (CeFe) $O_4$ nanocomposite was synthesized by substitution of A- and B- sites in $CuFe_2O_4$ using sol-gel nitrate-citrate route. Single phase powder XRD pattern shows spinel cubic structure with the lattice parameter value 8.3 Å. Average crystallite size calculated using scherrer's equation confirms that the particles size were in nanometer range which is supported by the structural investigation using scanning electron microscopy (SEM). SEM images show the particles colloidal aggregation and smaller size and shape. Energy-dispersive X-ray Spectroscopy (EDX) data supports that the purification of the sample which shows only the estimated metals present. The value of zeta potential 26.9mV was obtained, which rationalizes the observed excellent long-term stability of the colloidal suspension. FT-IR result exhibit the strong stretching peaks of Cu-O,Ni-O, Ce-O and Fe-O bonds. Both the A- and B-site dilution in the ferrites have predominant attention in Neel temperature which will influence the magnetic moment and the non-metallic behaviour leads to the ferrite sample in enormous changes in the structure-properties relations.

**NANP – 40**

## Synthesis of $BiVO_4$-$TiO_2$ for visible photocatalytic activity

**S. Shameena, K. Thirumalai, V. Thirupugazhmani, L. Ilavarasan and A.Ravi***

*PG & Research Department of Chemistry, Government Arts College, Tiruvannamalai*

**Abstract**

The visible light-responsive photo catalyst $BiVO_4$-$TiO_2$ was synthesized by hydrothermal method. The structural properties of the prepared Nano composite had been characterized using X-ray diffraction, scanning electron microscopy, transmission Electron microscopy, X-ray photo electron spectroscopy, photoluminescence spectroscopy. The experimental results of photocatalytic degradation also show that the novel composites exhibit remarkable visible-light photo catalytic activities for methylene blue dye degradation. The high visible photocatalytic performances are attributed to photo induced interfacial charge transfer in the heteronanostructure. This new composition is expected to show considerable potential applications in water purification.

**NANP – 41**

# Enhanced photoelectrochemical response in $SrTiO_3$ nanocomposite with various supporting material-A comparative study

**K. Thirumalai*[1], A. Ravi[1], J. Madhavan[2] and M. Swaminathan*[3]**

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**Abstract**

The development of photocatalysts that can generate hydrogen via water splitting under sunlight or destroy environmental pollutants has been one of the major areas of interest during the past few decades. The advantages of $SrTiO_3$ are that it is highly robust and can split water even in the absence of external bias potential. A composite material ($SrTiO_3$) containing Sr, Ti and O elements was prepared by a facile thermohydrolysis method. For supporting different rare earth oxides and noble metal were introduced. Various characterization methods such as X-ray powder diffraction, UV-vis diffuse reflectance spectroscopy, scanning electron microscopy and transmission electron microscopy were employed to investigate the structure and optical properties. The activities of the samples were evaluated by the photocatalytic degradation of methylene blue under visible light irradiation and the current densitywere measured by electrochemical methanol oxidation. The results showed prepared nanomaterial exhibits higher Photo-electrocatalytic activity than the bare material for methanol electrooxidation and splitting of water.

**NANP – 42**

# In-situ generation of AgNP into Cellulose matrix using Psidium guajava (Guava) leaf extract as reducing agent – a green approach

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**Abstract**

Silver nanoparticles (Ag NPs) were *in situ* generated in Cellulose matrix using *Psidium guajava* (Guava) leaf extract. These prepared Cellulose nanocomposite films were characterised by Fourier transform infrared spectroscopic (FTIR), energy dispersive X-ray analysis (EDX), scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques and their antibaterial studies were performed again five bacteria. The X-Ray analysis showed decrease in the crystallinity of composites over the matrix. The enhancement of tensile properties of cellulose was occurred due to rigidity of silver nanoparticles. The nanocomposite films demonstrated good tensile properties showing the reinforcing effect of silver nano particles in the composites. These nanocomposites shown good antibacterial activity against *E.coli, bacillus, pseudomonas* and *staphylococcus*. With the improved mechanical, thermal stabilities, along with good antibaterails activity makes these ccomposites suitable for medical and food packing applications.

**NANP – 43**

# In–situ generation of Ag/Cu bimetallic NPs in Cotton fabrics using Azadirachta indica leaves

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**Abstract**

The authors generated, *in-situ,* Silver (Ag) and Copper (Cu) nanoparticles (NPs) through green means and embedded in cotton fabric. In this work *Azadirachta indica* (Neem) leaves were used as reducing agent for synthesis of Ag/Cu NPs at room temperature. The developed nanocomposite cotton fabric was characterizations using XRD, FTIR and SEM/EDS. The X-Ray diffractograms confirmed the formation of nanoparticles representing their corresponding reflection planes. The average size of the nanoparticle is about 70nm and presence of Ag/Cu NPs was confirmed from EDS and scanning electron microscopy. The infrared spectra (FTIR) revealed that C=C groups were involved in the reduction process. This nanocomposite fabric possesses outstanding antibacterial activities for *gram-positive* and *gram-negative* bacteria make them suitable for medical/dressing, food package applications, besides other.

**Keywords:** Azadirachta indica, Cotton fabrics, in–situ generation, medical dressing / food package applications.

# Nd-Gd Co-Doped Cawo4 Nanocrystals - Synthesis and Characterization

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**Abstract**

This paper reports the synthesis of neodymium (Nd)-Gadolonium co-doped calcium tungstate (CaWO4) nanocrystals (NCs). The thus synthesized NCs were analyzed for phase identification using x-ray diffraction (XRD). The XRD pattern reveals that the formed NCs are in the average size of around 39 nm. A scanning electron microscope (SEM) image shows that the NCs are in the form of rectangular shapes. The presence of rare earth ions in the Nd-Gd :CaWO4 NCs is confirmed by energy dispersive analysis of the x-rays (EDAX). To further confirm the presence of rare earth ions, photoluminescence and photoluminescence excitation studies were carried out on these NCs. Emissions related to Nd3+ ions were only observed under 587 nm excitation, and the peaks were assigned to the characteristic 4F3/2–4I9/2, 4F3/2–4I11/2 and 4F3/2–4I13/2 transitions of the Nd ions. No Emissions related to Gd3+ were recorded and effect of the presence of Gd in the matrix is almost non-existing when compared to the data earlier reported by us.

**Keywords:** nanocrystals, calcium tungstate, rare earth ions, photoluminescence.

**NANP – 45**

# Urea and Brij 35 Inhibits the Growth of Nano Hydroxyapatite Developed on SBF using Biomimetic Assisted Ultrasound Method

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## Abstract

The present work deals with a novel chemical precipitation technique for synthesizing Hydroxyapatite (HAP $Ca_{10}(PO_4)_6(OH)_2$) by ultrasound assisted Biomimetic method. Calcium nitrate tetra hydrate $Ca(NO_3)_2 \cdot 4H_2O$ and diammonium hydrogen phosphate salts $(NH_4)_2HPO_4$ were utilised as a precursors. Tris hydroxyl methyl amino methane(TRIS) are used as a buffer, Urea and Brij 35 as an additive dissolved in 1.5 concentrated simulated body fluid SBF at 37 °C and pH of 7.4 for 15 days synthesised through sonochemical method. The hydroxyapatite formation is controlled by decomposition of the urea added to the suspension. The crystalline phase, chemical composition and crystallite size of the obtained samples were characterized by X-ray powder diffraction (XRD). The molecular structure and surface morphology were characterised using Fourier transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM) technique. The results suggest that the ultrasound irradiation, additives are the important factors which affects the formation of uniform and homogeneous distribution of bioceramic material. HAP powder is obtained with high degree of crystallinity, purity with minimal agglomeration. The as synthesised powder is to be tested further for its biocompatibility.

**Keywords:** Sonochemical, Biomimetic, Brij 35, Urea, Hydroxyapatite

# CFD analysis and Experimental studies on the performance of Heat Pipe Solar Collector (HPSC) using Al and $TiO_2$ nanofluids

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**Abstract**

The Sun has been bringing out its energy for billions of years and it is renewable, clean and inexhaustible. Depending on needs there are two possibilities in which the solar energy can be used by converting into electrical energy and thermal energy. This article addresses CFD analysis and experimental studies on the thermal performance of Heat pipe solar collector (HPSC) using $Al_2O_3$ and $TiO_2$. The improvement in thermal performance by using nanofluids in the heat pipes has been discussed. The main purpose of the CFD analysis and the experimental investigations are comparing the enhancement of the thermal performance of the two types of nano fluids such as $TiO_2$ (50 nm) & $Al_2O3$ (50nm) in the heat pipe solar collector. Readings were taken for the heat pipe solar collector with two various working fluids ($TiO_2$ & $Al_2O_3$) at the concentration of 0.2 % (by vol.) at different operating conditions. From the study, it recommends that efficiency of HPSC increases when Aluminium is used comparatively $TiO_2$ used as a working fluid.

**Keywords:** $TiO_2$ nanofluids, Al nanofluids, heat pipe, solar collector, CFD analysis

**NANP – 47**

# Antifungal Activity of Silver Nanoparticles Synthesized using Cissus Vitiginea Leaf Extract

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## Abstract

In recent years, resistance to commercially available fungicides by phytopathogenic fungi has been increasing and has become a serious problem. So, the search for new fungicides and alternatives is of paramount importance to combat newly emerging resistant strains of fungal pathogens. One solution would be nanotechnology which enhances antimicrobial activity of materials by converting them to nanoparticles. The improved antimicrobial activity of nanoparticles compared to their salts is due to their unique properties *i.e.* large surface area to volume ratio. It has been known that silver and its compounds are effective antimicrobial agents. Keeping this in view, in the present study was to evaluate the antifungal activity of silver nanoparticles synthesized from *Cissus vitiginea* leaf extract. Antifungal activity against *Candida albicans* and *Aspergillus flavus* was investigated along with standard control, chloramphenicol. The synthesized AgNPs exhibited a potent antifungal activity against tested fungal strains. Result of this study indicated that AgNPs have remarkable potential as an antifungal agent in treating infectious diseases.

**NANP – 48**

# Shock Wave Induced Switchable Magnetic Phase Transition Behaviour of $ZnFe_2O_4$ Ferrite Nanoparticles

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**Abstract**

The present work was designed to investigate the impact of shock waves on Zinc Ferrite nanoparticles ($ZnFe_2O_4$) NPs. The test material was prepared by precipitation method and shock waves recovery experiment was done by table top pressure driven shock tube. The Mach number 2.2 shock wave with different number of shock pulses 50,100 and150 was utilized.The Shock wave induced changes in structural, morphological and magnetic properties were noticed by various analytical techniques such as powder X-ray Diffractometer (PXRD), scanning electron microscopy (SEM) and vibrating sample magnetometer (VSM). The obtained PXRD results shown, there are no significant structural changes occurred but grain size changes were observed. Switchable paramagnetic to super -paramagnetic behaviour was observed during the shock wave loaded conditions. The mechanism of this magnetic phase transition effect was discussed.

**Key words**: $ZnFe_2O_4$ Ferrite NPs, Shock waves, Grain size, Magnetic phase transition

**NANP – 49**

# Size and Morphology - Controlled Synthesis of Hydroxyapatite Nanocrystal by Precipitation Method

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**Abstract**

Hydroxyapatite chemically donated as $Ca_{10}(PO_4)_6(OH)_2$ is one of the most important biominerals of interest in the broad group of calcium phosphate-based bio ceramics and the main inorganic constituent of bone and teeth. Especially its used to excellent biocompatibility, bioactivity and also osteoconductive properties. In this work, thiourea substituted HAP Nano crystalline were synthesis using precipitation method from aqueous solution of calcium nitrate, potassium dihydrogen phosphate and the presence of thiourea. The synthesised sample were physically characterized such as X-ray diffraction analysis, scanning electron microscopy and FTIR. The results showed high crystalline HAP nanoparticles and SEM photograph showed that the size of the crystal was well controlled by the reaction parameters such as reaction time, temperature and the molar ratio of Ca/P.

**Keywords:** Hydroxyapatite, precipitation method, Nanostructure,

# Polymer Papers

**POLP – 1**

# Synthesis and Characterization of Novel Liquid Crystalline Random Copolyester

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## Abstract

In the present work, a novel random copolyester (P1DID) based on Diethyleneglycol, 2, 5 - Ditertiarybutylquinol with isophthaloyl chloride as different diols and diacid chloride monomers was synthesized by solution polycondensation method. Solubility was checked in common organic solvents. Qualitative structure analysis of the polymer was carried out by UV, FTIR and $^{1}$H NMR spectroscopy. The thermal analysis of copolyester was carried out by TGA and DSC studies. The thermal behavior of the copolyester was found to be very sensitive based on its chemical structure and thermal stability. The texture, morphology and crystallinity of the polyester were monitored using SEM and XRD. The results of the investigation reveal that the synthesized polymer was found to possess liquid crystalline nature.

**Keywords:** Copolyester, polycondensation, liquid crystalline, TGA, and XRD.

**POLP – 2**

## Synthesis and Charecterisation of Aliphatic Polyester Nanocomposite - Application in Drug Delivery

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**Abstract**

The potential interest in biodegradable polymers comes from the eco-friendly degradation ***via*** microbial action which transforms the polymers into carbon dioxide and water resulting in a pollution-free natural system. To improve the polymer properties several methods adopted one of the important methods is incorporation of nanoparticle in polymer matrix to synthesis nanocomposites. One of the great advantages of nanoparticles incorporation in the polymer is the ability to tune the chemical, physical and biological properties of polymer which is useful in drug delivery applications in medicine.The incorporation of Nano hydroxyapatite into aliphatic polyester also improves their mechanical strength greatly. Present study was carried out by synthesising poly (sorbitol citrate) PSC biodegradable aliphatic polyester using catalyst free direct melt polycondensation and nano Hydroxy Apatite using Sol-gel method.Nano hydroxyapatite-polysorbitol citrate polymer nanocomposite synthesisedusing ultra sonication method. Biodegradable polyester and its nanocomposites werecharacterised by spectral studies like FT-IR, NMR. Further UV- visible spectral analysis also performed for the nanohydroxyapaptite and polyesternanocomposite.Powder XRD andSEM analysis of the nanocomposite and polyester, explain about the crystallinity and morphology of the nanocomposite and polyester. Predetermined amount of drug loaded in the polyester nano composite and the drug releasing efficiency calculated. This polyester nanohydroxy apatite composite exhibit high releasing capability.

**Keywords:** Nanohydroxyapatite, polymernanocomposite-nHA, nanodrugloader

**POLP – 3**

# Effect of Mg $(CF_3SO_3)_2$ concentration on structural and electrochemical properties of ionic liquid incorporated polymer gel electrolyte membrane

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**Abstract**

In the present study, magnesium ion conducting polymer gel electrolytes based on polyethylene oxide (PEO) containing 1-Ethyl-3-methylimidazolium tetrafluoroborate (EMIM-$BF_4$) as ionic liquid are investigated. The electrolyte membrane samples are prepared using the standard solution casting technique. Differential scanning calorimeter (DSC), X-ray diffraction (XRD), Scanning electron microscopy, Atomic force microscopy (AFM), cyclic voltammetry (CV) Fourier Transform Infrared spectroscopy (FTIR) techniques are employed to study the influence of cation-polymer interactions on structural and electrochemical properties of the prepared polymer gel electrolyte films. Electrical Impedance spectroscopy technique has been utilized to study the electrical conductivity, dielectric and modulus properties of the gel polymer electrolytes.The optimized polymer gel electrolyte membrane with 6 wt.% of $Mg(Tf)_2$-salt shows maximum ionic conductivity of $9.36 \times 10^{-5}$ S $cm^{-1}$ at room temperature.

**Keywords**: Polymer gel electrolyte, Ionic liquid, Dielectric and Modulus analysis.

**POLP – 4**

# Synthesis and Characterization of Alternating Copolymer of Vanillin Schiff's Base with Ethyl Acrylate

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## Abstract

An exhaustive literature survey reveals that there are only a few reports on the synthesis of 1:1 vanillin based alternating copolymer using ethyl acrylate as electrophilic monomer, which impelled a research drive to synthesis alternating copolymer by mixing 4-hydroxy-3-methoxy benzylidene-4'-hydroxy aniline that acts as a schiff base with ethyl acrylate in 1:1 mole ratio. 10ml of acetonitrile and hydroquinone monomethyl ether(0.1g) was added as radical inhibitor. The resulting reddish brown copolymer was precipitated from excess diethyl ether and dried at 50$^{o}$C. The physical characteristics such as solubility and intrinsic viscosity of the synthesized copolymer were determined. A probable mechanism for the alternating copolymerization was also proposed. The chemical structure of the synthesized copolymer was investigated by IR spectra and $^{1}$H NMR spectra.

**POLP – 5**

# Biomedical and Pharmaceutical Applications of PEG 400 Copolyesters Using Dodecanedioic acid and Dodecane diol

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**Abstract**

This paper describes about novel aliphatic biocompatible polymers prepared from polyethyleneglycol (PEG 400) moieties by melt condensation of dodecanedioic acid & 1, 12- dodecane diol. The synthesized copolyesters were determined by viscosity measurements and the structural elucidation was confirmed by FTIR, $^{1}$H NMR and $^{13}$C NMR spectra. IR spectra of the random copolyester showed characteristic absorption peaks for ester carbonyl stretching group. $^{1}$H NMR spectra of the copolyester exhibited the characteristic peaks of methylene protons of diols and diacids. $^{13}$C NMR spectra of copolyester showed characteristic resonance lines for carbons at different environments. The thermal analysis of the synthesized copolyester was carried out using Differential Scanning Calorimetry and Thermo gravimetry Analysis. The DSC analysis of the copolyester indicated the melting temperature (Tm) and TGA analysis of the copolyester indicated decomposition temperature (Td). Both the studies confirmed that the copolyester were thermally stable. The amorphous / crystalline nature of the copolyester was identified by wide angle X-ray diffraction studies. The XRD studies indicated that the copolyester arrived a peak value in the range of 20˚ - 30˚ which influenced the amorphous character of the copolyester. The molecular weight of the copolyester was confirmed with Gel Permeation Chromatography studies. Hence the synthesized copolyester were applied and used as antibacterial, antifungal, antibiofilm, antioxidant, anticancer, hydrolytic degradation, anti inflammatory and in controlled drug release studies.

**Keywords:** Polycondensation, Antibiofilm, Weightloss, Antioxidant and Drug release.

**POLP – 6**

# 4, 4'-Dihydroxybiphenyl - Aversatile Monomer for the Synthesis of Aliphatic-Aromatic Random Copolyester with Anti-Cancer Activity

**T. Sivaramakrishnan[1], N. Mahadevan[2], G. Annamalai[3] and G. Elango[4]**

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**Abstract**

In this communication we present our recent work related to the synthesis and characterization of a new aliphatic-aromatic random copolyester, PBID with improved properties synthesized using 1,4-butane diol, 4,4'-dihydroxybiphenyl and benzene-1,3-dicarbonyldichloride by direct solution polycondensation method. A thorough literature survey revealed that 4,4'-dihydroxybiphenyl induces inhibition of melanogenic activity in melanoma cells and showed Oestrogen-like properties in MCF-7 cells. The synthesized copolyester PBID was characterized by determining its inherent viscosity, solubility, thermal stability (DSC), UV-Vis, FTIR and $^{1}$H-NMR spectroscopy. Three dimensional molecular structure of the polymer was studied by wide Angle X-ray diffraction (WAXD) technique and the texture of the liquid crystalline polyester was identified using the photomicrographs obtained using optical microscopy and the nature of the polyester was interpreted by a combination of the these experimental methods. The in vitro cytotoxicity and the anti-proliferative effects of the synthesized copolyester, PBID was tested against HeLa cell line using the MTT method.

**Keywords:** Copolyester, 4, 4'-dihydroxybiphenyl, DSC, Cytotoxicity

**POLP – 7**

# Synthesis and characterization of certain novel random copolyesters

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**Abstract**

In the present investigation, we report on the synthesis of twonew random copolyesters namely PQIP and PQICbased on monomers: 1, 2-propane diol and 3-chloro-1, 2-propane diol as spacer groups and benzene-1, 3-dicarbonyldichloridewith an aromatic diol namely benzene-1, 4-diol to form semi-flexible liquid crystalline polyesterssynthesized using the solution polycondensation method. The polyesters were characterized by solubility studies, viscosity measurements, UV-€Vis., FTIR and $^{1}$HNMR spectral methods. The thermal properties were studied using differential scanning calorimetry and Thermo Gravimetric Analysis. We demonstrate that the chemical structure, morphology, physical integrity and surface property of the synthesized copolyesters can be controlled by simply changing the monomers. These novel polyesters exhibit versatility in thermal properties, morphology monitored using Scanning Electron Microscopy (SEM) and crystallinity studied using wide AngleX-ray diffraction (WAXD) technique and theirmesomorphic nature were interpreted by a combination of these experimental studies. The synthesized polyesters are multifaceted and their flexibility enhances their application effectively in the design of high-volume, low cast parts as well as critical, more expensive componentsfor engineering.

**Keywords:** Polycondensation, mesomorphic, WAXD

**POLP – 8**

## Evaluation of Corrosion Inhibition Efficiencies of Poly Aminothiophenols on Mild Steel in 1M Hydrochloric Acid Solution

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**Abstract**

The applicability of conducting polymer to enhance the corrosion resistance on metals in an acid environment is gaining greater significance as corrosion inhibitors. The inhibition performance of the isomers of poly(aminothiophenol) on mild steel in 1M hydrochloric acid solution is studied by electrochemical methods and weight loss method and their results are compared. The results show that the inhibition efficiency is found to increase with increasing concentration of the inhibitor. The maximum inhibition efficiency is observed for all the three polymers at the optimum concentration of 500 ppm. The inhibition action of poly (aminothiphenol) is explained in terms of adsorption which can form protective films on the surface of the mild steel. The anticorrosion activities carried out by potentiodynamic polarization method show that the inhibitor is of a mixed type and the electrochemical impedance spectroscopic technique exhibits capacitive loop indicating that the corrosion reaction is controlled by charge transfer process. The results obtained from the electrochemical methods are in good agreement with the weight loss method. The result clearly shows that the isomers of poly(aminothiophenol) act as a good corrosion inhibitor on mild steel in 1M HCl solution.

**Keywords:** Aminothiophenol, Conducting polymers, Corrosion, Mild steel, Electrochemical studies.

**POLP – 9**

# Heteropoly Acid Loaded Zeolites Catalyzed Aminolysis of Poly (Ethylene Terephthalate) Wastes

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**Abstract**

Polyethylene terephthalate (PET) is a most produced multifunctional polymer for the manufacturing of water bottles, soft drinks bottles, food packaging, synthetic fibers as well as adhesive materials.Zeolite–13X and Zeolite–4Acatalysts impregnated with 5.0 wt % of phosphotungstic acid (PWA) and phosphomolybdic acid (PMA) were synthesized using wet impregnation method and were characterized by BET and XRD analysis. In the present investigation we have explored the depolymerization of waste PET beverage bottles using aminolysis reaction catalyzed by supported phosphotungstic acid (PWA) and phosphomolydic acid (PMA).The supported catalysts were obtained by wet impregnation of PMA and PWA over zeolite supports such as Zeolite–13X and Zeolite–4A. The depolymerisation of PET polymer wastes have been successfully achieved by using 5wt% phosphotungstic acid and phosphomolydic acid loaded Zeolite -13X and Zeolite –4Acatalysts using aminolysis reaction at 150-170 °C. With respect to HPA, phosphotungstic acid (PWA) afforded 90% yield of aminolysed products where as phosphomolybdic acid (PMA) afforded 85% yield. PWA and PMA exchanged Zeolite -13X and Zeolite– 4Acatalysts effectively catalysed depolymersation of PET polymer wastes using ethanolamine, ethylene diamine, 1,3-diaminopropane and phenyl hydrazine, 3-Amino-1-propanal, 2-Amino-2-methyl-1-propanol as aminolyting agents. The yield of depolymerized product was found to be higher for PWA loaded Zeolite-13X and Zeolite–4A as compared to PMA loaded Zeolite –13X and Zeolite–4A. The surface area, pore volume the Zeolite has been evaluated by nitrogen adsorption and desorption studies, XRD, NMR, FT-IR. The yield of depolymerized product, BHETA and DPTPH was found to be higher for PWA loaded Zeolite-13X and Zeolite–4A as compared to PMA loaded Zeolite-13X and Zeolite–4Acatalysts.In comparison of yield of BHETA and DPTPH, 5wt% of PWA loaded Zeolite-13X as well as Zeolite–4Aafforded 85-90% yield of the depolymerized products.

**POLP – 10**

## Synthesis and Characterization of Certain Random Aliphatic Copolyesters

**A. Kesavan[1], T. Rajakumar[1], R. Nanthini[2], M. Karunanidhi[3] and A. Ravi [1*]**

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*[2]PG and Research Department of chemistry, Pachaiyappa's College, Chennai*

*[3]Department of chemistry, Government Arts College, Udumalaipet*

**Abstract**

Biodegradable aliphatic random copolyesters Poly (sorbitol sebacate -co-sorbitol citrate) and Poly (mannitol azelzte -co- mannitol Citrate) were synthesized from sorbital, and D-mannitol, citric acid,azelaic acid,sebacic acid through direct melt polycondensation with titanium tetra isopropoxide as a catalyst. These polyesters were characterized by FT-IR and FT-NMR spectral analysis and viscosity measurements.These crystallinity of polyesters studied using X-ray diffraction analysis. Thermal properties have been analysed using differential scanning calorimetry. Drug loaded and these polymers will be used as a drug loaded and eco- friendly packaging materials.

**Keywords**: Biodegradable polyesters, Drug loader, Eco-polymers

**POLP – 11**

# Quantification of Picric Acid on Nanospherepolypyrrole Modified Electrode by Stripping Voltammetry Method

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[3] *Departmetn of Chemistry, Bharathiyar University, Coimbatore*

**Abstract**

The electrochemical studies of picric acid were carried out in acidic, neutral and basic buffer media at bare glassy carbon (GC) and polypyrrole modified GC electrode. Cyclic Voltammogram (CV) of picric acid exhibited three reduction peaks at -0.4, -0.8 and -1.5V (*vs.* Ag/AgCl) and two oxidation peaks at 0.8 and 1.4V (*vs.* Ag/AgCl). Among the various pH studied, highly sensitive response was observed at pH 1.0at the optimal pH.The effect of scan rate was studied between 25 and 500 $mV.s^{-1}$.CV results revealed the adsorption-controlled reaction at the electrode surface. The GC electrode was modified with polypyrrole conducting polymer film to enhance the electrocatalytic activity of the reductive species. Atomic force microscopy (AFM) images showed the nanosphere morphology of the polypyrrole film, which was coated uniformly on the electrode surface. Under optimum experimental conditions, the influence of concentration on the stripping signal was studied. The linear range of detection was found between 50 ppb and 250 ppb with the lower limit of detection of 10±3 ppb.

**Keywords**: Picric acid; Polypyrrole; AFM; Stripping Voltammetry

**POLP – 12**

## Heteropoly acid loaded Zeolites Catalyzed Aminolysis of Poly (Ethylene terephthalate) wastes

**G. Jeya, M. Anbarasu, R. Dhanalakshmi, V. Vinithaand and V. Sivamurugan***

*PG and Research Department of Chemistry, Pachaiyappa's College, Chennai*

**Abstract**

Polyethylene terephthalate (PET) is a most produced multifunctional polymer for the manufacturing of water bottles, soft drinks bottles, food packaging, synthetic fibers as well as adhesive materials.Zeolite–13X and Zeolite–4Acatalysts impregnated with 5.0 wt % of phosphotungstic acid (PWA) and phosphomolybdic acid (PMA) were synthesized using wet impregnation method and were characterized by BET and XRD analysis. In the present investigation we have explored the depolymerization of waste PET beverage bottles using aminolysis reaction catalyzed by supported phosphotungstic acid (PWA) and phosphomolydic acid (PMA).The supported catalysts were obtained by wet impregnation of PMA and PWA over zeolite supports such as Zeolite–13X and Zeolite–4A. The depolymerisation of PET polymer wastes have been successfully achieved by using 5wt% phosphotungstic acid and phosphomolydic acid loaded Zeolite -13X and Zeolite –4Acatalysts using aminolysis reaction at 150-170 °C. With respect to HPA, phosphotungstic acid (PWA) afforded 90% yield of aminolysed products where as phosphomolybdic acid (PMA) afforded 85% yield. PWA and PMA exchanged Zeolite -13X and Zeolite– 4Acatalysts effectively catalysed depolymersation of PET polymer wastes using ethanolamine, ethylene diamine, 1,3-diaminopropane and phenyl hydrazine, 3-Amino-1-propanal, 2-Amino-2-methyl-1-propanol as aminolyting agents. The yield of depolymerized product was found to be higher for PWA loaded Zeolite-13X and Zeolite–4A as compared to PMA loaded Zeolite –13X and Zeolite–4A. The surface area, pore volume the Zeolite has been evaluated by nitrogen adsorption and desorption studies, XRD, NMR, FT-IR. The yield of depolymerized product, BHETA and DPTPH was found to be higher for PWA loaded Zeolite-13X and Zeolite–4A as compared to PMA loaded Zeolite-13X and Zeolite–4Acatalysts.In comparison of yield of BHETA and DPTPH, 5wt% of PWA loaded Zeolite-13X as well as Zeolite–4Aafforded 85-90% yield of the depolymerized products.

**POLP – 13**

# Acoustical and Stability studies on Polyvinyl Alcohol a Biodegradable Polymer

**G.M. Rajesh[1], S. Jayakumar[1], N. Dharani Rajan[1], A. Ravi[2] and G.S. Gayathri[3]**

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## Abstract

The Polyvinyl alcohol (PVA) is a synthetic polymer that is soluble in water. It is effective in film forming, emulsifying, and has an adhesive quality.PVA is a biodegradable polymer and environmental friendly. PVA bags used in sports fisheries to attract fishes. Since PVA is soluble in water it breaks down.When PVA bags containing pellets and these bags dipped in water attract fishes towards it. The chemical formula for the polyvinyl alcohol (PVA) is $(C_2H_4O)$ x.The various concentrations of PVA with water is prepared. The ultrasonic velocity, density and viscosity of the mixture are measured using the ultrasonic interferometer and ostwaldviscometer respectively.The acoustical parameters have been studied for aqueous polyvinyl alcohol. The acoustical parameterssuch as specific acoustic impedance (Z), freelength ($L_f$), viscous relaxation time ($\tau$), attenuation factor ($\alpha$), absorption co-efficient ($\alpha/f^2$), internal pressure ($\pi_i$) and free volume ($V_f$) have been estimated using the experimental data of velocity, density and viscosity of Polymer Solution. The stability constant (k) had been determined by Yoshida & Osawa method and Kannappan method.Statistical analysis had been determined in aqueous solution of polyvinyl alcohol. The standard deviation of these solutions is 693.8 and the variance is 481369.5. When PVA is dissolved in water, $H_2O$ molecule penetrate into free space of polymeric chain and causes bulging of the film. Presence of Hydroxyl groups in PVA is responsible for the intermolecular interaction of Polymer – solvent molecules.Both water and PVA is polar in nature forms strong Hydrogenbonding interaction between solute and solvent. Inter and Intermolecular bonding takes place between solute andsolvent molecules.Molecular diffusion of PVA depends on degree of polarity, degree of hydrolysis, molecular weight, temperatureand concentration.Short branched chain, PVA (solute) forms strong intermolecularHydrogen bonding with water (solvent) compared with other solvents.

**Keywords:** Biodegradable, absorption co-efficient, polarity.

**POLP – 14**

# Ultrasonic, Stability, frequency Acoustic Spectra, Scaled Particle Theory Studies and Statistical Analysis of Aqueous Polyvinyl Pyrolidine, Polymer

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**Abstract**

Polyvinyl Pyrolidine is a non ionic polymer and it is a protein acceptor. PVP is soluble in water and other polar solvents.Its chemical formula is $(C_6H_9NO)_n$. PVP is used as binder,stabilizer, adhesive, complexing agent and in resins. Ultrasonic velocity, viscosity and density studies on aqueous solutions of PVP of Molecular Weight 40,000 have been carried out. From the velocity, density and viscosity values, various Acoustical Parameters, specificacousticimpedance (z), adiabatic compressibility ($\beta$), intermolecular free length ($L_f$), viscous relaxation time ($\tau$), attenuation factor ($\alpha$), absorption coefficient ($\alpha/f^2$), internal pressure ($\pi_i$) and free volume ($V_f$) have been computed. All these parameters have been discussed to throw light on the polymer solute solvent interaction. The stability constant of polymer in solution, gives the stability and the nature of interaction.

The frequency acoustic spectra (FAS) of ultrasonic waves is determined from low frequency ($f_L$) to high frequency ($f_h$). From the frequency Acoustic Spectra the bandwidth of the aqueous polymer solution obtained is 3000 m/s. Lebowitz and Reisshave developed a formulation called scaled particle theory, which has been used to find out radial distribution function. These values are compared with standard values.Statistical Analysis of ultrasonic velocity in the polymer solution shows the mean value is 1322 4 m/s.The standard deviation of velocity obtained is 42.60.The higher standard deviation the lesserwill be the variation in the observation.PVP is amphiphilic in nature. The hydrophilic nature of PVP involves the presence of interaction between carbonyl group and polar solvent.

**Keywords:** Nonionic, stabilizer, stability constant, scaled particle theory.

**POLP – 15**

# Effect of Mg $(CF_3SO_3)_2$ Concentration on Structural and Electrochemical Properties of Ionic Liquid Incorporated Polymer Gel Electrolyte Membrane

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**Abstract**

In the present study, magnesium ion conducting polymer gel electrolytes based on polyethylene oxide (PEO) containing 1-Ethyl-3-methylimidazolium tetrafluoroborate (EMIM-$BF_4$) as ionic liquid are investigated. The electrolyte membrane samples are prepared using the standard solution casting technique. Differential scanning calorimeter (DSC), X-ray diffraction (XRD), Scanning electron microscopy, Atomic force microscopy (AFM), cyclic voltammetry (CV) Fourier Transform Infrared spectroscopy (FTIR) techniques are employed to study the influence of cation-polymer interactions on structural and electrochemical properties of the prepared polymer gel electrolyte films. Electrical Impedance spectroscopy technique has been utilized to study the electrical conductivity, dielectric and modulus properties of the gel polymer electrolytes.The optimized polymer gel electrolyte membrane with 6 wt.% of $Mg(Tf)_2$-salt shows maximum ionic conductivity of $9.36 \times 10^{-5}$ S $cm^{-1}$ at room temperature.

**Keywords**: Polymer gel electrolyte, Ionic liquid, Dielectric and Modulus analysis.

# Spectroscopy Papers

**SPEP – 1**

## Spectroscopic and Thermal investigations on $B_2O_3 – MnO_2 – ZrO_2$ Glasses

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[2]*Department of Physics, Government Arts College, Chidambaram - 608 102*

**Abstract**

The ternary glass system of $B_2O_3 – MnO_2 – ZrO_2$ with different compositions of $ZrO_2$ are prepared by melt quench technique. XRD profiles are used to confirmed the amorphous nature of the glasses. SEM analysis is carried out to study the morphological modification created by the modifier oxide. IR technique is used to investigate the structural changes with respect to composition in the glass systems and functional groups at different modification levels. Differential thermal analysis is used to identify the glass transition temperature, crystallization temperature and melting temperature of the glass samples. The glass stability factor and Hruby's parameter are calculated from the above mentioned temperatures. The properties and structural features of glasses are discussed in terms of relative of zirconium ions.

**Keywords**: Glass, Melt quench technique, XRD, SEM, FTIR, DTA

**SPEP – 2**

# Continuous Monitoring of Hypothyroid Disorder Using Blood in an Adult Woman Patient Using FTIR-ATR Spectroscopic Technique

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## Abstract

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.

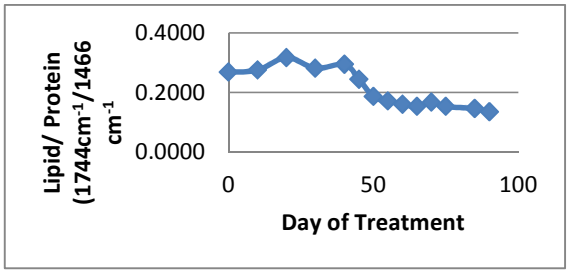


Fig. 1 Variation in the lipid-protein ratio as obtained from the absorbance at 1744 $cm^{-1}$ and 1466 $cm^{-1}$ after normalization 1550 $cm^{-1}$ respectively. The circle denotes the values deduced for the healthy group.

**SPEP – 3**

# Investigation of Acne Vulgaris a skin Disease using Hair tissues & Characterization - FTIR-ATR

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## Abstract

Acne vulgaris is a chronic skin disease which occurs due to inflammation of the hair follicles and sebum producing (sebaceous) glands of the skin called pilosebaceous unit and the anaerobic propionic acne bacterium, P.acne. Human sebum is dominantly made up of 57.5% of triglycerides and fatty acids, 26% wax esters, 12% Squalene and 4.5% Cholesterol. The increased level of Androgen hormone, sebum lipid composition and P.acne over growth induces monocytes and pro inflammatory cytokines. They attract neutrophils, basophils, and T cells to the pilosebaceous unit and drive epithelial hyper proliferation i.e., Acne vulgaris. The actual biomolecular changes due to acne vulgaris disease are present in the blood and in the sebum and also in the noninvasive sample of human scalp hair follicles. The main objectives of the present study are to analyze human scalp hair follicles samples using FTIR-ATR spectrum to compare and discriminate spectral signatures of healthy subjects and diseased acne samples through acne bio-markers in Protein, Amide I, Amide II and Squalene (LDL) present in tissue components using the method of internal ratio parameters.

**Keywords:** Acne Vulgaris, FTIR-ATR, Sebum, Sebaceous glands, P.acne, Squalene.

**SPEP – 4**

# Spectroscopic and Quantum Chemical Calculations of 9-Octadecenoic acid from leaves of Aavaram

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**Abstract**

We disclose a detailed DFT study and phytochemical study of *Cassia auriculata* product, 9-octadecenoic acid has been carried out. The present work is optimized molecular geometry and vibrational frequencies in the ground state are calculated by using the DFT and B3LYP methods with 6-31G+(d,p). Theoretically concluded FT-IR spectra of title molecule have been made on the basis of the calculated potential energy disruptions (PED). The stability and charge delocalization of the molecule was studied by the natural bond orbital analysis. The molecular electrostatic potential (MEP) shows the negative, the positive potential sites and determining the stability of the molecule was computed using B3LYP /6-31+G (d,p) basis set analyzed. A study on the Mulliken atomic charge and other electronic properties were performed by the DFT method. The HOMO-LUMO energies and the energy gap were determined by the time-dependent (TD-DFT) method.

**SPEP – 5**

# Spectroscopic, Quantum Computational and Molecular Docking Study of 4- Phenylbutyrophenone

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## Abstract

The title compound, 4-phenylbutyrophenone (4PBP), Characterized by FT-IR, FT-Raman and UV-vis spectral analysis. The optimized molecular geometry, the vibrational modes, the infrared intensities, and the Raman scattering activities were calculate by using density functional theory (DFT) B3LYP method with 6-311++G(d,p) basis set. The values are almost equal to the experimental XRD data. The computed HOMO and LUMO energies show that charge transfer within the molecule. NBO analysis was performed to study the stability of the molecule and donor-acceptor interactions. The hyperpolarizability calculation shows the present material has a reasonably good NLO property. The reactive areas are calculated by molecular electrostatic potential (MEP) and Fukui functions. The thermodynamic properties (heat capacity, entropy and enthalpy) of the CPPM calculated at different temperatures.

**Keywords:** FT-IR, FT-RAMAN, NBO, HOMO-LUMO

**SPEP – 6**

# Study of Molecular Structure and Vibrational Assignments of 3-Ethyl-4-Methyl-N-[2-(4-{[(Tran-4-Methylcyclohexyl) Carbamoyl] Sulfanoyl} Phenyl) Ethyl]-2-Oxo-2, 5-Dihydro-1h-Pyrrole-1-Carboxamide (Glimepiride) By Density Functional Theory

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**Abstract**

Theoretical and Experimental spectra (vibrational) of 3-Ethyl-4-methyl-N-[2-(4-{[(tran-4-methylcyclohexyl) carbamoyl] sulfanoyl} phenyl) ethyl]-2-oxo-2, 5-dihydro-1H-pyrrole-1-carboxamide (Glimepiride) were examined. The FTIR-ATR and FT-Raman spectra of Glimepiride in the solid phase have been recorded in the region of 4000-450cm$^{-1}$ and 4000-50cm$^{-1}$ respectively. Theoretical calculations were executed by density functional theory method using 6-31G (d,p) basis set of Gaussian 09W software program. Using the potential energy distribution (PED) calculations, the complete vibrational assignments of wavenumbers were calculated. The optimized molecular geometry, atomic charges and vibrational frequencies in the ground state were calculated. The experimental spectra coincide convincingly with theoretically produced spectrograms of title compound. The obtained vibrational wavenumbers are in good agreement with the experimental data. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies were estimated. By applying Natural Bond Orbital (NBO) analysis, the stability of molecules arising from hyper-conjugative interactions and charge delocalization were evaluated. The molecular electrostatic potential (MEP) surface was achieved over the optimized geometry of the molecule to access the chemical reactivity of the molecule. Mullikan population analysis on atomic charges also calculated.

**SPEP – 7**

# Spectroscopic, Quantum Computational Calculations and Structural Investigation of corynan-17-ol, 18, 19-didehydro-10-methoxy, acetate by GC-MS, Fourier Transform Infrared (FT-IR) UV-Vis, NBO, HOMO–LUMO Energies Molecular Docking Studies

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**Abstract**

This study aimed to evaluatethe isolated from leaves of corynan-17-ol,18,19-didehydro-10-methoxy, acetateand its structure was characterized using, Gas chromatography mass spectrometry [GC–MS], fourier transform infrared spectroscopy [FT-IR] and UV–Vis spectroscopy.Corynan-17-ol, 18, 19-didehydro-10-methoxy, acetate of isolated compound. Density functional theory calculations are carried out for the first time for geometric, electronic and spectroscopic properties of (corynan-17-ol, 18, 19-didehydro-10-methoxy, acetate). Atomic charges, donor-acceptor NBO hyper conjugative interactions, Ionization potential and electron affinities, HOMO-LUMO gap and molecular electrostatic potential were also computed at B3LYP/6-311++G (d,p) level.

**SPEP – 8**

# Spectroscopic and Quantum Chemical Investigations on D-Limonene

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## Abstract

In the present study, the combined experimental and theoretical analysis on D-Limonene, chemoprevention activity compound has been investigated by FT-IR, FT-Raman, NMR and UV-Vis spectroscopic techniques with the help of high level of the quantum chemical calculations. The molecular geometry optimization, vibrational frequencies, chemical shifts and electronic energies were calculated and discussed. Besides, D-Limonene is a stereochemical compound, which is identified from the natural extract of orange, lemon, mandarin, lime, and grapefruit using GC-MS techniques. The obtained experimental and theoretical finding shows a good conformity, these compounds were analyzed for anti-tumor activities with their protein targets using Molecular docking studies. Docking results showed best Glide energy, Docking score, H-bonding interactions compared with molecular targets and has the potential to prevent or treat breast cancer.

**Keywords**: Vibrational spectra, NMR spectra, Electronic spectra, GC-MS, DFT

**SPEP – 9**

## Molecular structure, spectroscopic (FT-IR and NMR) and theoretical studies on piperidone oxime picrate

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**Abstract**

A piperidin-4-one oxime picrate was synthesized and characterised by FT-IR and $^{1}H$ and $^{13}C$ NMR spectra. The compound the experimental data were compared with the theoretical data. The stability of the molecule due to hyper-conjugative interaction and charge delocalization was studied by NBO analysis. The UV-Vis spectral data calculated by using the DFT method were correlated with the experimental values. The calculated HOMO and LUMO energies revealed that charge transfer occurs within the molecule and Mulliken charges were also obtained. The higher energy difference between HOMO and LUMO indicates hardness stability and reactivity of the compounds. The electrical dipole moment (μ) and first hyperpolarizability (βo) values have been computed using DFT B3LYP/ 6-31G(d,p) method. Molecular electrostatic potential (MEP) analyses were performed to predict the reactive sites of the molecule. The calculated first hyperpolarizabilty is high suggesting an extended p-electron delocalization over the picryl ring and piperidone moiety which is also responsible for the nonlinear optical property of the molecule.

**Keywords**: Picrate, DFT, HOMO–LUMO, NLO, MEP.

# Spectral Analysis and Vibrational assignments on FT-IR, FT-Raman, NMR and Docking, Antibacterial studies of 2-Methoxypyridine-5-boronic acid (2MP5BA) by Using DFT

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**Abstract**

The geometrical parameters, nuclear magnetic resonance (NMR)and vibrational frequencies of the 2-Methoxypyridine-5-boronic acid (2MP5BA) have been performed using density functional theory (DFT) B3LYP method with 6-311++G(d,p) basis set. The experimental Infrared and Raman spectra were obtained in the region 4000-400cm$^{-1}$ and 3500-100cm$^{-1}$ respectively. In addition these, HOMO and LUMO energies and thermodynamic parameters were presented. The $^{1}$H &$^{13}$CNMR chemical shifts were calculated by the gauge independent atomic orbital (GIAO) method and compared with the experimental data. Firmness of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. From the title molecule various ligand are using in the cervical cancer protein by docking. From these 2MP5BA has been screened to antimicrobial activity and found to exhibit antibacterial effects.

**Keywords:** FT-IR, FT-Raman,$^{1}$H &$^{13}$CNMR, HOMO – LUMO, Docking and Antibacterial Activity.

**SPEP – 11**

# Screening the Bioactive Constituents of Solanum Nigrum Using FTIR-ATR, UV-Vis & GC-MS Techniques and Confirming the Antihistamic Activity Using Molecular Docking Studies

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**Abstract**

The present study has been carried out to characterise the bioactive constituents present in the Ethanolic extract of Solanum nigrum leaves (Solanaceae) using FTIR – ATR and UV- Vis Spectroscopic techniques. This plant is a traditional medicinal plant used to treat various ailments in mankind. The bioactive constituents of the plant Solanum nigrum are Flavonoids, Tannins, Terpenoids, Saponins and Alkaloids. The Ethanolic extract of Solanum nigrum leaves contains Flavonoids and Tannins. FTIR – ATR spectroscopy is an established time saving method to characterise and identify the functional groups present in the extract. The occurrence of bands for Phenols and polyphenolic compounds confirmed the presence of Flavonoids and Tannins. The presence of bioactive constituents of Solanum nigrum has also been identified by observing the bands corresponding to electronic transitions observed in UV spectrum. GC-MS studies have been carried out to separate the various bioactive components based on their volatility. Separated each component has the capability of curing various ailments such as antibacterial, anti-inflammatory, antioxidant , antihistamic , anticancer activities etc . In the present study the antihistamic activity is considered and this has been confirmed using the molecular docking studies.

**SPEP – 12**

# Individual and Combined Toxicity of $Ni^{2+}$ / $Cr^{6+}$ Ion on Muscle Tissues of Edible Fish Studied Using Spectroscopic Technique

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**Abstract**

Pollution of freshwater lakes, rivers, streams and groundwater has reached alarming proportions. Also, the discharge of metals from polluting sources usually consists of mixtures rather than of the individual metals. The importance of heavy metal nickel and chromium and its toxic effect on aquatic organism are discussed. The response of biota to individual-metal-exposure may differ from its response to that of multiple metals, as mixtures of metals may interact antagonistically, synergistically or additively. In addition, the toxicity of an element depends on its chemical form, concentration and physico-chemical factors. Bio-accumulation pattern of heavy metals on the selected organs of *Cirrhinus mrigala* was studied using ICP-AES technique. Accumulation was highest in Gill for chromium concentration (BCF=21.382).In the case of chromium, Cr(VI) after entering the cell it is readily reduced to Cr(III). This intracellular reduction of Cr(VI) to Cr(III) helps maintain a low level of chromium. Also, when the animals are exposed to nickel and chromium simultaneously increased absorption of nickel and chromium was observed in all the tissues. Increased bioavailability of nickel and chromium in the case of their combined exposure signifies the greater toxicity of the metal mixture compared to that of the individual metal exhibiting synergism among these metals. In the present investigation the observed data indicate that *Cirrhinus mrigala* could be suitable monitoring organisms to study the bioavailability of water-bound trace metals in freshwater habitats.

**Keywords:** Heavy metals, Nickel, Chromium, Synergism, Antagonism

**SPEP – 13**

# Thermal and Structural Properties of Mixed Alkli Transition Metal Iorns in Sodium Borate Glass

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**Abstract**

Glasses with composition 20 $Na_2$ – O - (80 –x) $B_2O$ X $Li_2$ O (NBL) and 20 $Na_2$-O- (80-x) $B_2$ $O_3$ X $Li_2O$ (where x=o to 10 is steps 2 mol %) where synthesis by conventional melt quenching method. The obtained glass were characterized by X ray diffraction (XRD), gthermogravimetric analysis (TGA) differential thermal analysis (DTA) , and Fourier transform infrared spectroscopy (FTIR). The amorphous phase of the prepared glass samples was conformed from their XRD, TGA, and DTA profiles. DTA profiles yielded date transition temperature (Tg) and thermal stability (del T) rang of glasses FTIR spectra were interpreted terms of the structural transformation on glass network by the changing composition . FTIR spectral study reveals the existence of Bo 3 and Bo4 groups with Li – O – Li and W – O – W vibrations in the present glasses. The presence of varied types like di, tetra, penta, and ortho borate groups are confirmed in the glass matrix.

**SPEP – 14**

# Eelectrochemical and in-vitro behavior of Graphene Oxide-Calcium Deficient Apatite thin layer coating on surgical grade 316LSS for Biomedical Applications

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**Abstract**

The objective of this work is to design and development of graphene based bioceramic composite. The composition of graphene bioceramic composite is Hydroxyapatite/β-Tricalcium phosphate reinforced Graphene oxide (HAp/ β-TCP/GO) in three different ratios**.** The crystalline structure, chemical composition, morphology and elemental analysis of the developed composite were characterized using analytical techniques such as X-Ray Diffraction (XRD), Fourier Transform Infra red (FTIR) Spectroscopy, Raman Spectroscopy, Field Emission Scanning Electron Microscopy (FESEM) and Energy Dispersive Spectroscopy (EDS). The developed material has coated on surgical grade implant metal and evaluates the corrosion inhibition behavior. In order to investigate the effect of graphene oxide on the in-vitro bio mineralization, the developed composite was immersed in Simulated Body Fluid (SBF) solution for various time periods (0, 7, 14 and 21 days) and the results indicate that the reinforcement of graphene oxide promotes the growth of hydroxyl apatite layer on the surface of composite discs. Further the developed composite of β-TCP/HAp reinforced graphene oxide can be used as a potential candidate material for biomedical applications.

# Synthetic Material Papers

**SYMP- 1**

## Synthesis of 1, 4-Dihydropyridine Derivatives in Aqueous Mediumassisted with Microwaveirradiation

**V. Vinitha, G. Jeya, M. Anbarasu, R. Dhanalakshmi and V. Sivamurugan***

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**Abstract**

Zn[(L)proline]2 was found to be an effective water soluble homogeneous catalyst for the synthesis of 1, 4-dihydropyridine derivatives, as one of the most important pharmaceutical compounds using the one-pot three component condensation reaction of aldehydes, β-dicarbonyl compounds, □-dicarbonyl compounds in aquoeus medium assisted with microwaveirradiation. This new methodology has been several benefits such as high yields (98%), short reaction time (2-5 min), safety, an environmentally friendly clean process. The process utilises low microwave power and reduces the cost, since water is used as medium. The Lewis acid catalysed Zn [(L) proline]2 was easily prepared, recyclable and reusable. All the synthesised derivatives were characterized by FT-IR, 1H &13C-NMR, MS and elemental analysis.

**Keywords:** Zn [(L)proline]2, 1,4-dihydropyridine.

**SYMP- 2**

# Evaluation of Anti-Biofilm and Anticancer Activity of 4 - Chlorobenzylidene Substituted Thiadiazine Containing Bridged Carbazole Derivative.

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**Abstract**

Structurally unique and functionality enriched heterocyclic systems are of great significances in chemically and biologically related research areas. The importance of carbazole derivatives are evidenced from the fact that the skeleton of it could be found in many biologically active molecules, natural products, therapeutic agents and photoelectrical materials. N-(4-chlorobenzylidene)-5-(1,2,3,4-tetrahydro-9H-carbazol-1-yl)- 6H- 1,3,4-thiadiazin-2-amine has synthesized by four stages as follows, Fischer's indolization (stage1), bromoacetylation using bromoacetyl bromide (stage2), thiadiazine ring formation using thiosemicarbazide (stage3) and chlorobenzylidene substituted thiadiazine containing carbazole derivative using 4-chloro benzaldehyde. The synthesized compound has been confirmed using spectral analysis viz, FTIR, 1H & 13C NMR and Mass spectroscopy. The synthesized compound evaluated for anti-biofilm and anticancer activity. The result shows the synthesized compound found to have excellent anticancer and anti-biofilm activity.

**Keywords:** Anticancer, Anti-biofilm, bromoacetyl bromide, Ciprofloxacin.

**SYMP- 3**

# Novel Ph – Tunable Non – Toxic Hydrogels of Pyrrole-2-Carboxylic Acid and Ethylenediamine Derivatives: Synthesis and Characterization

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**Abstract**

The pH sensitive biopolymeric hydrogel has been synthesised using stoichiometric amount of Citric acid, Ethylenediamine and Pyrrole-2-carboxylic acid in ethanol medium by condensation polymerisation. FT-IR, NMR, TGA, DSC and SEM analysis were used to characterise the prepared hydrogel. Swelling behaviour of hydrogel in various pH(3 to10) were also studied to examine their drug delivery capacity. The synthesised hydrogels were also subjected to antibacterial activity against gram positive s.aureus and gram negative E.Coli using zone inhibition method. The studies showed that pH sensitive biopolymeric hydrogel could be used as a drug delivery system, in view of their swelling and prolonged drug release characteristic in acidic pH.

**Keywords:** Biopolymeric hydrogel, pyrrole-2-carboxylicacid, swelling equilibrium, antibacterial activity etc.

# Solvent Effects on UV Spectra of (E)-3- (Benzo[D][1,3]Dioxol-5-Yl)-1-(1-Methy-1h-Pyrrol-2-Yl) Prop-2-En-1-One (Bdpp) in Various Organic Solvents

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## Abstract

Chalcones have much attention due to the wide spread range of biological applications in pharmatutical field. Chalcones derivatives exhibit antioxidant, antifungal, anticancer activity etc., and they posses important role in organic synthesis. The absorption spectra of some biologically active chalcone constitutes in various solvents of different polarities with various physical properties have been studied at room temperature. A solvent effect on wave number of the absorption band maxima( ƛmax) were discussed using the following solvent parameters; Refractive index(N)Dielectric constant (D) and empirical Kamlet-Taft solvent parameters π*(dipolarity/polarizability),α(hydrogen bond donating capability) and β(hydrogen bond accepting ability) using multilinear regression method . The solute solvent interactions were determined on the basis of multi Linear Salvation Energy Relationship (LSER) concept. The solvate chromic behavior was explained in detailed manner.

**SYMP- 5**

# Design, Target Specific, Highly Diastereoselective Synthesis and Spectral Characterization of Carbazol-3-Yl- Pyranoquinolinyl-2-Phenylacrylic Acid Diasteromers as Potential A - Glucosidase Inhibitors

**K. Venkatapathya[1], C. J. Magesh[1]*, G. Lavanyaa[1], R. Sathishkumar[2] and S. Premaa[1]**

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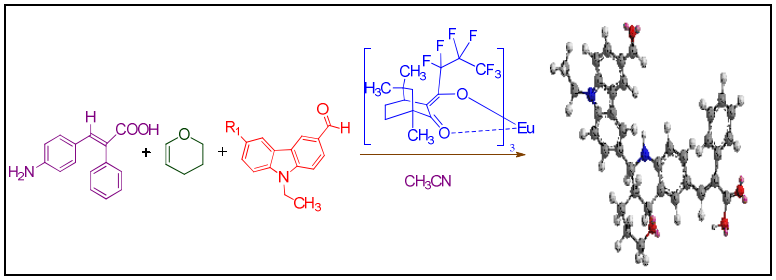
*[2]PG & Research Department of Physics, Arignar Anna Govt Arts College, Cheyyar,*

## Abstract

In the present investigation we report the first target specific, highly diastereoselective synthesis of new class of Carbazol-3-yl- pyranoquinolinyl-2-phenylacrylic acid diastereomers and evaluation of their invitro α-glucosidase inhibitory activity. All the products were thoroughly characterized by 1H-NMR, 13C-NMR, FT-IR, Mass spectral and CHN analysis. A highly diastereoselective target specific route of synthesis for the biologically active diastereomers were developed by using chiral catalyst Europiumtris[3-heptafluoropropylhydroxylmethylene]-(-)-camporate (A). It was found that among a set of 4 diastereomeric products obtained, exodiasteromers of carbazol-3-yl- pyranoquinolinyl-2-phenylacrylic adducts exhibited relatively high α-glucosidase inhibitory activity. The newly synthesized compounds exhibited IC50 values in the range of (0.80 ± 0.02 - 48.3 ± 0.94µM) as compared to standard acarbose (IC50= 0.85± 0.32µM). It was found that five compounds were found to be more active than standard acarbose. It was also found that unsubstituted compound or compounds with chlorine or methoxy substituent showed potential α-glucosidase inhibitory activity. However a reversal in activity was observed with Nitro substituent where in the endodiastereomers were found to be more active than exodiastereomers. Molecular docking studies were used for design of the compound and understand the mode of binding between the compound and target enzyme. A plausible mechanism for the diastereoselective synthesis was also proposed.



# Synthesis of bis(indolyl)methane derivatives using Zn (L) Proline$_2$/MCM-41 catalyst

**R. Dhanalakshmi, G. Jeya, M. Anbarasu, V. Vinitha and V. Sivamurugan***

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**Abstract**

Bis(indolyl)methane analogous using indole with substituted aldehydes/ketones were synthesised in desired yield by multi-component condensation by MCM-41 impregnated with Zn(L)Proline$_2$as recyclable and non-toxic catalyst. The vibrindole derivatives (BIM) has significant material due to its pharmacological activities like anticancer, antibacterial, antibiotics, analgesic and anti-inflammatory. They are also highly beneficial in promoting good estrogen and increase the body's natural metabolism of hormones. In this procedure, we have synthesized cyclo condensation using substituted carbonyl compounds with indole in excellent yields with highly efficient, heterogenous supported catalyst. All the synthesized BIM derivatives were characterised by different spectral techniques.

**Keywords:** Bis(indolyl)methane (BIM), MCM-41, ZnP catalyst.

**SYMP- 7**

# Ultrasonic Velocity, Density and Viscosity Measurements of Para Substituted Aromatic Derivatives of Ketone

**G. S.Gayathri[1], S. Jayakumar[2], N. Dharani Rajan[3], G.M.Rajesh[4], S. Bangaru Sudarsan Alwar[5] and R.Sambasivam[6]**

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**Abstract**

Ultrasonic techniques are non-destructive testing method which directs us to understand the type of intermolecular interaction in the binary liquid mixtures. Intermolecular interactions have been obtained as a result of attraction or repulsion among the various components present in the liquid mixtures. Aromatic ketones derivatives and Benzene have wide application in industries like pharmaceuticals, dyes, perfumes, polymers, solvent extractions etc. In the present study, the thermos acoustical parameters like Free length, Free volume, internal pressure and excess parameters like excess adiabatic compressibility, excess free length, excess molar volume have been computed for the binary solid-liquid mixtures of 4-Bromoacetophenone-Benzene,4-Nitroacetophenone-Benzene and 4-Hydroxyacetophenone-Benzene applying the measured values of ultrasonic velocity, density and viscosity of various mole fraction range at 308 K. Aromatic ketone derivatives like 4-Bromoacetophenone, 4-Nitroacetophenone, 4-Hydroxyacetophenone are polar in nature, whereas Benzene is a nonpolar molecule. The electron withdrawing natures of these ketones are tangled by the resonance effect which in turn results in the calculated parameters. These parameters indicate the presence of strong dipole-induced dipole intermolecular interactions existing between the Para substituted aromatic derivatives of ketone and benzene molecules. The excess parameters used to correlate the strength of interaction between the unlike molecules.

**Keywords:** Ultrasonic Velocity; thermos acoustical parameters; Aromatic Ketones; Resonance effect; dipole-induced dipole interactions.

**SYMP- 8**

# Synthesis of Zirconium Oxide Nanoparticles using Calotropis Gigantes Leaf Extract and Antibacterial and Antifungal Activities

**T.Balasankar**

*Chemistry Section (Feat), Annamalai University*

**Abstract**

Synthesized nano particles have an incredible application in biomedicine owing to its simplicity, eco-friendly properties and low cost. The present study aims to determine the green synthesized zirconium oxide nano particles from *calotropis gigante* an leaf extract. Synthesis condition were optimized for maximal and narrow size range synthesis ofziirconium oxide nano particles. The result nano powder was characterized using various analytical techniques, such as UV-VIS spectroscopy, FT-IR Spectroscopy, X-Ray Diffraction and Transmission Electron Microscopy (XRD), X-Ray diffraction studies crystalline nature of the nano particles indicating particle size within the range .Hence an easy effective green approach for synthesis of zirconium oxide nano particles with efficient antibacterial and antifungal activity is reported in the study.

**SYMP- 9**

## Biogenic synthesis of stannic oxide nanoparticles –literature review

**K. Vedhapriya and Dr. G. Balaji**

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*Thiru.A.Govindasamy Government Arts College, Tindivanam.*

**Abstract**

In the past few years stannic oxide ($SnO_2$) has gained a lot of interest because of its outstanding range of applications in different field such as catalysis, energy storage, sensors, dye-sensitized solar cells, medicine etc.,. Green synthesis is one of the eco-friendly method for preparing nanoparticles without the use of venomous Chemicals .The green and bio-based route for the synthesis of metal and metal oxide nanoparticles has earned much heed by using various plant and their parts, bacteria, fungus, and biological materials. Among this plant extract is the simplest approach because of its low cost , abound resource and simple operation requirement, Plant phytochemicals which have antioxidant property is mainly responsible for the preparation of metal and metal oxide nanoparticles .

**Keywords:** biogenic, $SnO_2$, antioxidant, phytochemical

# Biosynthesis of Colloidal Copper Oxide Nanoparticles using Psidium Guajava L. Leaf Extract and its Physicochemical Characterization

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[2]*St. Joseph College of Arts and Science (Autonomous), Cuddalore.*

[3]*Research Scholar, Holy Cross College (Autonomous), Trichy.*

**Abstract**

In the present investigation, plant mediated bio-synthesis of copper oxide nanoparticles is synthesized using *Psidium guajava* leaf extract and were further characterized using Fourier transform infrared spectroscopy (Presence of biomolecules), UV-vis spectroscopy (250-300 nm), Field electron scanning electron microscope (40 to 65 nm), Energy dispersive x-ray analysis (Cu, O elements), X-ray diffraction analysis (face-centered cubic structure), Particle size analyser (120 nm). This confirms that copper oxide nanoparticles are well formed and synthesized. This confirms that the copper oxide nanoparticles can be produced in large scale and can be implied for prevention of food, crops and drug delivery system.

**SYMP- 11**

## Ingenuity Comparison of Aluminum Doped Cobalt Ferrite and Barium Doped Cobalt Ferrite as Anode for Lithium - Ion Batteries Synthesized by Sol – Gel Technique

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*Department of Physics, SRM University, Vadapalani Campus, Chennai - 600026*

**Abstract**

The CoFe2O4, AlCoFeO4 and Ba0.5CoFe1.67O4 anode materials for advanced lithium storage have been prepared by a Sol-gel technique. The Compounds under investigation were synthesized and the effect of doping on the structure and microstructure has been analyzed using Powder X-ray Diffraction, Scanning Electron Microscopy and energy dispersive X-ray spectroscopy. The substitution of small quantity of dopant (Al3+ and Ba2+) in place of Fe3+ slightly shifts the diffraction peaks of CoFe2O4 towards the lower and higher angle respectively. Comparing the SEM images of CoFe2O4, AlCoFeO4 and Ba0.5CoFe1.67O4, the grains of AlCoFeO4 are fused more than other compounds proves that the conductivity will be increased by replacing Fe3+ by Al3+ in CoFe2O4. Hence this behavior can be helpful in reduction and oxidation of metal nanoparticles which in turn can enhance the capacity of anode material. The EDS values of CoFe2O4, AlCoFeO4 and Ba0.5CoFe1.67O4 confirms the presence of Co, Fe, O, Al and Ba elements in the corresponding samples. Pure and composite ferrite Aluminum as anode materials in the form of nanoferrites have large surface area can give improved battery performance at high current rate. These compounds demonstrates the great potential for applications in energy storage. The synthetic effects of all components result in the enhancement of lithium storage performance through accelerating the electron/ion transfer and increasing the structural and interfacial stability.

# A Study on Thermal, Acoustic and Optical Properties of Disodium Tartrate

**M.Sathish[1], K.Vadivel[2], A. Antony Lawrence[3] and M. Marshal Arunkumar[3]**

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[2]*Thiru Kolanjiappar Government Arts College, Virudachallam.*

[3]*Joseph Arts and Science College, Villupuram.*

**Abstract**

Viscosity studies are performed in aqueous solution of Di-Sodium tartrate in the concentration range of 2% to 20% at different temperatures 303K, 308K, 313K and 318K. In this case, the relative viscosity increases with the increase in concentration and decreases with the increase in temperature. For all the systems, the relative viscosity is minimum at lower concentration (2%) and at a higher concentration range (20%) it is maximized. It may be due to more frictional force developed between the layers of the solution. The activation energy increases with increase in concentration. The activation energy is minimum at 2% concentration and maximum at 20% concentration. From this, it may be concluded that more energy is required to move the molecules inside the structure with increase in concentration. The density results show a uniform increase with the increase in concentration of aqueous solutions of Di-sodium tartrate at 303 K. Refractive index studies are performed for Disodium tartrate in water in the concentration range of 2% to 20 % at 303K. It is observed that the refractive index increases with the increase in concentration. The intermolecular free length for aqueous solutions of Disodium tartrate decreases with the increase in concentration. The classical absorption coefficient for aqueous solutions of Disodium tartrate increases gradually with the increase in concentration.

**Keywords:** Di-Sodium tartrate, free length, relative viscosity.

**SYMP- 13**

# Template Synthesis and Characterization of Transition Metal Complexes of 13-Membered Tetraamide Macro Cycle 11,13-Dimethyl-1,4,7,10-Tetraazacyclotrideca-4,6,10,13-Tetraene-5,6-Diol

**B. Vimala[1] and Selvan[*2]**

*[1]Department of Chemistry, Mother Teresa Women's University, Kodaikanal*

*[*2]Department of Chemistry, Government Arts College for Women, Nilakottai*

**Abstract**

Metal complexes with open coordination sites have found wide use in molecular recognition. They serve as binding sites in the development of chemosensors, to study metalloenzyme function in bioinorganic chemistry, or to direct supramolecular self-assembly. Lewis-acidic metal complexes can target a large variety of Lewis basic functional groups, which makes them very suitable for the design of synthetic receptors. Coordination to metal ions occurs typically with large enthalpies compared to those for hydrogen bond formation, salt-bridges, or dipole-dipole interactions. This gives the opportunity to study molecular recognition and self-assembly in solvents competing for binding, such as water, using coordinatively unsaturated metal complexes as binding sites. Synthesis of multidentate macrocyclic ligands by the metal template method has been recognized as offering high-yielding and selective routes to new ligands and their complexes.

The present investigation achieves the Template Synthesis and Characterization of series of Transition Metal Complexes of 13-Membered Tetraamide Macro Cycle 11,13-dimethyl-1,4,7,10-tetraazacyclotrideca-4,6,10,13-tetraene-5,6-diol with metals of Cu, Co, Ni, Mn and Zn, and all the newly synthesized complexes are subjected to the detailed experimental analysis by governing their characteristic features and structural elucidation.

**Keywords:** Coordination complexes; Macrocyclic ligand; Schiff-base macrocyclic complexes; polyazamacrocycles.

**SYMP- 14**

# A biological approach for synthesis of copper oxide nano particles by fenugreek *( Trigohella sp.L)* leaf extract and its antibacterial activity

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*[2]Department of Physics, DG Govt Arts College, Mayiladuthurai, Tamilnadu,*

*[3]Department of Engg Physics, FEAT, Annamalai University, Annamalainager, Tamilnadu*

**Abstract**

The present investigation, the development of copper oxide nano particles (CuO Np) from leaf extract of fenugreek where copper oxide acts as the precursor. The X -ray diffractio (XRD) analysis shows that the crystalline structure, functional groups of the samples were identified by using Fourier Transmission Infrared (FT-IR) Spectroscopy. Their shape, structure and composition were assessed by Scanning Electron Microscopy (SEM) and energy dispersive spectroscopy (EDX). The results indicated that synthesized CuO Nps were spherical shape with particles size 20 to 30 nm. The presence of flavonoids and their interaction with the CuO Nps were confirmed using FT-IR. Antibacterial activities of the CuO Nps were studied against pathogenic gram positive Staphylococcus (S.aureus) and gram negative Escherichia coli (E. coli).

**SYMP- 15**

# A Study on Thermal, Acoustic and Optical Properties of Disodium Tartrate

**M.Sathish[1], K.Vadivel[2], A. Antony Lawrence[3], and M. Marshal Arunkumar[3]**

*[1]St.Joseph College of Arts and Science (Autonomous), Cuddalore.*

*[2]Thiru Kolanjiappar Government Arts College, Virudachallam.*

*[3]Joseph Arts and Science College, Villupuram.*

**Abstract**

Viscosity studies are performed in aqueous solution of Di-Sodium tartrate in the concentration range of 2% to 20% at different temperatures 303K, 308K, 313K and 318K. In this case, the relative viscosity increases with the increase in concentration and decreases with the increase in temperature. For all the systems, the relative viscosity is minimum at lower concentration (2%) and at a higher concentration range (20%) it is maximized. It may be due to more frictional force developed between the layers of the solution. The activation energy increases with increase in concentration. The activation energy is minimum at 2% concentration and maximum at 20% concentration. From this, it may be concluded that more energy is required to move the molecules inside the structure with increase in concentration. The density results show a uniform increase with the increase in concentration of aqueous solutions of Di-sodium tartrate at 303 K. Refractive index studies are performed for Disodium tartrate in water in the concentration range of 2% to 20 % at 303K. It is observed that the refractive index increases with the increase in concentration. The intermolecular free length for aqueous solutions of Disodium tartrate decreases with the increase in concentration. The classical absorption coefficient for aqueous solutions of Disodium tartrate increases gradually with the increase in concentration.

**Keywords:** Di-Sodium tartrate, free length, relative viscosity.

# Synthesis, Characterization of Novel 2-((2- (benzothiazol-2-yl)hydrazono)methyl) naphthalen-1-ol (NBS) and its application for Sensing of Fluoride ions

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**Abstract**

Acid catalyzed naphthalene based chemosensor 2-((2-(benzothiazol-2-yl)hydrazono) methyl) naphthalen-1-ol (NBS) was synthesized (Scheme 1) by taking 2-hydroxy benzaldehyde and 2-hydrazinylbenzothiazole as a starting materials and the product was characterized utilizing analytical techniques namely FT-IR, NMR, Mass spectrometry, UV-Visible spectroscopy. The compound **3** utilized as colorimetric chemosensor for selective sensing of fluoride ions. The particular sensing of fluoride ion is naked eye with a dissimilar colour variation. Fluoride ion sensing mechanism has been studied by UV-visible and $^{1}$H NMR titration investigations. The $^{1}$H NMR titration data describes that deprotonation of OH and N-H protons by $F^-$ as an obvious stage in the sensing of fluoride ion. Furthermore, the studies was also carried out for reproduction of deprotonated **3** utilizing trifluoroacetic acid as protonating agent. Furthermore, synthesized NBS were also coated with XAD-7 beads and subjected to the fluoride ion sensing.

**Keywords:** NBS, Fluoride Sensing, UV-visible spectroscopy, NMR titration.

# Thin Films

**THFP – 1**

## The Effect of Thickness on Structural, Optical and Electrical Properties of Nickel Oxide Thin Films Prepared by A Low-Cost Sol-Gel Spin Coating Technique.

**S. Anusha[1], Dr. C. J. Sreelatha[1]*, G. Ravindher[1] and P. Chandu[1]**

*[1]Department of Physics, Kakatiya University, Warangal, Telangana state.*

**Abstract**

Nickel oxide is the one of the best material for fabricating electrical devices. Nickel Oxide thin films were synthesized on a glass substrate by a spin coating method at 3000 rpm. The nickel acetate tetra hydrate Ni(Ac)2 .H2O use starting precursor and monoethanolamine (MEA) was added as catalyst. These deposited films were pre-heated at 150$^{O}$c for 10min and then annealed in air at 400-700$^{O}$C temperatures. The coated films were analyzed by XRD, UV-Vis-NIR, SEM, EDX, and Raman Spectroscopy. SEM and EDX studies confirmed the surface and the elemental analysis of the prepared films. The crystalline sizes of films increase with film thickness. X-ray diffraction studies confirmed the polycrystalline structure of Nickel oxide. The spectral studies were recorded by Raman spectroscopy. Electrical properties studied by four probe method. The thin film sheet resistance and resistivity were increased with increasing film thickness. Optical properties such as transmission, absorption, and band gap analysis were done by UV-Vis-NIR spectroscopy technique for different thickness of Nickel oxide thin films. The transmittance of films will decrease as the thickness of films increasing.

**THFP – 2**

# Studies on Structural, Optical and Magnetic Properties on Influence of Carbon Content in $Sno_2$

**S. Ashok[1], E. Priyadharshini[2] and S. Srinivasan[3]**

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*St. Peter's Institute of Higher Education and Research, Avadi, Chennai – 54, Tamilnadu*

*[2,3]Department of Physics, Presidency College, Chennai, 600005, Tamil Nadu*

**Abstract**

In the present work, pure and carbon doped $SnO_2$ was synthesized by hydrothermal method. The prepared samples were thermally treated at various temperatures (400,450,500°C) for 3 hours. The $SnO_2$ nano powders were structurally, optically and magnetically characterized by XRD, UV-Visible and VSM analysis separately. From XRD, the $SnO_2$ nano particle belonging to tetragonal crystal structure with space group ($P4_2/mnm$ 136) was identified with the lower cut off wavelength. Transparency and energy gap values were determined from UV-Visible spectral measurements. Magnetic properties of the $SnO_2$ were studied using VSM technique. The present work focused on investigates the structural, optical and magnetic properties of pure and carbon doped $SnO_2$ nano powder prepared by hydrothermal method. The X-ray diffraction analysis shows the rutile phase tetragonal crystal structure. The crystallite sizes were calculated using Scherer formula for the various peaks obtained in the XRD pattern. The energy gap values are calculated by using UV-Visible spectral analysis. The ferromagnetic properties of pure and carbon doped $SnO_2$ nano powder was analyzed with VSM measurements.

**THFP – 3**

## Opto-Electrical Properties of Cuo Thin Film Prepared by JNS Pyrolysis Technique

**N. Jhansi[1], K. Mohanraj[1, 2], R. Raman[1] and D. Balasubramanian[1*]**

*[1*]Raman Research Laboratory, PG & Research Department of Physics, Government Arts College, Tiruvannamalai-606603*

*[2]Department of Physics Graduate Institute of Photonics, National Changhua University of Education, Changhua 500, Taiwan.*

**Abstract**

CuO thin films are prepared at different substrate temperatures such as 300, 400, 500 and 600˚C using JNS pyrolysis technique. The XRD result reveals that the synthesized sample possesses polycrystalline nature with monoclinic phase and it depicts that the crystallite size varieswith the substrate temperature. UV-Visible spectrometer is used to record the transmittance spectrum. The Tauc's relation is used to calculate the bandgap of CuO and it is found that the bandgap depends on substrate temperature. The SEM image showsthat theparticles are agglomerated together and form a golf ball-like structure. The EDS results confirm the presence of Cu and O. The dependence of electrical conductivity with the substrate temperature has also been studied.

**Keywords:** CuO thin films, JNS pyrolysis, electrical conductivity.

**THFP – 4**

# Investigations on Dielectric Measurement and Electronic Spectroscopic Analysis of Vermiculite

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**Abstract**

Vermiculite is a hydrated magnesium-aluminium-iron silicate. It has been used as a refractory material, especially as liner or coating material in the boilers, which are at very high temperatures. The present work is aimed to make an investigation with reference to its insulating property with the raw and exfoliated form of vermiculite. The dielectric measurements were carried out to analyze the insulating property of raw and exfoliated vermiculite samples. It is observed that dielectric constant and dielectric loss of vermiculite decrease with increase in frequency. The UV-Visible-Diffused reflectance technique is used to analyze the band gap energy of the raw and exfoliated vermiculites. It is noted that there is an increase in the insulating property of the exfoliated vermiculite as compared to that of raw vermiculite.

**THFP – 5**

# The First Recyclable, Nanocrystalline Cds Thin Film Mediated Eco-Benign Synthesis of Hantzsch 1, 4 Dihyropyridines, 1, 8-Dioxodecahydroacridine and Polyhydroquinolines Derivatives.

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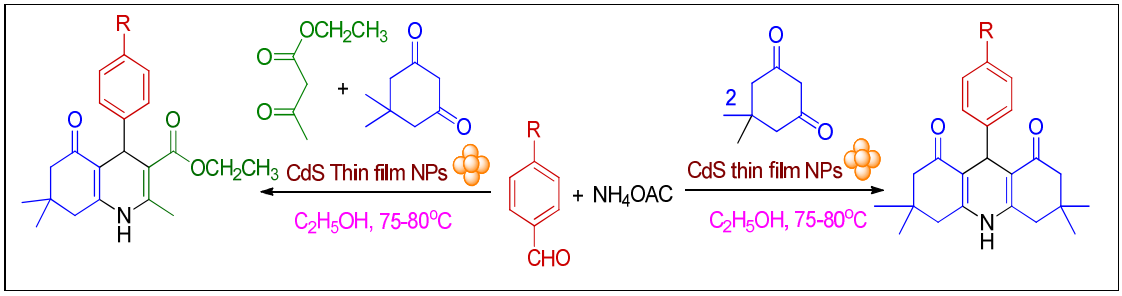
*[1*]PG & Research Department of Chemistry, Arignar Anna Govt.Arts and Science College, Cheyyar.*

*[2]PG & Research Department of Physics Arignar Anna Govt.Arts and Science College, Cheyyar*

*[3]Department of Chemistry, B.S Abdur Rahman Crescent Institute of Science and Technology, Vandalur, Chennai*

**Abstract**

In the present study, we report a recyclable, nanocrystalline CdS thin film mediated efficient one-pot, three component synthesis of Hantzsch 1, 4 Dihydropyridine in good yields. The catalyst is also effective for the efficient synthesis of Polyhydroquinoline and 1, 8-dioxodecahydroacridine derivatives in good to excellent yields. The CdS thin film catalyst was prepared by chemical bath deposition (CBD) technique. The cadmium sulphide thin film was characterized by powder XRD and FT-IR studies. The average crystallite size (D) was calculated from powder XRD by using Scherrer formula and SEM analysis. The elemental composition of the CdS thin film was established by EDS analysis. The effect of temperature, substituent's, catalyst loading and mole ratio on the reaction was also studied. All the products were thoroughly characterized by $^{1}$H-NMR, $^{13}$C-NMR, FT-IR, Mass spectral and CHN analysis. A plausible mechanism for the CdS thin film catalysed synthesis of 1, 4 DHP's is proposed. The heterogeneous catalyst could be easily recovered from the reaction mixture and successively reused at least five times without loss of activity.



**THFP – 6**

# Synthesis of Cadmium Sulphide (Cds) Thin Films by Chemical Spray Deposition Technique and Its Characterization

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*Department of Physics, Periyar Maniammai Institute of Science & Technology, Vallam, Thanjavur.*

**Abstract**

Cadmium Sulphide is a n-type semiconductor and it is perfectly suitable for a window layer in thin films based solar cells due to its desirable electrical and optical properties. CdS thin films have been coated on glass substrate around $300^0$C by spray pyrolysis technique. Cadmium acetate and Thiourea in different concentrations were used as precursors. The fabricated films are characterized by various methods. Their structural properties were studied by X-ray diffraction, morphological properties are studied by SEM, and optical studies determined by UV-VIS spectrometry.

**Keywords**: CdS, Spray pyrolysis, XRD, SEM-EDAX, UV-VIS.

**THFP –7**

# Effect of Concentration of Cadmium Acetate and Thiourea on the Formation of Cds Thin Films and Their Characterization

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*[3]Department of Physics, Karunya Institute of Science and Technology, Coimbatore*

**Abstract**

CdS thin films were deposited on the glass substrate for five different molar concentrations of precursor using spray pyrolysis technique. For the thin film preparation, different precursor concentrations (0.025M, 0.05M, 0.1M, 0.15M and 0.2M) of cadmium acetate with equimolar concentration of thiourea were dissolved in 20 ml of double distilled water. Well cleaned glass substrates were placed on the heater and the distance between the tip of the nozzle and surface of the substrate was maintained at 18 cm. A constant flow rate of 3 ml/min was maintained for all the samples to be deposited on substrates maintained at 400°C. The precursor molar concentrations of 0.025M, 0.05M, 0.1M, 0.15M and 0.2M have been named as PC1, PC2, PC3, PC4 and PC5, respectively. The films were characterized by structural and optical properties. The cubic phase of CdS thin film has been observed by XRD analysis. The SEM images show that PC3 has better uniformity with minimum defects in the deposition of thin films. The optical band gap was measured to be in the range of 2.16-2.43 eV. Photoluminescence spectra show that the emissions are at 518-525 nm. The thin film of PC3 sample has finite emission property beyond which there is a broad emission in the green region. It is concluded that, PC3 is the optimum precursor concentration for the better structural and optical properties of CdS thin films.

**Keywords:** Cadmium sulphide; Spray pyrolysis; Morphology; VSM

# Judd-Ofelt analysis and luminescence studies on $Dy^{3+}$ -doped different Phosphate glasses for white light emitting material applications

**B. Nagaraja Naick[1], S. Damodaraiah[2] and Y.C. Ratnakaram[2*]**

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## Abstract

This article reports detailed analysis of trivalent dysprosium ($Dy^{3+}$) doped alkali and alkaline earth phosphate glasses prepared by melt quenching technique. From X-ray diffraction (XRD), Scanning electron microscope (SEM) and $^{31}P$ solid-state Nuclear Magnetic Resonance (NMR) spectral investigations, the structural properties have been evaluated. The optical absorption spectra of these $Dy^{3+}$ doped phosphate glasses have been analyzed and discussed using Judd-Ofelt (J-O) theory and intensity parameters ($\lambda$= 2, 4, 6) have been evaluated. Different radiative parameters such as radiative lifetimes ($\tau_R$), branching ratios ($\beta r$) and emission cross sections ($\sigma_P$) have been calculated in all the alkali and alkaline earth phosphate glasses and compared. Emission from $^4F_{9/2}$ state has been identified and the measured lifetimes have been obtained from the decay curves and compared with calculated lifetime values. The CIE chromaticity co-ordinates have been measured from the photoluminescence spectra. Hence the obtained results suggest that the present $Dy^{3+}$ -doped glass matrices are potential candidates for yellow and white light emission applications.

**THFP – 9**

## The Kinetic Mechanism of Single-Step Electrochemical Deposition of $Cuinse_2$ Thin Film

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**Abstract**

Photovoltaic power generation has been emerged as a very important non-conventional energy source. Copper indium selenide ($CuInSe_2$) is a ternary semiconductor compound offering good possibilities for thin film photovoltaic applications because it has a direct energy gap of 1.02 eV. The benefits electrochemical deposition can provide are convenient and inexpensive production of large are solar cells, utilizing a technology readily adaptable to industrial production. In the present work describes thermodynamics and kinetics constituent of the electrochemical deposition mechanism of $CuInSe_2$. It will be shown that the mechanism of $CuInSe_2$ phase formation goes through a number of consecutive reactions. The formation of Cu + In + Se phases proceed the assimilation $CuInSe_2$ compound formation. Under the conditions of electrochemical deposition all three elements in the one-step electrochemical deposition process, the formation of Cu + Se and In + Se phases are controlled by diffusion of selenium and also the insertion of indium based phases into the film depends on the applied potential. This work describes associated model used to determine the fluxes of copper, indium and selenium species to the cathode and relative concentration of deposited solid phases.

**THFP – 10**

# Structural and Luminescence Properties of Mn2+ Ions Doped Calcium Strontium Borophosphate Glasses

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**Abstract**

Calcium strontium borophosphate glasses doped with Mn2+ ions and borate and phosphate as variable were prepared using conventional melt quenching technique. XRD and FTIR studies revelaed the amorphous nature.he structure of obtained glasses were examined by means of use: X-ray diffraction (XRD) and fourier transform infrared (FT-IR). XRD analysis confirmed amorphous nature of glass samples. The doping of Mn2+ ions(1– 5mol%) shows no significant changes in FTIR spectra. Optical properties were studied by measuring the near infrared photoluminescence (PL) spectra. These glasses exhibited green emission peak (582 nm) which is assigned to a transition from the upper 4T1g ->6A1g ground state of Mn2+ ions. The decay curves of 4T1g level were examined and found in agreement with the reports that they are strongly depend on Mn2+ concentrations. These glasses have to be studied further for their potential applications as luminescent optical materials.

**Keywords:** Borophosphate glass FT-IR Luminescence properties

**THFP – 11**

## Studies on some physical Properties of $Mn^{2+}$, $Ni^{3+}$, $Co^{2+}$ doped bioactive glasses.

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**Abstract**

The results of spectroscopic, thermal, optical, dielectric and ac conductivity properties of Mn2+, Ni 3+ and Co 2+ ions doped bioactive glasses in the chemical composition of Na2O-LiBr-CdO-B2O3-P2O5 glasses. For these glasses, absorption spectra have been measured in the (UV-Vis-NIR) region and are analysed. From XRD profiles, the amorphous nature of the doped glasses has been confirmed. EPR sprectra were recorded and the studies agreee with the reported spectra at room temperature. The spectra were assigned and analysed. Glass transition temperature (Tg) and crystallization temperature (Tc) are evaluated using DSC data. The dielectric constant and dielectric loss, ac conductivity (σac) and electrical modulus were reported at the room temperature in the frequency range of 1 Hz to 1 M Hz. It is found that the dielectric properties are decreasing as the ac conductivity increases with an increase in frequency variation because of hoping of electrons between different valence states. As reported earlier, the high value of dielectric constant at low frequencies could be due to space charge polarization. It is noticed that the transition metal (Mn2+, Ni 3+ and Co 2+) ions separately exhibited paramagnetic behaviours in the reported glass matrix.

**Keywords:** Bioactive glasses; EPR, DSC, FTIR, XRD, dielectric studies

**THFP – 12**

# Bioactivity of Strontium Doped Boro-fluoro/Choloro-phosphate Disordered Glasses

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**Abstract**

Bioactive glasses with composition Na2O-LiF-SrO-CaO-B2O3-P2O5 and Na2O-LiCl-SrO-CaO-B2O3-P2O5 were prepared by the traditional melt-quench method. Bioactive glasses are able to bond to bone by forming hydroxyl carbonate apatite layer on their surfaces. The in vitro bioactivity test was conducted on the prepared glass samples by using simulated body fluid (SBF), which confirms the formation of hydroxyl carbonate apatite layer on the glass samples. X-ray diffraction (XRD) characterization showed the amorphous nature of glasses. For surface morphology the prepared glasses have been characterized by Scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) confirmed the formation of hydroxyl carbonate apatite layer formation.

**Keywords:** Bioactive Glass; Strontium; Simulated body fluid; Borophosphate glass; in vitro

**THFP – 13**

# Fabrication and Characterisation of Poly (Vinyl Alcohol) / Methyl Cellulose / Graphene Oxide Nanosheets

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**Abstract**

Poly (vinyl alcohol) (PVA), PVA/Methyl cellulose (MC) and PVA/MC/graphene oxide (GO) films were prepared by solution casting method. The prepared composites were characterized by infrared spectroscopy (ATR-FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM). Mechanical properties of the composite were also studied. ATR-FTIR investigation indicated that hydrogen bonding existed between the interface of GO and PVA-MC. Scanning electron microscopy and X-ray diffraction analysis showed that GO was uniformly dispersed in PVA-MC matrix. The tensile strength of the neat PVA film, PVA/MC composite, and PVA/MC/GO film were studied. Introducing MC into PVA caused a significant improvement in tensile strength than pure PVA and incorporating GO into PVA/ MC matrix led to a further increase. These findings suggested that the developed composite possess the prerequisites and can be used in the water treatment.

**Keywords:** Poly (vinyl alcohol), methyl cellulose, graphene oxide nanosheets.

**THFP – 14**

# Effect of $Na_2O$ on the Elastic and Thermal properties of $B_2O_3$–CdO– $Na_2O$ glasses

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**Abstract**

Glasses in the system $60B_2O_3$–(40-x) CdO– $xNa_2O$ with different $Na_2O$ contents (0, 3, 6, 9 and 12 mol %), have been prepared by standard melt quenching technique. Elastic properties, DTA studies have been employed to study the effect of $Na_2O$ on the structure of the prepared glass system. The absence of Bragg's peaks and presence of broad hump in the XRD pattern confirms the amorphous and homogeneous nature of the prepared glass samples. Density and ultrasonic velocity (shear and longitudinal velocity) of all the glass samples was measured using Archimedes principle and pulse echo overlap techniques respectively. Elastic properties, Poisson's ratio and microhardness have been calculated using ultrasonic velocity and density. The variations of above parameter with respect to the composition are analyzed in terms of structural changes in the glass network. The results of the glasses reveal that the borate network consists of $BO_3$ and $BO_4$ units and is affected by the increase in the concentration of $Na_2O$ content.

**Keywords:** XRD, DTA, Ultrasonic velocity

**THFP – 15**

# FTIR, Morphology and Thermal Stability Studies of Lithium Doped Cadmium Borate Glasses

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**Abstract**

Using standard melt-quench technique, lithium doped cadmium borate glasses having composition $60B_2O_3$ - (40- x) CdO - $xLi_2O$ (Where x = 3, 6, 9 and 12 mol %) are prepared. The amorphous nature of the sample was confirmed by XRD measurement. Studies of structural and thermal properties have been carried out for different compositions, in order to understand the effect of lithium oxide on the structure of cadmium borate glasses. The results of the infra red spectra indicate that boron exist in both $BO_3$ and $BO_4$ units and no boroxol ring formation takes place in the structure. The morphology of the samples were studied from SEM analysis. The samples in bulk form are subjected to differential thermal analysis (DTA) to assess the glass transition temperature (Tg), crystalline temperature (Tc) and melting temperature(Tm). The results suggest that the structure is modified by the substitution of $Li_2O$.

**Keywords:** XRD, FTIR, SEM, DTA.

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