



# EASWARI ENGINEERING COLLEGE

(AUTONOMOUS)

25<sup>th</sup> YEARS  
INSPIRING YOU  
TOWARDS EXCELLENCE  
& A BRIGHT FUTURE  
ITS STARTS NOW... ITS STARTS HERE...

## INTERNATIONAL VIRTUAL CONFERENCE ON MATERIALS RESEARCH (IVCMR- 21)

26<sup>th</sup> & 27<sup>th</sup> August 2021

## BOOK OF ABSTRACTS

Organised by:

Department of Physics  
EASWARI ENGINEERING COLLEGE  
Ramapuram, Chennai- 600 089.



**INTERNATIONAL VIRTUAL CONFERENCE  
ON  
MATERIALS RESEARCH  
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*Organised by*  
*Department of Physics*  
*Easwari Engineering College(Autonomous)*  
*Ramapuram, Chennai - 600 089*  
*Tamil Nadu , India*  
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## **PREFACE**

**EASWARI ENGINEERING COLLEGE (AUTONOMOUS)**, a unit of SRM Group of Educational Institutions for higher learning was instituted in the academic year 1996-1997 and is one of the leading Engineering colleges in Tamil Nadu which is affiliated to Anna University, Chennai. The college offers eleven Under-Grauate and six Post-Grauate Programs covering Engineering & Technology and Management. The college has a strong Industry-Interaction with reputed National and International organizations.

The Department of Physics is conducting a two days **International Virtual Conference on Materials Research (IVCMR - 21)** on 26<sup>th</sup> – 27<sup>th</sup> August 2021. The discovery and development of new materials represent a national core competency that is essential for scientific progress and long-term economic growth. The search for new or advanced materials is driven by need to improve existing technologies based on novel functionalities of materials. Virtually every technology is material limited. The conference will provide an opportunity for the young researchers to have interactions with eminent scientists from all over India in a single platform and it focuses on new perspectives to identify new challenges and breakthroughs in the field.

In this conference 08 invited talks will be delivered and 80 papers will be presented for discussions.

The faculty members of Physics department express their sincere thanks to Chairman – Ramapuram and Trichy campus, Co-Chairman, Chief Director, Director, Principal and Vice-Principal for their inspiration, support and guidance.

Also the organizing committee thanks all the invited speakers, authors and participants of **IVCMR - 21** for their fullest cooperation for the successful conduct of the conference.

*With Regards*

**Dr. S. Nirmala**  
*Convener*  
**IVCMR-21**

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# SRM Group of Educational Institutions



**Dr. R. Shivakumar, M.D.,**

## CHAIRMAN'S MESSAGE

I am glad that the Department of Physics, Easwari Engineering College (Autonomous) is organizing International Virtual Conference on Materials Research (IVCMR-21) on 26<sup>th</sup> and 27<sup>th</sup> August 2021.

Rapid advances in technology have dramatically increased the importance of materials science and engineering to society. The prominent change in materials science during the last two decades is active usage of computer simulation methods to find new compounds, predict various properties, and as a result design of new materials. Materials science underpins every product and process on which our modern society depends and you cannot make it without materials. Continued progress in all aspects of technology relies on proper education of materials scientists and engineers and active progress in materials research and development.

I am confident that this conference will provide an excellent platform for the research scholars to engage in healthy deliberation and exchange their ideas with one another.

I extend my full support and wish this conference all success.

*R. Shivakumar*

**CHAIRMAN**  
SRM Ramapuram & Trichy Campus

---

No. 50, Bharathi Salai, Ramapuram, Chennai - 600089, Phone: +91 4392 3256 / 3098



## SRM Group of Educational Institutions



Mr. S. Niranjan, M.S.,

### Co-Chairman's Message

It is very gratifying to note that the Department of Physics, Easwari Engineering College [Autonomous] is organizing an [IVCMR 2021] **International Virtual Conference on "Materials Research"** on the 26<sup>th</sup> and 27<sup>th</sup> of August 2021.

Material Scientists and Engineers not only engage themselves in developing materials for new applications but also strive to improve the existing materials to enhance their performance by making the materials useful and valuable that can benefit the society. This continuous development of new materials has promoted the growth of innovative industrial sectors whose productive activities have solved many a real world problem and a harbinger to the progress of technology.

I am sure the erudite discussions among eminent Scientists and Researchers will provide a pathway in the development of Science and Technology.

I am extending my Best Wishes to all the members of the Organising Committee to make this conference a grand success.

A handwritten signature in black ink, appearing to read 'N. S.' followed by a stylized surname.

Co-Chairman

SRM Ramapuram & Trichy Campus

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No. 50, Bharathi Salai, Ramapuram, Chennai - 600089, Phone: +91 4392 3256 / 3098



# EASWARI ENGINEERING COLLEGE

(AUTONOMOUS INSTITUTION)

A Unit of SRM Group of Educational Institutions & Run by Valliammai Society  
Approved by AICTE & Govt. of Tamil Nadu, Affiliated to Anna University Chennai, ISO 9001:2015 Certified  
Bharathi Salai, Ramapuram, Chennai - 600 089.



**Dr.R.S.KUMAR**  
B.E (Hons.), M.Tech., Ph.D., FIE  
Principal

17-07-2021

## MESSAGE FROM PRINCIPAL



I am happy that the Physics Department, Easwari Engineering College (Autonomous) is organizing International Virtual Conference on Material Research (IVCMR-21) on 26<sup>th</sup> and 27<sup>th</sup> August 2021.

Materials are of the utmost importance for engineers, as the usage of the appropriate materials is crucial when designing systems. As a result, materials science is an increasingly important part of an engineer's education. With the development of Science &Technology, new materials appear and are widely used all over the world, and they give tremendous impetus to product design. I hope the conference will describe how these new materials affect the product design and discusses about the development of new materials and their applications in some typical products like nano materials, ceramic materials, green materials, composite materials and functional materials.

I congratulate the Head of the Department of Physics and her team of faculty members for their efforts in organizing this International Virtual Conference.

I also wish them all the best in making this event a grand success.

  
**PRINCIPAL**

Ph.: 044 - 4392 3041, 4392 3100, 2249 1130, 2249 0853  
principal@eec.srmrmp.edu.in Web : [www.srmeaswari.ac.in](http://www.srmeaswari.ac.in)

## PROGRAM SCHEDULE

	TIME	PROGRAMME
<b>DAY 1 : 26.08.2021 - Thursday</b>		
	<b>9.45 am - 10.00 am</b>	<b>Inaugural Function</b> <b>Chief Guest : Dr. Sulekha Chattopadhyay , Ph.D</b> California Public Utilities Commission
<b>Session 1</b>	<b>10.00 am -11.00 am</b>	<b>Invited Talk: 1</b> <b>Dr. Sulekha Chattopadhyay , Ph.D</b> California Public Utilities Commission <b>Title : Environmental policies and emerging Technologies</b>
<b>11.00 am - 11.20 am</b>		<b>Tea Break</b>
<b>Session 2</b>	<b>11.20am - 12.20pm</b>	<b>Invited Talk: 2</b> <b>Prof. G.Vaitheeswaran</b> Advanced Centre of Research in High Energy Materials , University of Hyderabad.  <b>Title : Computational study of energetic solids under hydrostatic pressure</b>
<b>12.20 pm - 1.30 pm</b>		<b>Lunch Break</b>
<b>Session 3</b>	<b>1.30 pm - 2.30 pm</b>	<b>Invited Talk: 3</b> <b>Dr. Mohd Taazeem Ansari</b> Department of Applied Sciences & Humanities, Jamia Millia Islamia, New Delhi, India  <b>Title : Quantum simulation of Miniaturized nano components using graphene, GNRs, CNTs, and Allied Materials for electronic devices as well as sensing applications</b>
<b>Session 4</b>	<b>2.30 pm - 4.00 pm</b>	<b>Paper Presentation</b> <b>( Abstract ID from MR 001 to MR 055)</b>
<b>Session 5</b>	<b>4.30 pm - 5.30 pm</b>	<b>Invited Talk: 4</b> <b>Prof. Christopher Shuck, Ph.D</b> Department of Materials Science & Engineering A.J. Drexel Nanomaterials Institute (DNI), US  <b>Title : M Xenes: 2D Transition Metal Carbides and Nitrides</b>

## PROGRAM SCHEDULE

	<b>TIME</b>	<b>PROGRAMME</b>
<b>DAY 2 : 27.08.2021 – Friday</b>		
<b>Session 6</b>	<b>9.00 am -10.00 am</b>	<b>Invited Talk: 05</b> <b>Prof. Goutam Chattopadhyay</b> Senior Scientist, NASA – Jet Propulsion Lab, Pasadena, California, US.  <b>Title : Mars Landing and Related Technical Challenges</b>
<b>Session 7</b>	<b>10.00 am -11.00 am</b>	<b>Invited Talk: 06</b> <b>Prof. Bidushi Bhattacharya, Ph.D.</b> TEDx Speaker, Thought Leader, Ex-NASA Astropreneur University of California, Los Angeles  <b>Title : An Overview of Materials and Manufacturing in the Commercial Space Sector</b>
<b>11.00 am - 11.20 am</b>		<b>Tea Break</b>
<b>Session 8</b>	<b>11.20am – 12.20pm</b>	<b>Invited Talk: 07</b> <b>Raghavan Chinnambedu Murugesan</b> ERDF Research Associate Enabling Technologies &Innovation Competences Challenge (ETICC) Aston Institute of Photonic Technologies  <b>Title : 2D Materials for Optoelectronic Applications</b>
<b>12.20 pm – 1.30 pm</b>		<b>Lunch Break</b>
<b>Session 9</b>	<b>1.30 pm - 2.30 pm</b>	<b>Invited Talk: 08</b> <b>Dr. N.Vijayan</b> Principal Scientist BND Division CSIR-National Physical Laboratory New Delhi.  <b>Title : Why precise measurements are important for Scientific research?</b>
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**INVITED TALK – 1****Environmental Policies for Emerging Technologies**

**Dr. Sulekha Chattopadhyay , Ph.D**

*California Public Utilities Commission*

*California*

**ABSTRACT**

To date, technological advances have led to a consistent increase in economic and industrial growth. The thriving transportation and communication sectors have lifted millions out of poverty, and given hope for a brighter future. This should be something to celebrate. However it has come at a very high price for us and more importantly our future generations. The unprecedented demand for energy has made climate change by far the biggest challenge to the very existence of life on earth as we know it. Today, carbon dioxide concentration levels are approximately 414.5 parts per million. As a consequence, we are experiencing increases in the occurrence of wildfires, severe droughts, and flooding.

Fortunately, scientists and engineers are at the forefront of this issue, developing technologies that will support a more sustainable growth in transportation and communication sectors among others. Their success depends on the renewable energy resources that need to become cost-competitive with fossil fuels. This requires a strong, consistent commitment from society which can only be achieved if we can translate the complexities of science and technology into meaningful environmental policies. My talk will explore some of the actions that are being taken in California.

**INVITED TALK – 2****Computational study of energetic solids under hydrostatic pressure****Dr. G. Vaitheeswaran\***

*School of Physics, University of Hyderabad, Hyderabad 500046, Telangana, India,*

\*E-mail: [vaithee@uohyd.ac.in](mailto:vaithee@uohyd.ac.in)

The main requirements of energetic materials are high performance, insensitiveness, eco-friendly nature so that these materials can find tremendous applications in both civil and military sectors. Ammonium Di Nitramide (ADN) is one of the most promising green energetic oxidizers for future rocket propellant formulations. In the present talk, I will discuss the structural, mechanical, and spectroscopic properties of ADN from first-principles theory. The obtained ground state lattice parameters, axial compressibilities, and equation of state are in good accord with the available experimental results. Strength of inter molecular interactions has been correlated using the calculated compressibility curves and elastic moduli. Discontinuities in the structural parameters and elastic constants are observed as a function of pressure. In addition, the computed infra-red(IR) spectra at ambient pressure reveal that ADN is found to have more hygroscopic nature over Ammonium Perchlorate (AP) due to the presence of strong hydrogen bonding. Pressure dependent IR spectra show blue- and red-shift of bending and stretching frequencies which leads to weakening and strengthening of the hydrogen bonding below and above 5 GPa, respectively. The abrupt changes in the calculated structural, mechanical, and IR spectra suggest that ADN might undergo a first order structural transformation to a high pressure phase around 5-6 GPa.

**INVITED TALK - 3****Quantum simulation of Miniaturized nano components using graphene, GNRs, CNTs and Allied Materials for electronic devices as well as sensing applications****Dr. Mohd Taazem Ansari**

*Department of Applied Sciences & Humanities,  
Jamia Millia Islamia, New Delhi, India*

**ABSTRACT**

The present talk is based on describing the electronic transmission and various other application-based perspectives in nano devices involving graphene, graphene nano ribbon (GNR), carbon nanotube (CNT), and Biphenylene network (BPN), etc at room temperature. As electrons propagate between the two electrodes (left electrode (LE) and right electrode (RE)) via a transmission channel in a streamlined manner, it shows negligible interactions with the ions and thus experiences no scattering during its movement from one end to another. This imparts ballistic nature to electron transport at the nano scale since at nanoscale quantum mechanical effect comes into play. The occurrence of ballistic transport gives rise to unique characteristics in nano devices. The transmission spectrum is the first step towards the analysis of possible electron transport through nano devices. It may be calculated at desired specific applied bias voltages, starting at 0 V and going up to 2.0 V. Non-equilibrium Greens function formalism (NEGF) is an effective tool to compute the electron transmission spectrum. It is based on solving the differential equation in the context of the many-body wave function. The corresponding eigen values and eigen functions are obtained by employing the Schrodinger equation. This forms the basis for calculating the transmission coefficient of electrons traveling from source (LE) to drain (RE) respectively. Instead, NEGF formalism in

coordination with density functional theory (DFT) incorporated into python-based programming software termed ATK-VNL tends to be a more efficient and precise computational technique. However, before calculating the transmission coefficient of electrons, the geometry of the device needs to be optimized (i.e., attainment of maximum force acting between the atoms). The maximum attained force desired to be small for obtaining accurate results. Further, the selection of suitable Monkhorst sampling points and exchange-correlation potential (LDA) too accounts for more accuracy.

Moreover, in context to sensing-based perspectives, the parameter to be analyzed is the adsorption energy and charge transfer. Also, for a steady adsorbed structure, a negative magnitude of adsorption energy and charge transfer between the sensing structure and gas molecule is desired. Further, to assist a more accurate sensor in the light of robust quantum mechanical calculations, for a system comprising of a large no of atoms, the simulation cannot be performed on PCs. It requires the use of high-performance computing (HPC), i.e., parallel computing using a computer cluster with commercial modelling and simulation software like the ATK virtual nano lab.

**INVITED TALK – 4****MXenes: 2D Transition Metal Carbides and Nitrides****Dr. Christopher Shuck***Post-Doctoral Researcher**A.J. Drexel Nanomaterials Institute (DNI)**Department of Materials Science & Engineering**Drexel University***ABSTRACT**

2D transition metal carbides and nitrides (MXenes) are an emergent, and potentially the largest, class of 2D materials discovered. MXenes have the general formula,  $M_{n+1}X_nT_x$ , where M is an early transition metal (Ti, Mo, Nb, etc.), X is C and/or N, and  $T_x$  represents the surface functional groups (O, OH, F, Cl, etc.). To date, more than 30 members of this family have been experimentally synthesized. They benefit from high electrical conductivity (up to 20,000 S/cm), tuneable optical properties from the UV to IR, hydrophilic surface, high mechanical strength, and a redox-capable surface. Since their discovery, MXenes have been used in a variety of applications, including electrochemical energy storage, electromagnetic interference shielding, biomedical, environmental remediation, catalysis, etc., with more novel applications being studied daily.

In this talk, I will overview MXenes, how they are synthesized, their properties (optical, electronic, and mechanical), and applications that they've been used in.

**INVITED TALK -5****Mars Landing and Related Technical Challenges****Dr. Goutam Chattopadhyay**

*NASA-Jet Propulsion Laboratory, California Institute of Technology  
4800 Oak Grove Drive, Pasadena, CA 91109, USA.*

**ABSTRACT**

NASA's Jet Propulsion Laboratory, which completed eighty years of its existence in 2016, builds instruments for NASA missions. Exploring the universe and our own planet Earth from space has been the mission of NASA. Robotics missions such as Voyager, which continues to go beyond our solar system, missions to Mars and other planets, exploring the stars and galaxies for astrophysics missions, exploring and answering the question, "*are we alone in this universe?*" has been the driving force for NASA scientists for more than six decades.

Fundamental science questions drive the selection of NASA missions. And to answer some of the fundamental science questions, NASA took multiple trips to the red planet Mars. Mars in its early history resembled a lot like our own planet. Landing on Mars is extremely challenging. In this presentation we will discuss those challenges and the technologies we developed to address them. We will also present an overview of the state of the art instruments that we are currently developing and layout the details of the science questions they will try to answer.

Rapid progress on multiple fronts, such as commercial software for component and device modelling, low-loss circuits and interconnect technologies, cell phone technologies, and submicron scale lithographic techniques are making it possible for us to design and develop smart, low-power yet very powerful instruments that can even fit in a Small Sat or Cube Sat. We will also discuss the challenges of the future generation instruments in

addressing the needs for critical scientific applications. The research described herein was carried out at the Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, USA, under contract with National Aeronautics and Space Administration.

**INVITED TALK - 06****An Overview of Materials and Manufacturing in the Commercial Space Sector**

**Dr. Bidushi Bhattacharya**  
TEDx Speaker, Thought Leader,  
Ex-NASA Astropreneur  
University of California, Los Angeles

**ABSTRACT**

Space technology is a part of our daily lives. Whether it's through satellite-based location services on our smart phones or space-based monitoring of fires and weather, we are becoming more reliant on products and services based in outer space. The advent of AI, combined with the miniaturization of electronics, has led to exponential growth in the space sector, much as the computer industry grew in the 1980's. Commercial Space, "New Space," will be worth \$2 Trillion within 20 years, and the demand for a space-knowledgeable workforce will continue to grow exponentially. What are some potential areas of opportunity? What is the role of the education sector in building this new workforce for the future?

**INVITED TALK-7****2D Materials for Optoelectronic Applications****Raghavan Chinnambedu Murugesan**

*Aston Institute of Photonic Technologies, Aston University, Birmingham B4 7ET, UK*

**ABSTRACT**

Two-Dimensional (2D) materials gained substantial research interest due to their exotic properties, which includes broadband optical response, strong and tuneable light-mater interactions and rapid relaxation dynamics. In this presentation, some of our recent studies on the optical and optoelectronic properties of 2D metal halide hybrid perovskites and transition metal-chalcogenides will be discussed. Growth of phase pure high-quality single-crystals, microstructural features, lasing with tuneable wavelengths, transport properties of 2D hybrid perovskites,  $(BA)_2MA_{n-1}Pb_nI_{3n+1}$  ( $n=1, 2$  and  $3$ ) and transition metal chalcogenides, HfSSe and  $Si_2Te_3$  will be presented

**INVITED TALK – 8****Why precise measurements are important for scientific research?****Dr. N Vijayan**

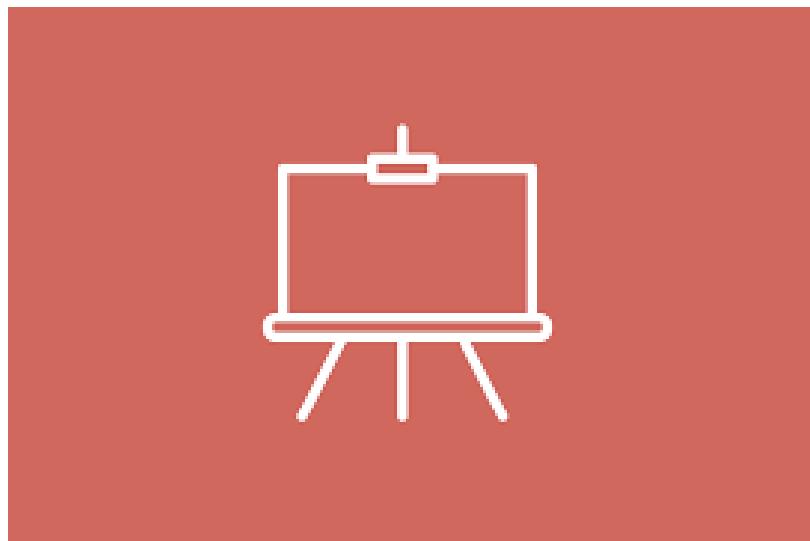
CSIR-National Physical Laboratory, New Delhi – 110 012.

E mail: [nvijayan@nplindia.org](mailto:nvijayan@nplindia.org)

**ABSTRACT**

Accuracy and precision are two main key factors for taking data and to perform scientific measurement. Accuracy signifies how close a measurement is to its actual value. This is essential because bad instrument, poor data processing or human mistake can lead to incorrect results that are not very nearby to the accurate one. Precision is how close a series of measurements of the same thing are to each other. Measurements that are imprecise do not properly identify random errors and can produce a widespread result. In research, new innovations are possible only by doing the accurate and precise measurements. Otherwise the whole research will not be used or considered for the corresponding work. To get accurate and precise results, the instrument to be calibrated by comparing with the reference material. In-House BND group is involved for the development of Indian Reference Materials in the area of sophisticated instruments such as Powder X-ray diffractometer and X-ray Fluorescence spectrophotometer. Powder X-ray Diffraction (PXRD) is one of the most widely used equipments in the country for the structural analysis of materials. However, to record accurate data, reference materials are essential. As of now, reference materials are imported. Measurement data from Powder X-ray diffractometer is not reliable, if the machine is not calibrated by reference materials. In India, many colleges/universities may not be able to afford the cost of imported reference material. The reference materials from CSIR-NPL will cost much less and can be used widely by stake holders like Bruker, Rigaku and Panalytical. Precise and accurate measurements, indirectly helps to improve our scientific outcome and also reflects in countries economy. CSIR-NPL has released  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, an Indian Reference

Material (BND) for the calibration of Powder X-ray diffractometers. The detailed discussion will be given during the conference.



## **CONTRIBUTORY PRESENTATIONS**

## Crystal and Molecular docking studies of 3-hydroxy-2-((2-hydroxy-4, 4-dimethyl-6-oxocyclohex-1-enyl) (4-methoxyphenyl) methyl)-5,5-dimethylcyclohex-2-enone with focal adhesion kinase inhibitors

K S Kiran<sup>a\*</sup>, Chandan R<sup>b</sup>, M.A Pasha <sup>c</sup>

<sup>a</sup>\*Department of physics, Faculty of Engineering and Technology, Jain Deemed to be University, Bangalore, Karnataka, India

<sup>b</sup> Department of physics, Research scholar, Jain deemed to university, Bangalore, Karnataka,

<sup>c</sup> Department of Chemistry, Bangalore University, Bangalore, Karnataka, India.

\*Corresponding author: Email: [kiranphy18@gmail.com](mailto:kiranphy18@gmail.com)

### ABSTRACT

In the present study crystal structure of 3-hydroxy-2-((2-hydroxy-4, 4-dimethyl-6-oxocyclohex-1-enyl) (4-methoxyphenyl) methyl)-5, 5-dimethylcyclohex-2-enone was determined using single crystal X-ray diffraction. Cyclohexane is a non planar molecule the shape of which vaguely resembles a chair. The conformation of cyclohexane molecule is constantly changing, with the atom on the left which is currently pointing down flipping up, and the one on the right flipping down. Further the structural feature was extrapolated to molecular docking studies with focal adhesion kinase (FAK) domain using Autodock to study its anti-cancerous property. The compound exhibited considerable bacterial inhibition of lower to moderate concentrations. We conclude that these derivatives can be used in medicine and have enormous potential as pharmaceutical agents due to their biological activities. The above titled receptor gain functional and structural insights into their mechanism of inhibition and explore its potential as an anticancer agent.

**Keywords:** Bis cyclohexyl diols, Docking, Focal adhesion kinase, anticancer

**Effect of humidity on secondary gamma radiation flux at Udaipur, India****Devendra Pareek***Department of Physics, Bhupal Nobles' University, Udaipur (313001), Rajasthan, INDIA***Corresponding author:** Email: deven.pareek69@gmail.com**ABSTRACT**

To observe the effect of humidity on secondary gamma radiation flux an experimental study was conducted at Udaipur ( $27^{\circ} 43' 12.00''$  N,  $75^{\circ} 28' 48.01''$  E), India on dates September 12, 14, 15, 16, 17 and 18 2020. Data files were stored in the computer for one hour using ground based NaI (Tl) Scintillation detector. The analyzed data showed the variation of secondary gamma radiation flux (SGR) with the presence of humidity in the atmosphere of the earth.

**Key Words:** Cosmic radiation, solar radiation, secondary gamma radiation, presence of humidity in atmosphere of Earth.

## Synthesis of Longest Cr doped Core-Shell Ge/GeO<sub>x</sub> Nanowire for their applications

**Amar S. Katkar**

*Department of Physics, Dr. B.N.P. Arts, Smt. S.G.G. Com. And Smt. S.A.M. Sci. College, Valvan,  
Lonavla,*

**Corresponding author:** Email: [amarkatkar@gmail.com](mailto:amarkatkar@gmail.com)

### **ABSTRACT**

Synthesis of ultralong, low diameter (High aspect ratio) and uniform nanowires could be useful for integration of multiple devices using one nanowire. In the present work simple vapour transport method was used to synthesize ultralong Cr-doped core-shell Ge/GeO<sub>x</sub> nanowires. The conditions such as substrate temperature, precursors and required dopants were optimized for the growth of uniform ultralong Germanium nanowires. After characterizations, the as prepared samples were utilized to investigate electrical and biological applications. The ultralong Cr-doped Ge/GeO<sub>x</sub> nanowires could be very useful in future for the fabrication of electronic and biological devices.

## A Novel Design and Development of an Automated JNSP System to Prepare Zinc doped Copper Oxide thin films for Ag/Zn:CuO/Si Structured Diode Application

**Jagadeesan V \* and R. Sakthivel**

*Department of Electronics, PSG College of Arts & Science, Coimbatore-641014, Tamilnadu,*

**Corresponding author:** Email:: vjpsgcas1@gmail.com

### **ABSTRACT**

Zinc-doped Copper oxide (Zn:CuO) thin films are deposited via well-designed automated jet nebulizer spray pyrolysis (JNSP) system for developing Ag/Zn:CuO/Si structured diode. The system is fitted with a microcontroller-based spray nozzle with an up/down movement to enable thin film deposition in an automated way. Zn:CuO thin films are deposited via an automated JNSP system with 1%, 3%, and 5% doping concentration. The characteristics studies and analysis of Zn:CuO thin films are studied. XRD examination showed that all of the Zn:CuO thin films have a monoclinic crystal structure. Surface morphological analysis of an automated Zn:CuO thin films showed spherical-shaped small grains. It is found that particles are closely packed and well covered. Additionally, elementary composition analysis (EDS) is carried through to finalize the 'Cu', 'O', and 'Zn' atoms in the deposited Zn:CuO materials. The least energy band gap of 1.90 eV and the highest conductivity of  $3.67 \times 10^{-8}$  S/cm is obtained for 3% Zn doped CuO. Based on the characteristics analysis and studies of automated Zn:CuO thin films, Ag/Zn:CuO/Si structured diode have been developed. Various diode parameters have been evaluated under light and dark conditions.

**Keywords:** nebulizer; microcontroller; thin film; junction diode; ideality factor

## Effect of solid state reaction method of luminescence and magnetic properties on ZnO nanoparticles

B.Arunkumar<sup>a</sup>, M.Jothibas<sup>b</sup>, A.Sindhya<sup>b</sup>, S.Johnson Jeyakumar<sup>b</sup>

<sup>a</sup>*Department of Physics, Sir Issac Newton College of Arts & Science, Nagapattinam-611 102, Tamilnadu, India.*

<sup>b</sup>*PG and Research Department of Physics, T.B.M.L. College, Porayar-609 307, Tamilnadu, India.*

**Corresponding author:** Email: bvarun2030@gmail.com

### ABSTRACT

In this work, pure ZnO nanoparticles were prepared by the method of solid state reaction using zinc acetate as a pioneer material. The synthesized ZnO nanoparticles were characterized by the various spectrographic tools. The crystallinity nature and lattice parameters are studied through the XRD patterns and the average crystallite size is found to be 34.5 nm. The absorption peak in the FTIR spectra confirms the presence of functional group, whereas a UV-Vis spectrum is used to determine the optical properties of the sample. Furthermore, surface morphology, electronic structure and the magnetic properties of the ZnO nanoparticles were studied by using the SEM, Photoluminescence and VSM studies respectively. This particular method of synthesis is simple and easiest method to obtain the pure ZnO nanoparticles with high crystallinity in nature. The obtained ZnO, have potential, engineering applications as materials for UV filtering shields with high transparency, luminescent materials without any toxic nature.

## Theoretical Investigation of Advanced Versatile Applications of Cold Spray Coatings in Additive Manufacturing and Repair of Components

**<sup>1</sup> M.Ashokkumar, <sup>2</sup> D.Thirumalaikumarasamy, <sup>2</sup> S. Deepak, <sup>2</sup> M.Mathanbabu and**

**<sup>2</sup> K.Mathivanan**

*<sup>1</sup> Annamalai University, Manufacturing Engg, Chidambaram.*

*<sup>2</sup>Government College of Engineering Bargur*

**Corresponding author: Email:** ashokleadsaero12@gmail.com

### **ABSTRACT**

Cold spray process (CS) comes under the family of thermal spray technology. There are numerous terms to represent the CS as cold gas dynamic spray, kinetic spray, high velocity powder deposition and kinetic energy metallization. In this process the coating is formed in the solid state by impingement of power particle with supersonic velocity on the coupon, below the recrystallization temperature of the coating powder, the unique feature of this process to develop a additive manufacturing (AM) components with free of oxidation when compared with other conventional AM and coating techniques, because it all need high temperature energy source to melt the feedstock coil/powder to develop AM components/coatings. Cold spray additive manufacturing (CSAM) is the powerful and emerging technique in the field of AM, still there are few flaws in this technique, to overcome this problem many researches are going on in CSAM and repair of components to meet the real time applications. This review focuses on summarizing the work done so far in CSAM and repair of components.

## Green extract influence on bis(melaminium)ltartrate 2.5hydrate using green synthesis

Manjula.C\*<sup>2</sup> and S.R.Thilagavathy<sup>1</sup>

*Department of Physics, Jeppiaar Engineering College, Chennai-119, Tamilnadu, India*

*Department of Physics, Easwari Engineering College, Chennai-89, Tamilnadu, India*

**Corresponding author:** Email: manjuks.mk@gmail.com

### ABSTRACT

Bis(Melaminium)L-tartrate 2.5Hydrate was prepared by mixing equimolar ratio of melaminium and tartrate. The above product was mixed with Aloe Barbadensis, Menthaarvensis, Plectranthusamboinicus, Calotropis gigantean extracts. The products obtained from these extracts were analyzed for their Antimicrobial activity. The absorption spectra for different extracts were obtained using UV-vis spectroscopy. The organic functional groups were determined using Fourier Transform Infrared analysis.

**Keywords:** Aloe Barbadensis, Plectranthusamboinicus

## Land and underwater rover using raspberry pi

Nithya S , Vijayalakshmi K , Parimala Devi M

*Department of Electrical and Electronics Engineering, SRMIST, Ramapuram, Chennai.*

**Corresponding author:** Email: nithyas@srmist.edu.in

### ABSTRACT

In the present scenario, the world is focusing on automation to increase efficiency, accuracy and consistency in operations by reducing human error. AOV is an autonomous rover that works automatically without any remote control but the user does not have enough control over the rover once it is designed and programmed. So, to give humans more command over the machine to rectify the error, we propose multipurpose rover that can be used in both land and water. In water, our rover will be controlled by the host ship or from land by a human. The data like water quality, water pressure, depth of the sea, the temperature of the water can be monitored in real time which can be used in numerous applications. The proposed design will be affordable and low maintenance as its structure will be made of PVC pipes and all the sensors will be connected with the Raspberry pi model 3B

**Keywords:** Multipurpose Rover, Automation,

## Influence of Ti on Structural and Morphological properties of ZnO nanoparticles and their Gas sensing activity

N.Nithya<sup>1</sup>, S.Gopi<sup>2</sup>, G.Magesh<sup>1</sup>, A.P.Arun<sup>3</sup>

<sup>1</sup> Department of Physics, PSGR Krishnammal College for Women, Coimbatore- 641004.

<sup>2</sup>Department of Physics, SRMV College of Arts and Science, Coimbatore

<sup>3</sup> Department of Mechanical Engineering, Kumaraguru College of Tech., Coimbatore- 641049.

Email Id: nithyanesakumar@gmail.com

### ABSTRACT

In this report, Pure and Ti doped ZnO nanoparticles were effectively synthesized through easy Co-precipitation method. The synthesized Ti - ZnO NP's were characterized by XRD, FESEM, UV-Vis, FTIR and PL. X-ray diffraction analysis proved the creation of the hexagonal wurtzite structure. The average crystallite size was found to be 25- 30 nm. The FESEM and TEM analysis verified that the sphere-shaped morphology for both ZnO and Ti - ZnO NP's. UV – Visible Spectroscopy confirmed that an increase in the optical bandgap involving the concentration of dopant Ti increases. The bandgap values were found to be 3.57-3.54 eV. FTIR spectra showed that the existence of the characteristic stretching and bending vibrational band of Zn – O bonding at 400-600 cm<sup>-1</sup> and shifts in vibrational bands were noticed for Ti - ZnO NP's. PL spectra of Ti - ZnO NP's at various concentrations show a strong UV emission band. SAED pattern proves the crystalline nature of synthesized samples. EDAX spectra confirm the existence of Ti, O, and Zn and verify that Ti<sup>4+</sup> ions are present in the ZnO lattices. The synthesized samples were investigated for various VOC's gases and the nanoparticles shows highest selectivity for ethanol gas. The response and recovery time were 11s and 9s. The stability was found to be 30 days.

**Keywords:** Ti - ZnO NP's, Structural Properties, Ethanol, Sensing Properties.

**Polyethylene glycol - chitosan incorporated Zinc Oxide nanoparticles with  
NN-Dimethyl  
curcumin as a drug carrier for Antiarthritic application**

**K.Priyadharsini <sup>a,b</sup> , M.Anbucbezhiyan <sup>b\*</sup>**

*a Department of Physics, Tagore Engineering College, Rathinamangalam, Chengalpattu Dt.,  
Tamil Nadu, India*

*b Department of Physics, SRM Valliammai Engineering College, Kattankulathur,  
Chengalpattu 603203, Tamil Nadu, India*

**\*Corresponding author e-mail:chezhiyan70@gmail.com**

## **ABSTRACT**

Polymer-based nanoparticles is found to be the more feasible one in drug delivery for innumerable diseases. Rheumatoid arthritis is an autoimmune inflammatory disease which has affected almost 0.5-1% of total population in the world. It is the disease which causes inflammation in the joints due the attack of various inflammatory agents. Antiarthritic activities are strongly related to the group of reactive oxygen species (ROS) in nanomaterials, due to their large surface areas, increase in oxygen vacancies and the diffusion capability of the reactant molecules and the release of active ions. In the current research work Chitosan coated ZnO nanoparticles were magnificently synthesized and the biocompatible nanocomposite N,N-Dimethyl Cur-PEG-CS-ZnO is got by coupling the carboxyl group of N,N-Dimethyl Cur-PEG to the amine group of CS-ZnO using hydrothermal method. Polyethylene glycol (PEG) enhances the biocompatibility, low toxicity and bio-safety of nanoparticles. Using PEG on nanoparticles prevents premature elimination of the drug from the bloodstream. Characterization techniques such as XRD, FTIR, UV-Vis, TEM and in-vitro drug release studies confirmed the structure formation, particle size and controlled drug loading and releasing performance of nanoparticles. Also, the results obtained from characterization, confirms the synthesized nanocomposite NNDMA Cur PEG CS/ZnO are capable of controlling the producing of auto-antigens which cause denaturation of proteins during inflammation.

**Keywords:** N,N-Dimethyl Curcumin, PEG, Hydrothermal method, Antiarthritic activity.

**Comparative Study on the Functional properties of Formic acid treated Modal and Cotton fabric.****K.Gnana Priya and T.Sasikala***Department of Chemistry, Sri Ramakrishna College of Arts and Science, Coimbatore.***Corresponding author e-mail:** gnnapriyak84@gmail.com**ABSTRACT**

Modal is a second generation regenerated cellulosic fiber and a variation of rayon. Modal is one of the most important cellulosic fibers obtained from the wood pulp of beech tree wood. Modal is very soft, shiny, and gives silk feel than mercerized cotton with the ability to absorb up to 50% more water than cotton. Fabric made from modal drape well and do not pile like cotton. Modal fabrics resist fading, shrinking and the build-up of hard water mineral deposits even after repeated washing. In this study, modal fabrics (woven and knitted) are selected and conventionally pre-treated and subjected with 98% formic acid which is a used for the bio process of cellulose polymeric materials, in different concentrations. The formic acid treated modal fabrics were then undergone different testing such as; Anti-Bacterial Assessment, Anti Odour Behaviour, Anti Odour Retention Behaviour, UV Protection factor. These treatments on modal fabrics were correspondingly compared with those of cotton for its effectiveness.

**Keywords** - Modal fabrics; Formic acid; Anti-Bacterial Assessment; Anti Odour Behaviour; Anti Odour Retention Behaviour; UV Protection factor.

**Analysis of switched reluctance motor with reduced torque ripple****Vijayalakshmi K***Department of Electrical and Electronics Engineering, SRMIST, Ramapuram, Chennai.***Corresponding author e-mail:** vijayalk1@srmist.edu.in**ABSTRACT**

Electric vehicles are becoming increasingly popular as the automotive industry & environmental effect grows. Switched reluctance motors are an excellent choice for high-speed aerospace applications due to their high speed, fault tolerance, and high-power density. The SRM, have numerous advantages with high-speed operation with the limitation of torque ripple. The main important factor to be considered for the reduction of torque ripple can be in terms of materials selected for the stator and the rotor core. By proper analysis it is found that the selection of materials plays a vital role in the reduction of the effect created by the excitation of rotor force on the stator.

## Numerical Analysis of CZTS and CIGS Solar Cell with $\text{In}_2\text{S}_3$ as buffer layer by SCAPS-1D

**Virang Shukla <sup>1 \*</sup> and Gopal Panda <sup>2</sup>**

<sup>1</sup> Department of Physics, Sarvepalli Radhakrishnan University, Bhopal, India

<sup>2</sup> Department of Physics, Sarvepalli Radhakrishnan University, Bhopal, India

**Corresponding author e-mail:** virangshukla\_1983@yahoo.co.in,

### ABSTRACT

The CZTS and CIGS Solar cell were simulated using SCAPS-1D Simulator.  $\text{In}_2\text{S}_3$  was used as buffer layer. Generally CdS is used as buffer layer. But it can create injurious effect on human health and cause environmental pollution. It can create absorption loss in solar cell due to low band gap. So  $\text{In}_2\text{S}_3$  is good substitute of CdS due to its stability and higher band gap. Fluorine doped tin oxide (FTO) was used as window layer and Au was used as back contact. The effect of thickness, defect density, carrier concentration of absorber layer, temperature, electron affinity and thickness of buffer layer was investigated using SCAPS-1D Simulator. The CZTS Solar cell shows 16.09% efficiency and CIGS shows 21.97% efficiency after simulation. The simulation was also carried out by replacing  $\text{In}_2\text{S}_3$  with CdS buffer layer with the aim of comparing output parameters.

**Key words:** CZTS and CIGS Solar cell, absorber and buffer layer thickness, temperature, defect density and carrier density of absorber layer, electron affinity of buffer layer.

**Nanomaterials : An Alliance of Dentistry and Engineering – A Review****Dr. S. Vidhya**

Department of Conservative Dentistry & Endodontics, SRM Dental College, Ramapuram,  
Chennai

**Corresponding author e-mail:** vidhyas@srmist.edu.in

**ABSTRACT**

Nanotechnology and nanomaterials have revolutionized the field of health science. Human tooth is composed of inorganic and organic components, which are assembled in the form of microscopic structures that give shape and functionality to the teeth in the oral cavity. With advances in medical science, the average life expectancy of humans has been remarkably prolonged. Hence, the natural human dentition is also expected to serve an increased period of retention in the oral cavity and serve the functions of aesthetics and mastication. Dental material science has metamorphosed from micro- to nanomaterials in an attempt to better integrate the materials with its substrate. The smaller size, increased surface area, enhanced surface area to volume ratio and better diffusion characteristics of nanomaterials compared to their microscopic counterparts are considered ideal requisites to enable this transformation.

Nanoscience forayed into restorative dentistry in the form of fillers in dental materials, especially resin composites, the most widely used esthetic restorative material in dentistry, which resulted in excellent polishability and heightened esthetics. Nano-hydroxyapatite, derived from natural sources like eggshells are showing promise as an excellent remineralizing agent with prospective use as anti-cavity toothpastes and desensitizing agents for tooth sensitivity. Silver nanoparticles have been widely researched as an effective antimicrobial agent to reduce bacterial adherence and colonization on prostheses as well as root canals of teeth. Nanochitosan and nanocalcium hydroxide have been proven to be effective antimicrobials and are recommended as an intracanal medicament for endodontic therapy.

This paper reviews the various applications of nanomaterials and nanotechnology that have improved the standard of patient care in dentistry.

## Ambient mass spectrometry using electrospun nanofibers for various analytical contexts

**Mohd Azhardin Ganayee, R. G. Hemalatha, and T. Pradeep**

*DST Unit on Nanoscience and Thematic Unit of Excellence, Department of Chemistry, IIT Madras,  
Chennai.*

**Corresponding author e-mail:**azhar1iitm@gmail.com

### ABSTRACT

In this work, an ambient ionisation mass spectrometry, DESI MS-based molecular analysis and imprint imaging using electrospun nylon-6 nanofiber mats are demonstrated for various analytical contexts. Uniform mats of varying thicknesses composed of ~200 nm diameter fibers were prepared using needleless electrospinning. Analytical applications requiring rapid understanding of the analytes in single drops, dyes, inks, and/or plant extracts incorporated directly into the nanofibers are discussed with illustrations. The possibility to imprint patterns made of printing inks, plant parts (such as petals, leaves, and slices of rhizomes), and fungal growth on fruits with their faithful reproductions on the nanofiber mats is illustrated with suitable examples. Metabolites were identified by tandem mass spectrometry data available in the literature and in databases. The results highlight the significance of electrospun nanofiber mats as smart surfaces to capture diverse classes of compounds for rapid detection or to imprint imaging under ambient conditions. Large surface area, appropriate chemical functionalities exposed, and easiness of desorption due to weaker interactions of the analyte species are the specific advantages of nanofibers for this application.

**Keywords:** Electrospinning, Nanofibres, DESI-MS, Smart Surfaces and Imprint Imaging

## Synthesis and electrochemical properties of $\text{ZnCo}_2\text{O}_4$ - PANI nanocomposite electrode for high-performance supercapacitor applications

P.Vijayamathubalan<sup>1</sup>, V. Venkatachalam<sup>2</sup>, R. Gunaseelan<sup>3</sup>, A. Antony Raj<sup>4</sup>,  
S. Selvakumar<sup>1\*</sup>

<sup>1</sup>PG and Research Department of Physics, Government Arts College for Men, Chennai-35

<sup>2</sup>Department of Physics, Sir Theagaraya College, Chennai-600021, India

Department of Physics, Pachaiyappa's college for Men, Kanchipuram- 631501, India.

<sup>4</sup>Department of Physics, St Joseph's College, Trichy- 620002, India.

\*Corresponding Author email: [drsskphy@gmail.com](mailto:drsskphy@gmail.com)

### ABSTRACT

In this work,  $\text{ZnCo}_2\text{O}_4$ /PANI nanocomposite was synthesized by hydrothermal and blending approach. The structural, morphology and functional compound of the electro-active material were analyzed by using XRD, HR-TEM and FT-IR. The morphology analyses reveal the nanoparticles  $\text{ZnCo}_2\text{O}_4$  decoded with PANI. The modified  $\text{ZnCo}_2\text{O}_4$ /PANI nanocomposite electrode was studied under three electrode testing condition for their electrochemical properties. The modified nanocomposite electrode exhibits the highest specific capacitance value of 789.4F/g at a current density of 5mV/s in 3M KOH with enhanced the capacitive performance because the effective presence of PANI on the  $\text{ZnCo}_2\text{O}_4$  nanoparticles. This method brings a viable, low-cost synthesis of metal oxide/PANI based composite with promising characteristics for the energy-storage applications in supercapacitors.

**Keywords:** Binary metal oxide, PANI, nanocomposite, electrochemical properties, supercapacitor

## Effects of different metal ions on optical properties and photocatalytic activities of zirconia nanoparticles

K. Anandan \* , K. Rajesh, K. Gayathri

*Department of Physics, AMET University, Chennai 603 112, Tamilnadu, India*

\*E-mail address: anand.ka@ametuniv.ac.in

### ABSTRACT

Optical and photocatalytic properties of pure and different metals ions doped zirconia ( $ZrO_2$ ) nanoparticles, synthesized via the facile precipitation process. The effects of the different metal ions on physic-chemical properties of zirconia were analysed by using different techniques. The structural properties of the synthesized samples were done by XRD and FTIR analyses, which confirm that the both pure and different metal ions doped zirconia nanoparticles reveal tetragonal structure with average crystallite size, are in good agreement with TEM results. Optical properties of the different metal ions doped  $ZrO_2$  nanoparticles were evaluated using UV-vis absorption and PL emission spectroscopies. The performances of the pure and different metal ions doped zirconia nanoparticles in the photocatalytic degradation of methyl orange dye under UV light were evaluated, degradation percentage (%) found and the results have been comparatively discussed. The detailed mechanism for degradation of MeO dye by using metal ions doped  $ZrO_2$  catalyst was discussed.

## Synthesis and Characterization of Zinc Telluride thin film as Interface Layer for CdTe Solar Cells

**Shivaji M Sonawane**

*Department of Physics, Bharatiya Jain Sanghatana's Arts Science & Commerce College Wagholi, Pune - 412207, Maharashtra.*

**Email Id:** sonawaneshivaji77@gmail.com

### **ABSTRACT**

Development of low ohmic and stable back contact is required for the fabrication of efficient CdS/ CdTe solar cells. CdTe material has a higher electron affinity (4.5 eV), therefore a high work function metal is required to form a good ohmic contact on p-type CdTe. Due to the non-availability of high enough work function metal, the best solution to overcome the contact problem is to introduce heavily doped p-type layer between the CdTe absorber and back contact to form a tunnel contact. The II-VI compound ZnTe is considered as a potential candidate for applications in the field of solar cells due their appropriate optoelectronics properties. ZnTe thin films have been synthesized using an electrodeposition process from an acidic aqueous solution by potentiostatic conditions on FTO substrates. The reaction mechanism has been studied by cyclic voltammetry with scan rate 5 mV sec<sup>-1</sup> to identify the deposition potential. ZnTe thin films electrodeposited at -0.95 V with respect to Ag/AgCl reference electrode. As deposited films are close to the stoichiometric composition. The band gap energy of ZnTe thin films is observed at 2.25eV by Vis- UV spectroscopy. X-ray diffraction, Raman spectra as well as SEM techniques have been employed to investigate the structure and surface morphology of as-deposited films. As deposited ZnTe layer has cubic structure with (111) preferential orientation. Globular surface morphology was observed from SEM micrograph. Zn rich layer are grown at growth potential - 0.95V.

## Investigation on Synthesis, spheroidization and spray deposition of plasma sprayed lanthanum zirconate thermal barrier coatings

**M.Mathanbabu<sup>1\*</sup>, D.Thirumalaikumarasamy<sup>2</sup>, M.Ashokkumar<sup>3</sup>, S. Deepak<sup>4</sup>,  
K.Mathivanan<sup>5</sup>**

*Government College of Engineering, Bargur, Krishnagiri-635104, India,*

*<sup>1,4,5</sup> Research scholar, Annamalai University, Annamalai nagar*

**E-mail:** mathanbabb@gmail.com

### **ABSTRACT**

During the last decade, research works were carried out to the development and manufacturing of ceramic thermal barrier coatings (TBC's) on turbine parts because the traditional turbine materials have reached the limits of their temperature capabilities. Formerly, yttria stabilized zirconia (8YSZ) has been utilized as the commercial material for TBC applications. However, the YSZ has the disadvantage that its operation temperature is about 1200°C for the long term application. TBCs have been widely used in hot section metal components in gas turbines either to increase the inlet temperature with a consequent improvement of the efficiency or to reduce the requirements of the cooling air. There are various ceramics that have been evaluated as TBC materials, and lanthanum zirconate (LZ) is one of the most promising among them. The properties specifically high-melting point, phase stability up to its melting point, low thermal conductivity, low sintering activity and oxygen-non transparent make the LZ a prospective TBC material for high-temperature applications. However, the production methods used to synthesize LZ are highly time consuming and the powder is not commercially available. Hence, in this investigation an attempt was made to synthesize, spheroidize and spray deposit LZ material by thermal plasma method. LZ has been synthesized by universal ball milling technique by a combination of La<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub> powders that is used as feedstock powder for plasma spray deposition. This investigation demonstrates the effectiveness of thermal plasma as a major materials processing method. Suitable characterization techniques have been studied for the material modifications after respective plasma processing exposures.

## Influence of various size and volume fraction of Suspended particles on the Rheological properties of Shear Thickening Fluids for Soft Armour Applications.

**S.Deepak<sup>1\*</sup>, D.Thirumalaikumarasamy<sup>2</sup>, M.Ashokkumar<sup>3</sup>, M.Mathanbabu<sup>4</sup> and K.Mathivanan<sup>5</sup>**

<sup>1,4,5</sup>*Research scholar, Government College of engineering, Bargur, Krishnagiri-635104, India. P*

<sup>2</sup>*Assistant professor (SG), Government College of engineering, Bargur, Krishnagiri-635104, India.*

<sup>3</sup>*Research scholar, Annamalai University, Annamalainagar, Tamilnadu, India.*

*E-mail: naamphd@gmail.com*

### **Abstract**

The shear-thickening phenomenon behaviour occurs in most of the concentrated colloidal dispersions such as clay – water, calcium carbonate – water, polystyrene – silicon oil, iron particles – carbon tetrachloride, titanium oxide – resin, silica – polypropylene glycol, and silica – polyethylene glycol have attracted the attention of protective systems development applications. The rheological properties of Shear Thickening Fluids (STF's) could be controlled by the composition of the carrier fluid molecular weight with chain length and solid particles influence of a few parameters, such as particle size, volume fraction and critical shear rate range. Based on the reviewed literature, including primarily the nature of solid phase are discussed considering many factors affecting shear thickening behaviour and the use of STFs in protective systems is reviewed. We include investigations of Important Parameters, particle size and volume fraction Influencing of Shear Thickening Fluid (STF).

**Keyword:** Shear Thickening Fluids; Soft Armour Applications; protective systems; carrier fluid PEG; synthesized nanoparticles.

**ZnS/rGO nanocatalyst for enhanced photocatalytic activity****Dr. M. Sathishkumar***Department of Electronics, Nehru Arts and Science College, Coimbatore, Tamilnadu, India.***Email :** mskeasc@gmail.com**ABSTRACT**

High performance hexagonal crystal structured reduced graphene oxide doped zinc sulfide (ZnS/rGO) nanocatalyst has been synthesized by a facile one step microwave irradiation method. Two different amount of rGO (5 and 10 wt%) has been prepared by reducing GO and were loaded into ZnS synthesis. The prepared ZnS/rGO was characterized by several modern X ray techniques. These results are suggested that prepared nanocatalyst samples are having improved structural and optical properties which more suitable for photodegradation of eosin yellow (EY) dye. The superior degradation efficiency of ZnS/rGO (10 wt%) can be attributed due to improved structural and optical properties with specific surface areas which may increase the migration of photogenerated charge carriers for efficient separation and generation of charge carrier.

**Keywords:** ZnS/rGO nanoparticles, microwave irradiation, Photocatalysis, Carbon materials, XPS

## Prediction of corrosion rate of AZ91D magnesium alloy in NaCl solution under salt fog environment

**K.Mathivanan<sup>1\*</sup> , D.Thirumalaikumarasamy<sup>2</sup>, M.Ashokkumar<sup>3</sup>, M.Mathanbabu<sup>4</sup> and S.Deepak<sup>5</sup>**

<sup>1,4,5</sup> Research scholar, Government College of Engineering, Bargur, Krishnagiri-635104, India.

<sup>2</sup> Assistant professor (SG), Government College of engineering, Bargur, Krishnagiri-635104,

<sup>3</sup> Research scholar, Annamalai University, Annamalainagar, Tamilnadu, India.

**E-mail:** mailtomathi806@gmail.com

### ABSTRACT

The corrosion behaviour of plasma-sprayed stellite coatings was evaluated using a salt fog test in NaCl solution at various chloride ion concentrations, pH values, and spraying times. The effects of PH, chloride ion concentration, and spraying time on the corrosion behaviour of Mg AZ91D alloys subjected to salt fog were investigated. Corrosion attack increased as the PH value and Cl ion concentration increased. By introducing the corrosion process parameters, an empirical relationship was developed to predict the corrosion rate of stellite coatings. Scanning electron microscopy (SEM) and X-ray diffraction were used to examine the corroded surface. The results revealed that chloride ion concentration and pH value had a significant influence on the corrosion deterioration of stellite coating. The stellite coatings were discovered to be extremely vulnerable to localised damage. It was unable to provide effective corrosion protection to Mg alloy substrates in solutions with acidic environments (pH 3), higher chloride concentrations, and spraying time.

**Keywords:** stellite;salt fog, magnesium alloy; PH value; Cl - ion concentration.

**Synthesis and characterization of nano-TiO<sub>2</sub> via different methods****R.Vijayalakshmi and V.Rajendran***Department of Physics, Thiruthangal Nadar College, Chennai, Tamilnadu, India**Department of Physics, Presidency College, Chennai, Tamilnadu, India***Email:** viji2302@gmail.com**ABSTRACT**

In this paper, we report the comparison between TiO<sub>2</sub> nanoparticles prepared via two different routes; i) via sol-gel route and ii) by hydrothermal method. It was found that when prepared under the same ambient conditions viz temperature, pressure etc. and keeping all the parameters same viz precursors, mole ratio, solvent etc; the nanoparticles prepared via sol-gel route were highly crystalline and had smaller crystallite size ( $\sim 7$  nm) as compared to the one prepared by hydrothermal method ( $\sim 17$  nm). The crystallinity and the crystallite size were examined by XRD and TEM. The band gap values of the TiO<sub>2</sub> nanoparticles were calculated to be 3.54 and 3.43 eV. Photoluminescence (PL) was also recorded for the two types of particles and results have been analyzed.

**Keywords:** sol-gel, hydrothermal, optical properties, nanomaterials, size effect.

**Synthesis of N'-(<sup>1E,2E</sup>-3-(benzo[d][1,3]dioxol-5-yl)-1-(2-methoxyphenyl)allylidene) furan-2-carbohydrazide and N'-(<sup>1E,2E</sup>-3-(benzo[d][1,3]dioxol-5-yl)-1-(3-methoxyphenyl)allylidene) furan-2-carbohydrazide.**

**R. Kavitha<sup>a</sup>, S. Nirmala<sup>b</sup>**

*<sup>a</sup>Department of Physics, Rajalakshmi Engineering College (Autonomous), Thandalam, Chennai - 602105, Tamilnadu, India*

*<sup>b</sup>Department of Physics, Easwari Engineering College (Autonomous), Ramapuram, Chennai-600089, Tamil Nadu, India*

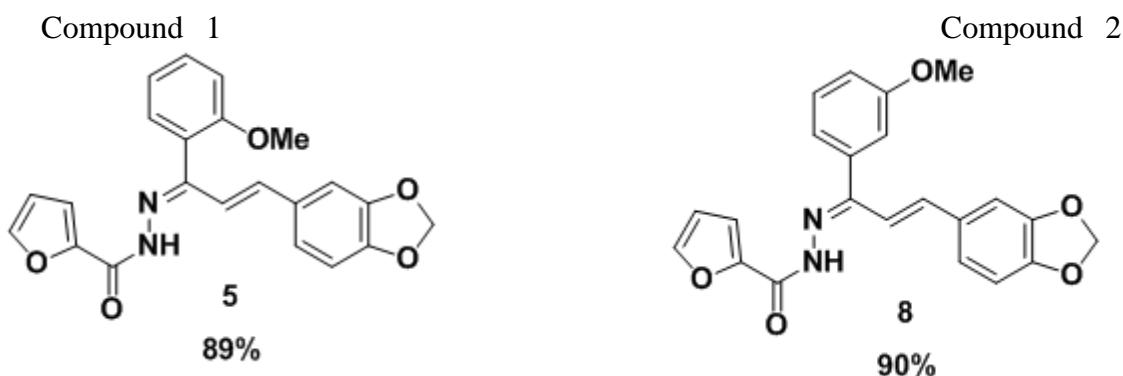
**Email:** kavitha.aishu@gmail.com

## ABSTRACT

The title compound 1, N'-(<sup>1E, 2E</sup>-3-(benzo[d][1,3]dioxol-5-yl)-1-(2-methoxyphenyl)allylidene) furan-2-carbohydrazide, C<sub>22</sub> H<sub>18</sub> N<sub>2</sub> O<sub>5</sub> crystallizes in monoclinic, achiral space group P21/c, planar. The dihedral angle between the plane of O4-C19-C20-C21-C22 and O1-O2-C1-C2-C3-C4-C5-C6-C7 is 4.93° and hence it is slightly tilted with each other. The molecules are linked in non-centrosymmetric. The dihedral angle between 1, 3-methylenedioxy and 3-methoxyphenyl molecule is 73.07°. The crystal system is stabilized by intermolecular hydrogen bonds. The structure was solved by direct method and refined by full matrix least square procedure to a final R = 0.0456 and wR = 0.0994 using 3456 reflections. Puckering of the molecule is stabilized by C-H...O and C-H...N interactions in addition to van der Waals force. The bond lengths of C1-C2, C1-C6 and C5-C6 are 1.358(4) Å, 1.374 Å and 1.363 Å respectively. The bond lengths of C5-H5 and C7-H7A are 0.9300 Å and 0.9700 Å respectively. N1-N2 is observed as 1.370(3) Å and here the aromatic C-H bond length is 0.9300 Å. The methyl hydrogen bond length is 0.9600 Å. A double bond is observed between C18-O3 and C18-N2. The bond angle may be varied due to the difference in bond length in oxygen substituted in five membered rings, which varies from 1.2 Å to 1.5 Å. In this compound 1, 1, 3 methylene dioxy is connected to N1 by weak van der Waals force. In practice the intermolecular interaction is produced due to acid and base interaction. Torsional angles between the planes C6-C1-C2-C13 and N1-C10-C11-C12 are 2.0 (5)° and 106.6 (4)°

respectively and have anticinal conformation. Plane C1-C6-O1-C7 has syn-periplanar conformation and its torsion angle is  $11.0^{\circ}$ . 1, 3-methylene dioxy five membered ring has envelope confirmations. The puckering parameter Q is 0.131 and  $\theta = 54.7^{\circ}$  and the envelope on C7 is observed in C6-O1-C7-O2-C1. Also total puckering is 0.187. The CCDC number is 2085276 and 2085277 for compound 1 and 2.

Scheme



The title compound 2, N'-( $(1E, 2E)$ -3-(benzo[d][1,3]dioxol-5-yl)-1-(3-methoxyphenyl)allylidene) furan-2-carbohydrazide, crystallizes in the triclinic, achiral space group P-1, planar. The dihedral angle between the plane of O1-O2-C1-C6-C7 and N1-N2-C9-C10-C11 is  $28.11^{\circ}$ . Same non-centro symmetric is also observed in compound 2. The crystal system is stabilized by intermolecular hydrogen bonds. The structure was solved by direct method and refined by full matrix least square procedure to a final  $R = 0.0506$  (1492) and  $wR = 0.1331$  (3581) using 3456 reflections and 1, 3-methylene dioxy five membered ring adopts envelope conformation. Puckering of the molecule is stabilized by C-H...O and C-H...N interaction in addition to van der waals force.

**3-Hydroxy-4-nitrobenzaldehyde: Spectral (FT-IR, FT-Raman and NMR) investigations, FMO, MEP, NBO analysis**

**K.Parimala<sup>a</sup>& S.Manimegalai<sup>a,\*</sup>**

*<sup>a</sup>PG & Research Department of Physics, Nehru Memorial College, Trichy-621007, India*

**E-mail:** mscmanimegalai@gmail.com

**ABSTRACT**

The structures of 3-Hydroxy-4-nitrobenzaldehyde were explored spectroscopically through FT-IR, FT-Raman  $^1\text{H}$  &  $^{13}\text{C}$  NMR. FMO, MEP, and NBO analysis were carried out by density functional theory (DFT). Different electronic properties of atomic charges, molecular electrostatic properties (MEP), chemical reactivity and absorption analysis have been studied by same method. In order to understand the interaction and stability of NBO analysis, molecular docking and MD simulation have been performed by various output like interaction energies, number of intermolecular hydrogen bonding, binding energy etc. have established the elucidate role of geometrical structure.

**Keywords:**FT-IR,FT-Raman, NMR, DFT, MEP

## Synthesis, Characterizations of Pure and Co<sup>2+</sup> Doped Iron Oxide Nanoparticles for Magnetic Applications

M. Subash<sup>a</sup>and R. Uthrakumar<sup>a\*</sup>

<sup>a</sup>Department of Physics, Govt. Arts College (Autonomous), Salem, 636 007, India

Emaiil : ukloyola@gmail.com

### ABSTRACT

In this research, we investigate the effects of pure and cobalt substitution on the size development, crystal erection, and attractive possessions of -Fe<sub>2</sub>O<sub>3</sub> nanoparticles, which were synthesised using the Sol-Gel process. X-ray Diffraction (XRD), scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX), and Fourier Transform Infrared Spectroscopy (FTIR) were used to analyse crystalline nature, magnitude, outline, and chemical composition of iron oxide (Fe<sub>2</sub>O<sub>3</sub>) nanoparticles (FT-IR). The change in direct band gaps is demonstrated by UV-Visible spectroscopy and compared to XRD findings. Furthermore, an XRD spectrum survey indicated that the material had a cubic structure. Scanning Electron Microscopy may be cast-off to characterise the morphologies and structures of iron oxides. The use of EDX to analyse elements revealed that cobalt doping had been successful. At room temperature, magnetic characteristics were resolute using a Vibrating Sample Magnetometer (VSM). Magnetic tests revealed that, when compared to pure and cobalt-doped nanoparticles, there is a significant difference. Furthermore, the doping content has a significant impact on magnetic characteristics.

## Investigations on the Growth and characterization of 2-amino-4-picolinium 4-hydroxybenzoate single crystals

R. Subash Chandra Bose<sup>a</sup>, R. Subramaniyan @ Raja<sup>b</sup>, H.Shankar<sup>b</sup>, K.Balasubramanian<sup>a</sup>,  
G.Vinitha<sup>c</sup>

<sup>a</sup>PG & Research Department of Physics, The M.D.T Hindu College, Tirunelveli- 627010, India.

<sup>b</sup>Department of Physics, KPR Institute of Engineering and Technology, Coimbatore-641407, India

<sup>c</sup>Division of Physics, School of advanced sciences, VIT Chennai, Chennai-600127, India

Email: [boseips@gmail.com](mailto:boseips@gmail.com)

### ABSTRACT

Supramolecular design has drawn a lot of interest in optoelectronic applications in the recent past. They are focused on interactions between hydrogen atoms. Many new organic single crystals have been identified using a molecular engineering approach, which is said to have scientific and technological applications [1]. 2-amino-4-picolinium-4-hydroxybenzoate (2A4P4HB) were grown as a single crystal using a controlled evaporation method in the present study. The lattice parameters of 2A4P4HB were affirmed using X-ray diffraction measurements. Using <sup>1</sup>H and <sup>13</sup>C nuclear magnetic resonance spectral studies, the proton and carbon position was determined. FTIR spectral study was carried out to investigate the functional groups of 2A4P4HB. Linear optical study was used to determine the cut off wavelength and the wide optical operating window. Thermogravimetric and Differential Thermal Analysis were used to examine the thermal properties of 2A4P4HB. Vickers microhardness testing was used to determine mechanical stability at room temperature. Meyer's law was used to investigate the hardness results. The Z scan measurements were performed on 2A4P4HB.

## The structural, optical, and electrical properties of nebulizer spray-deposited tin disulphide ( $\text{SnS}_2$ ) thin films with different substrate temperatures

R.Sarathkumar<sup>1</sup>, Pavan Kumar Naini<sup>2</sup>, V.Vijayanarayanan<sup>1</sup>, V. Aravindan, S.B.P Abirami  
Manickam Mahendran<sup>1\*</sup>

<sup>1</sup>*Smart Materials Lab, Department of Physics, Thiagarajar College of Engineering, Madurai*

<sup>2</sup> *Department of Physics, Matrusri Engineering College, Saidabad, Hyderabad- 500 059*

\*Email: [sk5557564@gmail.com](mailto:sk5557564@gmail.com)

### ABSTRACT

Tin disulphide thin films are prepared by nebulizer spray pyrolysis technique with the different substrate temperatures. The structural, electrical, and optical properties of  $\text{SnS}_2$  thin films are investigated. The X-ray diffraction (XRD) analysis revealed the polycrystalline nature, having a hexagonal structure with the preferential orientation along the (0 0 2) plane. The size of the  $\text{SnS}_2$  crystallization is determined by using the Full width half maximum value of the Bragg peak. The composition and surface morphological of  $\text{SnS}_2$  thin films are analyzed by Scanning Electron Microscope (SEM). Transmittance and absorption spectra of these films are determined in the wavelength range of 400-1110 nm. The optical band gap of tin disulfide thin films is decreased from 3.17 eV to 2.61 eV with an increase in substrate temperature. The absorption coefficient and activation energy are decreased with respect to substrate temperature.

**Key words:**  $\text{SnS}_2$ , XRD, SEM, Nebulizer Spray Pyrolysis

## Collagen from Fish Scales- Preparation, Characterization and Biomedical Application

**S.WeslenVedakumari**

*Faculty of Allied Health Sciences, Chettinad Academy of Research and Education, Kelambakkam, Chennai- 603 103, India.*

**Email:** drweslen@gmail.com

### **ABSTRACT**

Collagen, a naturally occurring protein has wide range of medical applications because of its biodegradability, low toxicity & immunogenicity. The main objective of the study was to extract collagen from spotted seer fish (*Scomberomorus guttatus*) and to investigate its role in wound healing. Acid-soluble collagens (ASC) were extracted from the skin, fin and tail of spotted seer fish (*Scomberomorus guttatus*) using the method of Piezet *al.*, Wound healing efficiency of spotted seer fish collagen was studied by creating full-thickness excision wounds in rats. Topical application of spotted seer fish collagen, once in two days, for 12 days resulted in complete healing of wounds on the 16<sup>th</sup> day. Granulation tissue collected on every fourth day of healing showed increase in hydroxyproline, hexosamine, uronic acid and total protein contents in collagen-treated rats. Histological analysis and tensile strength measurements further confirmed proper healing in collagen-treated rats. These results clearly indicate the wound healing efficiency of spotted seer fish.

## Heterogeneous nucleation and growth of SnSe thin films

A G Kunjomana<sup>a</sup>, Bibin John<sup>a</sup> Teena Mathew<sup>b</sup> and R Karthikeyan<sup>a</sup>

<sup>a</sup>Department of Physics and Electronics, CHRIST (Deemed to be University), Bangalore 560029

<sup>b</sup>Department of Physics, St. Thomas College, Palai, 686574, Kerala, India

E-mail : kunjomana.ag@christuniversity.in

### ABSTRACT

Thermal evaporation of tin mono selenide (SnSe) thin films was carried out under high vacuum ( $2 \times 10^{-6}$  mbar) using the coating unit, Model: 12A4D. The films prepared at room temperature were found to be amorphous as the vapor-solid interface is atomically rough due to multiple nucleations on the glass substrate. In order to limit the random heterogeneous nucleation sites, glass slides were ultrasonically cleaned and high tension cleaning was carried out prior to the thermal evaporation process. The distance between molybdenum boat and substrate was maintained as 20 cm with a filament current of 70 A. Good quality crystalline thin films were deposited at a substrate temperature, 220°C due to the evaporation of chemically homogeneous SnSe ingot and periodic addition of atoms on the atomically smooth interface. Powder X-ray diffractograms ensured the phase identification of crystal system to be orthorhombic with lattice parameters,  $a = 4.445 \text{ \AA}$ ,  $b = 11.501 \text{ \AA}$  and  $c = 4.150 \text{ \AA}$ . Chemical composition of the constituent elements was probed using energy dispersive analysis by X-rays, which enabled the right elemental atomic proportion, 50.03: 49.97. The optical characteristics of the films were probed using UV-Vis-NIR and photoluminescence spectroscopy. The optimization of optoelectronic parameters pave the way for the suitability of prepared thin films for energy harvesting applications.

## Control of Phase Transition on the Structural Properties of Antimony Chalcogenide Crystals

BibinJohn<sup>a</sup>, A G Kunjomana<sup>a</sup> and Teena Mathew<sup>b</sup>

<sup>a</sup>Department of Physics and Electronics, CHRIST (Deemed to be University), Bangalore 560029,

<sup>b</sup>Department of Physics, St. Thomas College, Palai, 686574, Kerala, India

E-mail : kunjomana.ag@christuniversity.in

### ABSTRACT

Antimony triselenide ( $Sb_2Se_3$ ) crystals have been prepared in bulk form by directional solidification method under vacuum environment ( $6 \times 10^{-3}$  mbar) to study the effect of structural properties as per the phase diagram of Sb-Se system. The growth runs were performed by suitably adjusting the temperature gradients using temperature controllers and slow cooling was done to harvest good quality crystals after a growth period of 48 h. When the temperature gradient was very low, perturbation in the melt-solid ( $\beta$ - $\beta$ ) interface induced rough surface with structural irregularities and compositional changes with poor mechanical strength. Optimization of supercooling by stabilizing the temperature gradient enabled atomically smooth interface, and thus produced structurally perfect, homogeneous crystals without any surface damage. The growth kinetics was systematically studied using optical and scanning electron microscopes and confirmed the layer by layer deposition of crystals as per the KSV mechanism. X-ray diffraction and energy dispersive analyses justified the monophase characteristics of the grown samples with good crystallinity and stoichiometry. The density of the cleaved crystals was calculated from XRD data (5.869 g/cm<sup>3</sup>), which is in well agreement with the value estimated from Archimedes principle. Micro-indentation studies revealed that the melt grown  $Sb_2Se_3$  crystals have appreciable mechanical stability.

## Structural and Antimicrobial studies for pure and silver doped copper oxide nanoparticles of different concentrations

D. Reshma Agnes Preethi<sup>1</sup>, A. Philominal<sup>1\*</sup>

<sup>1</sup>PG and Research Department of Physics, Holy Cross College, Tiruchirappalli-620002, India

E mail: reshmiagnespreethi14@gmail.com

### ABSTRACT

Nanoparticles had greatly involved in broad spectrum of applications like ceramics, gas sensors, microbial activity, absorbents and catalyst. In the midst of all native metals, Silver (Ag) nanoparticle has its own solely characteristics and plays a vital role in favourable catalytic, electrical conductivity, chemical stability, and antimicrobial activity. Therefore, the present work was carried out to implement the sustainable process by usage of indigenous medicinal plant Moringa Oleifera leaf extract as a reducing agent for synthesizing pure and silver doped copper oxide nanoparticles of various concentrations (2%, 5%, 10% and 15%) using Co- precipitation method. The phase and monoclinic structure was identified by X- ray Diffraction (XRD). It shows that peaks were good crystalline in nature and average crystallite size was found to be in the nanometer range. From Scanning Electron Microscopy (SEM), it is revealed that nanoparticles are appeared to be in spherical morphology. The elemental compositions like copper (Cu), oxygen (O) and silver (Ag) were confirmed by Energy Dispersive X-ray analysis (EDAX). The antibacterial and antifungal activity of pure and silver doped copper oxide nanoparticles for different concentrations were exhibited against fungal culture (*Candida albicans*, *Aspergillus flavus*) and for gram positive (*Staphylococcus aureus*, *Streptococcus aureus*, *Bacillus subtilis*) and gram negative bacterial strains (*Escherichia coli*, *Enterococcus aeruginosa*). By enhancing the concentration of silver as a dopant it shows excellent result towards antimicrobial behaviour against pathogens.

**Keywords:** Silver, Copper oxide nanoparticles, Moringa Oleifera, Antimicrobial activity.

## Synthesis, growth and characterization of Piperazinium Tetrabromo-cadmium (II) monohydrate single crystals

**S Sivaraj<sup>1</sup>, B Chidambaranathan<sup>1,\*</sup>, S.E Allen Moses<sup>3</sup>, S Abraham Rajasekar<sup>2</sup> and S Selvakumar<sup>\*1</sup>**

<sup>1</sup>*PG and Research Department of Physics, Government Arts College for Men (A), Chennai 600 035*

<sup>2</sup>*Department of Physics, Sir Theyagaraya College, Old Washermanpet, Chennai 6006021.*

<sup>3</sup>*Department of Physics, School of Arts and Science (SAS), Vinayaka Mission's Research Foundation, AVIT-Campus, Chennai 603 104.*

**E mail:** sivarajsettu424@gmail.com

### ABSTRACT

Piperazinium Tetrabromo-cadmium (II) monohydrate (PTBC) compound was successfully synthesized by using aqueous solution as solvent. The slow evaporation solution growth technique was used to grow a good optical quality single crystal of PTBC at room temperature. The structure of grown crystal was confirmed monoclinic by the values of unit cell parameters calculated using single crystal x-ray diffraction analysis. Fourier Transform Infrared spectroscopy is employed to identify the functional groups of the synthesized material. The lower cut-off wavelength of 234 nm for PTCB was revealed from optical transmittance spectrum. In photoluminescence spectrum, sharp emission peaks are observed, which indicates the blue (425) emission. The third order nonlinear optical susceptibility  $\chi^{(3)}$  of the material is measured using Z-scan technique and it is found to be  $2.6002 \times 10^{-12}$  esu.

**Keywords:** Slow cooling, Z-SCAN, UV-Vis-NIR studies

## Thermal conductivity investigation of TiO<sub>2</sub>-water nanofluids using ultrasonic method

Dr. M. Leena\*

Department of Physics, Thiruthangal Nadar College, Selavayal, Chennai – 600 051.

\*E mail: drleerithima@gmail.com

### ABSTRACT

In the present study, Titanium oxide (TiO<sub>2</sub>) nanoparticles (NP's) were synthesized by means of sol-gel method. Crystalline nature of synthesized TiO<sub>2</sub> NPs was confirmed by the X-ray powder diffractometry (XRD). The surface morphology and the size of particle of NPs were analyzed by high resolution scanning electron microscopic method (HRSEM). Phase composition in TiO<sub>2</sub> was identified by FT-Raman spectroscopy. The different concentration of TiO<sub>2</sub> NPs were dispersed into water and mixed thoroughly by using ultrasonication process to obtain nanofluid samples. The dispersion of nanoparticles in nanofluids is studied with the unique method of UV-visible spectrometer, which confirms that dispersion stability has prepared nanofluids. The value of thermal conductivity, ultrasonic velocity and density were measured for the different concentrations and temperatures of TiO<sub>2</sub> nanofluids. The acoustical parameters such as adiabatic compressibility, intermolecular freelength, and acoustic impedance were calculated from the experimental data. It was observed that ultrasonic velocity showed linearity with particle concentration, and the results were discussed. Also, the thermal conductivities of nanofluids have been calculated through ultrasonic method and the results were compared experimentally with the flash laser technique method.

**Keywords:** Nanofluids, TiO<sub>2</sub>, Ultrasonic velocity, Thermal conductivity.

## Synthesis and spectral characterization of 2 -methyl 8- quinolinol co-crystals

N.Jayasudha<sup>a</sup>, M.Suganya <sup>a</sup>, MadhukarHemamalini<sup>a\*</sup>, S. JoseKavitha<sup>a</sup>, A.Catherine Paul<sup>a</sup>

<sup>a</sup> Department of Chemistry, Mother Teresa Women's University, Kodaikanal.

Email.Id: [hemamalini2k3@yahoo.com](mailto:hemamalini2k3@yahoo.com)

### ABSTRACT

Co-crystals of 2-methyl 8-quinolinol with carboxylic acids in the 1:1 stoichiometric ratio were obtained by the slow evaporation method. In co-crystals at least one part is molecular and a solid at room temperature i.e. conformer and forms supramolecular synthons with a molecular or ionic, API (Active Pharmaceutical Ingredient). They were characterized by ultraviolet-visible spectrophotometry (UV), Fourier transforms infrared spectroscopy (FTIR). It shows the vibrational frequencies of the probable functional groups occupied in hydrogen bonding. The synthesis of the co-crystals and indicated the functional groups depends on the structure of the new supramolecular synthons.

**Keywords:** cocrystals,2-methyl8-quinolinol,carboxylicacids, UV Visible spectro photometry , Fourier Transforms Infrared Spectroscopy (FTIR).

## Assimilation of zinc metal ion with hydroxyapatite by co-precipitation technique- for dielectric studies

K.Poovendran<sup>1</sup>, K.S.Joseph Wilson<sup>2</sup>,

<sup>1,2</sup> PG and Research Department of Physics, Arul Anandar College (Autonomous), Karumathur.

\*E-mail: [poov4u@gmail.com](mailto:poov4u@gmail.com)

### ABSTRACT

The aim of the present work is to explore the doping effect of Zn metal ions on hydroxyapatite for different concentrations (0.2, 0.4, 0.6, and 0.8). The samples for the pure and Zn doped HAP are synthesized by wet chemical precipitation method. The properties such as the hexagonal structure and the particle size are identified by using XRD. The functional bands of PO, CO and OH are assayed through FTIR and also the surface morphological and particle shapes are studied through SEM. The elemental analysis such as zinc, calcium and phosphates are analyzed by EDAX. All the designed elements are studied and confirm the (Ca+Zn)/PO ratio is nearly 1.67 and no other elements were identified in this study. The morphological particles of needle shape and the nanoscale particle size and shapes are studied by using TEM. The electrical conductivity of the synthesized ZnHAp ceramic is mainly related to width of the channel and the polarizability. The dielectric loss and nyquist plots were studied by using an impedance spectroscopy.

## Electro chemical synthesis of oxides of Fe-Co for electro chemical sensing application

**M. Murugan, Dr. M. Kanagasabapathy**

*Department of Chemistry, Rajapalayam Rajus' College, Rajapalayam*

**E mail:** muruganmariappan793@gmail.com

### **ABSTRACT**

Hydroxides and Oxides of cobalt and iron are having noteworthy technological applications such as in supercapacitors, battery electrodes water splitting (Hydrogen / oxygen generation) catalysts, pharmaceutical and biochemical sensing devices. These materials can be fabricated by electro-deposition method. Electro-deposition is viable reproducible and relatively lucrative with better process control over the formed films but limited literature is available, based on the electrochemical deposition and electrochemical sensing is binary metal oxides and oxy hydroxides. The solids are characterized by XRD, FTIR, SEM and energy dispersive X-ray spectroscopy analysis using secondary electrons. The SEM images show formation of the Nano iron cobalt oxides micro structure average width less than 50 Nano meter. Mathematical and computation modelling should be carried out to estimate the primary, secondary current distribution, deposit composition and crystal lattice geometry elucidation. By using either individual or binary metal oxides/oxy hydroxides, electrochemical detection of few selective and simple bio-active pharmaceutical organic compounds such as diclofenac, methyl salicylate, phenacetin, quinhydrone, acetaminophen, salicylaldehyde derivatives etc., are planned.

## FTIR and FT-Raman, Molecular Geometry, Vibrational Assignments, Density Functional Theory Calculations for 3-bromo benzylbromide

**Dr. I . Monica Chandramalar <sup>a</sup>.Dr.V.P.Subhasini <sup>b,\*</sup>**

<sup>a</sup>*Department of physics, Jeppiaar Engineering College, Chennai-600119*

<sup>b,\*</sup>*Department of physics, Shrimathi Devkunvar Nanalal Bhatt Vaishnav College for women,  
Chrompet, Chennai -600044.*

**E mail :** vpsubhasini@gmail.com

### **ABSTRACT**

A complete vibrational analysis of 3- bromo benzylbromide have been performed according to SQM force field method based on ab initio and DFT calculation 6-311++G(d,p) basis set and their frequencies are compared. It is expected that DFT theories are reliable for predicting the vibrational spectra of 3BBB . The vibrational spectra of benzyl bromide have been extensively studied and analyzed. The aim of this work is to check the performance of B3LYP density functional force field of 3BBB with the use of the standard 6-311+G(d,p) and 6-311++G(d,p) basis sets. A detailed quantum chemical study will aid in understanding vibrational modes of this title compound. So in this present investigation, the vibrational wavenumbers, geometrical parameters, modes of vibrations, dipole moment, rotational constants, atomic charges. HOMO-LUMO energies, NMR analysis, First hyperpolarizability, Mulliken analysis and other thermodynamic parameters of 3BBB investigated using B3LYP calculations. Area of high, neutral and low electrostatic potential is determined for 3BBB

**Keywords:** Vibrational spectra, Mulliken analysis, HOMO LUMO, NMR, First Hyperpolarizability, 3BBB

## The role of nanotechnology in combating multidrug resistance in cancer cell

**Jayavardhini Bhoopathy<sup>1</sup>, Weslen Vedakumari Sathyaraj\***

*Faculty of Allied Health Sciences, Chettinad Academy of Research, and Education,  
Chettinad Hospital and Research Institute (CHRI), Kelambakkam, Chennai- 603 103, India.*

**E mail:** jaya96bho@gmail.com

### **ABSTRACT**

Chemotherapy is a form of chemical drug therapy that is used to kill fast growing cancer cells. But its success is severely hampered by the toxic side effects of chemotherapeutic drugs and development of resistance by cancer cells. Multidrug resistance (MDR) is the principal mechanism by which many cancers develop resistance to chemotherapy drugs and it remains a major challenge in the treatment of cancer. Multidrug resistance is associated with deformed lysosomal compartments due to release of cathepsin in tumor environment. Lysosome is a membrane-enclosed organelle that functions as an essential part of the digestive system of the cell. Cancer cells have relatively large lysosomes and are more fragile than those present in normal cells. Lysosomal-mediated cell death serve as a unique option to treat tumor cells. In this review, we focus on nanotechnology-based treatment to overcome multidrug resistance cancer cells.

**Keywords:** Nanotechnology, multidrug resistance, lysosome, cancer

## Synthesis and growth of bulk Urea-Succinic Acid single crystal and its characterization for Photonic Applications

**Debabrata Nayak<sup>1,2,\*</sup>, N. Vijayan<sup>1,2</sup>, Manju Kumari<sup>1,2</sup>, Kiran<sup>1,2</sup>, Subasis Das<sup>3</sup>, R.P. Pant<sup>2</sup>**

<sup>1</sup> *Academy of Scientific and Innovative Research, CSIR- Human Resource Development Centre, (CSIR-HRDC) Campus, Ghaziabad, Uttar Pradesh- 201002*

<sup>2</sup> *CSIR – National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi – 110012, India*

<sup>3</sup> *Department of Physics, University of Burdwan, Bardhaman, 713-104, India*

**E mail:** debabratanayak254@gmail.com

### ABSTRACT

A wide optical band gap material single crystal of Urea-Succinic Acid (USA) has been synthesized from their equimolar aqueous solution using slow evaporation solution growth techniques (SEST). The monoclinic, centro symmetric space group  $P_{21}/C$  of ingot has been confirmed by single crystal X-ray diffraction. Crystalline perfection and existence of point defects inside the titled compound single crystal has been assessed through high resolution X-ray diffraction (HRXRD) technique. The optical parameters like UV-cut off, optical transparency and optical band gap in electromagnetic spectrum have been obtained from UV-visible spectroscopy. The luminescence behaviour of synthesized material is investigated by photoluminescence spectroscopy. From time resolved PL the bi-exponential curve of major emission photons shows the presence defect state in between the band structure of single crystal. The self-focusing lasing action of the synthesized single crystal has been studied through by Nd-YAG nanosecond laser with wavelength of 532 nm. The nonlinear optical variables like nonlinear refractive (NLR) index ( $n_2$ ) and nonlinear absorption (NLA) coefficient ( $\beta$ ) of titled compound single crystal is evaluated from Z-scan measurement. The laser damage threshold of the USA single crystal is found to be  $1.69 \text{ GW/cm}^2$  for 1 pulse/second in the same laser used in Z-scan measurement.

## Investigation on growth and characterization of metal organic saltLithium Itaconate single crystal

Irbaz Shoeb<sup>1,2</sup>, N. Vijayan <sup>2\*</sup>, Neha Gupta<sup>2,3</sup>, Ravinder Kumar<sup>2</sup>, D. Nayak<sup>2</sup>, M. Kumari<sup>2</sup>  
and Kiran<sup>2</sup>

<sup>1</sup> Department of Chemistry, Aligarh Muslim University, Aligarh, Uttar Pradesh- 202002, India

<sup>2</sup>CSIR –National Physical Laboratory, Dr K. S. Krishnan Road, New Delhi 110 012, India

<sup>3</sup>Lajpat Rai College, Shahibabad, Ghaziabad -Uttar Pradesh- 201005

E-mail: [Irbazshoeb01@gmail.com](mailto:Irbazshoeb01@gmail.com)

### ABSTRACT

Single crystals are very important for making any solid state electronic devices. Particulalry, NLO active crystals will show extraordinary applications in telecommunication and laser based devices. In the present study single crystal of Lithium Itaconate has been successfully grown by SEST (Slow evaporation solution growth technique) at room temperature. Powder X-ray diffraction analysis was employed to estimate the cell parameters and to understand the structure for the grown crystal. The functional group present in title compound was accomplished using Fourier transform infrared spectroscopy. The optical transparency and the band gap energy were elucidated by utilizing UV-visible spectrum. The Photoluminescence spectral studies revealed the photon excitation in the crystal system. Analysis of aforementioned techniques revealed that Lithium Itaconate crystal can sever as a promising aspirant for advanced non linear optical applications. Keywords: Crystal growth, Non-linear optical material, X-Ray Diffraction.

## Bio-Synthesis of Cobalt Oxide Using Aristolochia Indica Bark Extract and its structural, optical and morphological analyses

S. Thangewari<sup>a,b</sup>, and Dr. K. Amudhavalli<sup>a\*</sup>

<sup>a</sup>Department of Physics, V.O.Chidambaram College, Thoothukudi- 628 008. Tamil Nadu, India.

<sup>b</sup> Research Scholar, Affiliated to Manonmaniam Sundaranar University, Abishekapatti,

Tirunelveli- 627 012. Tamil Nadu, India.

E mail: thangam8991@gmail.com

### ABSTRACT

This research work reports on the bio-synthesis and the main physical properties of  $\text{Co}_3\text{O}_4$  nanoparticles by a completely green process using Aristolochia Indica natural extract as an effective chelating agent. Their surface/interface and optical properties are reported. The electrochemical activity, crystalline structure, morphology and optical properties of  $\text{Co}_3\text{O}_4$  nanoparticles were studied using various characterization techniques. The X-ray diffraction (XRD) and Energy Dispersive X-ray Spectroscopy (EDS) analysis confirmed the formation of  $\text{Co}_3\text{O}_4$  nanoparticles. The Fourier Transform Infrared Spectroscopy (FTIR) spectrum shows stretching vibration of  $\text{Co}_3\text{O}_4$  nanoparticles. The average size of the  $\text{Co}_3\text{O}_4$  nanoparticle observed from scanning electron microscopy (SEM) images is found to be 21 nm. The functional group was identified with the help of FTIR. The optical properties were calculated by UV and PL characterization. The optical characterization clearly gave the information about direct band gap 1.9 and 2.7 eV for core and 2.3 eV for core shell.

**Key words:** bio synthesis, Aristolochia Indica, physical and optical properties

## Biosynthesis and Characterisation of Samarium Oxide nanoparticles

**A.Vinothini<sup>1</sup> and Dr.A. Mathavan<sup>2</sup>**

<sup>1</sup> Research scholar,P.G. and Research Department of chemistry, V.O.Chidambaram college, Tuticorin, Tamilnadu

<sup>2</sup>P.G. and Research Department of chemistry, V.O.Chidambaram college, Tuticorin, Tamilnadu.  
Email: [jashvinothini@gmail.com](mailto:jashvinothini@gmail.com)

### ABSTRACT

Samarium oxide nanoparticles was successfully synthesised in a greener way by using the extract of *vigna radiata*. They are characterized by various techniques like UV-DRS, FT-IR, XRD and FESEM. A well-defined absorption peak was observed in the UV-visible absorption spectroscopy. The band gap energy of samarium oxide nanoparticles are 3.05eV which is well agreement with the previous literature. Sm-O-Sm stretching frequency vibration was observed at around 530 cm<sup>-1</sup> and in which confirmed that the presence of metal oxide nanoparticles. From XRD data average crystallite size is 41 nm. The sharp peaks are obtained and they are crystalline in nature.XRD results shows that the formation of cubic crystal structure.

**Key words:** Biosynthesis, nanoparticles, UV-DRS, FT-IR, XRD, FESEM.

## Investigation on Growth, Structural, Optical and dielectric properties of Ammonium Pentaborate (APB): A Nonlinear Single Crystal

Kiran<sup>1,2\*</sup>, N. Vijayan<sup>2</sup>, Debabrata Nayak<sup>1,2</sup> and Manju Kumari<sup>1,2</sup>

<sup>1</sup>*Academy of Scientific and Innovative Research (AcSIR), CSIR-HRDC Campus, Ghaziabad, Uttar Pradesh- 201 002, India*

<sup>2</sup>*CSIR- National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi 110 012, India*

\*Email: [kiran999nm@gmail.com](mailto:kiran999nm@gmail.com)

### ABSTRACT

Single crystals are playing remarkable role in the development of recent technology due to enormous applications in optical device fabrication, electronics, fiber optic communications, materials engineering, etc. The nonlinear optical crystals of inorganic materials are having good mechanical and thermal properties. Ammonium penta borate (APB) was found to be a good candidate for above said applications. APB single crystal was grown by slow evaporation solution growth technique at room temperature. A saturated solution was prepared from commercially available ammonium penta borate as solute and deionised water as solvent. The harvested crystal was subjected to different characterizations to check its suitability for device fabrications. The structure of the grown ingot was confirmed by powder X-ray diffraction technique. Transmittance ability and optical parameters of the grown ingot were assessed using UV-Vis., spectral analysis and the band gap was calculated using Tauc plot. The luminescence behaviour of the titled compound has been examined by photoluminescence (PL) spectroscopy. The third order nonlinear optical property was confirmed by Z-scan studies. The shock damage threshold and dielectric properties has been studied for the titled material. The observed results will be presented in detail.

## Studies of Lanthanum Oxide Doped L-Alanine Alaninium Nitrate NLO Crystal

G. Krishnamoorthia, R. Uvarani\*

*<sup>a</sup>PG and Research Department of Physics, Thiruvalluvar Government Arts College, Rasipuram-637401, Tamilnadu, India.*

E mail: gkmphysics@gmail.com (R. Uvarani)

### ABSTRACT

A pure L-alanine alaninium nitrate (LAAN) single crystals doped with lanthanum oxide ( $\text{La}_2\text{O}_3$ ), urea ( $\text{CH}_4\text{N}_2\text{O}$ ) and glycine ( $\text{C}_2\text{H}_5\text{NO}_2$ ) were developed from fluid solution by slow evaporation at room temperature. X-ray diffraction result reveals that LAAN crystallites with system with space bunch P21 and cell parameters  $a=7.836 \text{ \AA}$ ,  $b=5.428 \text{ \AA}$ ,  $c=12.809 \text{ \AA}$  and  $\beta=94.25^\circ$ . These parameters were marginally changes for doped crystals compared to pure LAAN crystal. The UV results shows that the great transmission property of the doped LAAN crystal within the whole visible region guarantees its reasonableness for SHG applications. The presence of dopants within the LAAN crystal was further affirmed through ICP studies. The functional groups were analyzed through Fourier change infrared spectra investigation. The microhardness and dielectric study at 100 Hz was found to be broadly higher than that of pristine LAAN. The ac conductivity was found to extend after doping due to the induced defects in crystal lattice. The grown crystals were also subjected to second harmonic generation (SHG) efficiency tests and it was found to be  $\text{La}_2\text{O}_3$  doped LAAN crystal is 2.8 times greater than that of KDP.

**Keyword:** Growth from solution; Doping; X-ray diffraction; Nonlinear optical material; Dielectric properties.

## Growth, Optical, and Thermo Electrical Properties of An Organic Nonlinear Optical Crystal: Brucinium Hydrogen Fumarate Sesqui Hydrate

**K. Gayathri<sup>1\*</sup>, R. Swadhi<sup>1</sup>**

<sup>1</sup>Department of Physics, Academy of Maritime Education and Training, Kanathur-603112,

\* E-mail: [gskrithick@gmail.com](mailto:gskrithick@gmail.com) (K. Gayathri)

### **ABSTRACT**

Single crystals of Brucinium Hydrogen Fumarate Sesqui hydrate, an Organic nonlinear optical material, were grown by slow solvent evaporation technique at room temperature. The grown crystals were subjected to different characterization analyses. The lattice dimensions were verified from the single crystal X-ray diffraction analysis. The functional groups present in the infrared and Raman spectrum gives structure of the compound and optical behavior of the crystal was obtained from UV-Vis analysis. The nature of variation of dielectric constant with frequency at different temperature was investigated. Thermogravimetric analysis carried out for the crystal exhibits a melting point at 73.80°C. Relative powder second harmonic generation efficiency is tested by high intensity Nd:YAG laser as a source and confirmed by the emission of green light. The chemical etching study was carried out using deionized water with ethanol (1:1) ratio as an etchant. The mechanical behaviour has also been studied by Vicker's microhardness test.

**Keywords:** Growth from solution, X-ray diffraction, Organic compounds

## Mineralogical characterization of rock samples collected from Paleolithic archaeological site of Attirampakkam, Tamil Nadu using FTIR and XRD techniques

A.Tamilarasi<sup>1</sup> A.Chandrasekaran<sup>1\*</sup>

<sup>1</sup>Sri SivasubramaniyaNadar College of Engineering (Autonomous), Chennai-603110, Tamilnadu

Email: [chandrasekarana@ssn.edu.in](mailto:chandrasekarana@ssn.edu.in); Tel; +91-9566759835

### ABSTRACT

In the present work, rock samples have been collected from Paleolithic archaeological site Attirampakkam, Tamil Nadu, India to assess the presence of mineralogical composition of samples using Fourier Transform infrared-spectroscopic (FT-IR) technique and these identified minerals are confirmed by using X-Ray Diffraction (XRD) technique. From FT-IR spectra the presence of minerals such as quartz, orthoclase, microcline, kaolinite, montmorillonite, dolomite, aragonite, and palygorskite minerals are identified in rock samples. In this samples quartz is the majorly presented mineral and crystallinity index of quartz ( $\text{SiO}_2$ ) is estimated for all the samples by comparing the ratio of intensity of the characteristic peak at 778 and 695  $\text{cm}^{-1}$  with the corresponding ratio for a standard sample. In rock samples, calculated crystallinity index of quartz is greater than 1 and shows that the disordered in nature. Additionally some more minerals such as hematite and rutile are identified in rock samples by X-ray diffraction technique. This extensive study shows that the archeological rock samples are wide variation in mineral composition.

**Keywords:** Rock, Paleolithic archaeological site, FT-IR, crystallinity index, XRD

## Synthesis and Biological Applications of TiO<sub>2</sub> Nanoparticles

**P.Maheswari<sup>1\*</sup>, Harish<sup>2</sup>, K.D.Nisha<sup>2</sup>, Ganesh Munuswamy Ramanujam<sup>2</sup>, M.Navaneethan<sup>3</sup>, S.Ponnusamy<sup>2</sup> and Hayakawa<sup>3</sup>.**

<sup>1</sup>*Department of Nautical Science, VISTAS, Thalambur - 603 103, India,*

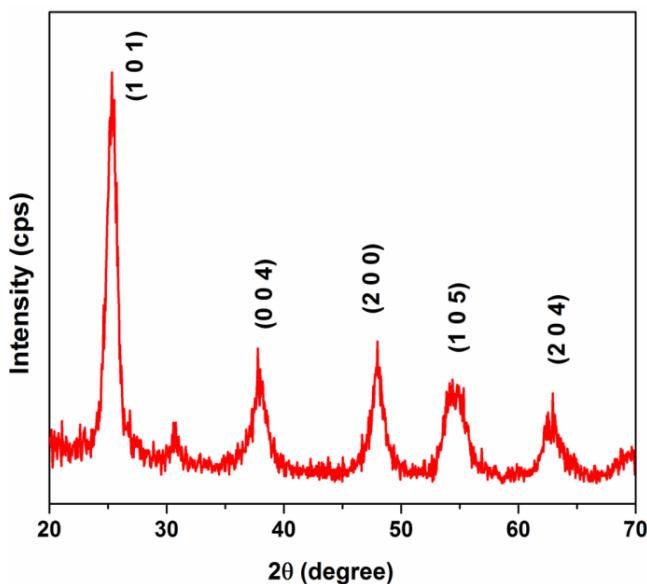
<sup>2</sup>*Department of Physics, SRM University, Kattankulathur-603 203, India,*

<sup>3</sup>*Research institute of Electronics, Shizuoka University, 3-5-1 Johoku, Naka-ku, Hamamatsu, Shizuoka 432 - 8011, Japan*

\* E-mail : [maheshvels23@gmail.com](mailto:maheshvels23@gmail.com)

### ABSTRACT

The main goal of this study was to synthesis TiO<sub>2</sub> nano particles by hydrothermal method. From the past, it was studied that the TiO<sub>2</sub> nano particles showed excellent antibacterial property. X- Ray diffraction studies revealed that the nano particles were highly crystalline. EDX showed that the particle consist of only Ti and O and no other impurities were found in it. The high concentration of the precursor showed that the particle size is increased with different morphology. The synthesized TiO<sub>2</sub> nanoparticles were tested against Gram positive and Gram negative bacteria.



**Key Words:** Crystalline, optical properties, EDX, antibacterial activity.

## Mineralogical and physic-chemical characterization of industrial lake sediments of Ranipet district, Tamil Nadu by spectroscopic techniques

V.Sathish<sup>1</sup>, A. Chandrasekaran<sup>1\*</sup>

<sup>1</sup>Sri SivasubramaniyaNadar College of Engineering (Autonomous), Chennai-603110, Tamilnadu

Email: [chandrasekarana@ssn.edu.in](mailto:chandrasekarana@ssn.edu.in); Tel; +91-9566759835

### ABSTRACT

In the present study, we present the physico-chemical and mineralogical characteristics of industrial lake sediments of Ranipet district, Tamil Nadu, India. In, sediment characterization, % of sand, silt, clay and pH and electrical conductivity (EC) of sediment samples were measured to identify its level of quality. In addition to that, major and minor minerals such as quartz, feldspar, clay mineral groups like (kaolinite and montomorilinte), carbonate mineral like calcite and organic carbon were identified by FT-IR technique and confirmed by X-ray diffraction technique. Also relative distributions of minerals are studied for sediments by calculating the extinction coefficient. This study proves that an infrared and X-ray diffraction spectroscopic investigation on sediments is found to be an ideal tool for mineral analysis in sediments. Pearson correlation analysis was performed between the physic-chemical properties and extinction co-efficient of minerals to know the existing relation between them.

**Keywords:** Lake Sediments, physic-chemical properties, FT-IR, XRD, extinction coefficients

## Green biosynthesis of platinum nanoparticles using plant-mediated extracts – a review

Jone Magadelin B<sup>1</sup>and Dr. AjithSinthuja S<sup>2\*</sup>

<sup>1</sup>*Ph.D. Research Scholar, Department of Chemistry, Holy Cross College (Autonomous), Nagercoil*

<sup>2</sup>*Department of Chemistry, Holy Cross College (Autonomous), Nagercoil-629004.*

E-mail: ajithsinthuja22@gmail.com

### ABSTRACT

Platinum nanoparticles (Pt NP's) have superior physicochemical properties and great potential in biomedical applications. Eco-friendly and economic approaches for the synthesis of Pt NP's have been developed to overcome the shortcomings of the traditional physical and chemical methods. Various biogenic entities have been utilized in the green synthesis of Pt NP's, including mainly plant extracts, algae, fungi bacteria, and their biomedical effects were assessed. Other biological derivatives have been used in the synthesis of Pt NP's such as egg yolk, sheep milk, honey, and bovine serum albumin protein. The green approaches for the synthesis of Pt NP's have reduced the reaction time, the energy required, and offered ambient conditions of fabrication. This review highlights the state-of-the-art methods used for green synthesis of Pt NP's, synthesis parameters, and their reported biomedical applications.

**Keywords:** Green synthesis, biosynthesis, platinum nanoparticles, anticancer, antioxidant, antibacterial, antifungal.

## Nanocrystalline Cobalt iron oxides for Stress Sensitivity.

S. G. Kakade<sup>1</sup> and Y. D. Kolekar<sup>2</sup>

<sup>1</sup> Department of Physics, Sir Parashurambhau College, Pune, Maharashtra, India-411030,

<sup>2</sup> Department of Physics, Savitribai Phule Pune University, Pune, Maharashtra, India-411007

Email: [sgksp189@gmail.com](mailto:sgksp189@gmail.com)

### ABSTRACT

The rare earth ion substituted nanocrystalline cobalt iron oxides were synthesized using sol gel auto-combustion method. The obtained samples were characterized using X-ray diffraction, FE-SEM microscopy and Raman spectroscopy to understand the effect on structural properties due to the rare earth ion substitution such as Erbium. X-ray diffraction patterns confirm the pure phase formation and the solubility limit. X ray diffraction pattern, scanning electron microscopy confirms the nano-dimension and Energy-dispersive X-ray spectroscopy (EDX) helps to confirm the concentration of the dopant. Raman Spectroscopy has been utilized to confirm the site occupancy and induced strain due to the substitution of rare earth ions in the inverse spinel structure of cobalt ferrite matrix. The M-H hysteresis shows the decrease in saturation magnetization and increase in coercivity with the substitution of dopant. This may be due to the decrease in A-B super exchange coupling. The piezomagnetic measurements and induced magneto-strictive derivative measured using p3 strain indicator authenticates the use of synthesized samples for piezomagnetic and stress sensitivity applications.

**Keywords:** Cobalt Ferrite, Nanoparticles, Stress sensitivity properties

## Synthesis and Characterization of Curcumin based Fluorescent sensor for sensing of Copper(II) ion in solution medium

R. Mahalakshmy\*

Department of Chemistry, Thiagarajar College, Madurai-625 009, Tamilnadu, India

\*Email: [mahalakshmy\\_chem@tcarts.in](mailto:mahalakshmy_chem@tcarts.in)

### ABSTRACT

Fluorescent sensors developed from Schiff base conjugated molecules have wide application and useful because of their chelating properties, better sensitivity, selectivity and low cost. Optical properties of such sensors get increased due to the forceful complexation with the metal ions. Schiff base contains O and N donor atoms show specific selectivity towards the metals and they have received much attention in biological as well as environmental system. Therefore, it is important to develop a fluorophore with coordination site for the binding of certain metal ions.

In the present work, we have attempted to examine the curcumin modified conjugated molecule as a fluorescent chemosensor for the selective detection of copper ion. The chemosensor has been prepared by the condensation of Curcumin and  $\alpha$ -Naphthylamine. The synthesized chemosensor has been characterized by IR, UV-Visible,  $^1\text{H}$ NMR, and GC mass spectroscopic techniques. The metal complexes of this chemosensor have been prepared by in-situ method by adding an appropriate aliquot of each metal calculated amount of the ligand stock solution. After the addition of  $\text{Cu}^{2+}$  to the chemosensor a new absorption band among 300-400 nm appears, while the other metal ions caused negligible changes of the absorption spectra. Binding affinity toward  $\text{Cu}^{2+}$  is found to be of higher magnitude compared to the other three cations mentioned. In fluorescence spectroscopic technique, the sensor showed quite moderate fluorescence emission due to the isomerization of  $\text{C}=\text{O}$  double bond in the excited state; however, after addition of  $\text{Cu}^{2+}$ , the sensor exhibited selective, sensitive and prominent fluorescent quenching response toward  $\text{Cu}^{2+}$  over a wide range of metal ions, such as  $\text{Al}^{3+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Hg}^{2+}$ ,  $\text{K}^+$ ,  $\text{NH}_4^+$ ,  $\text{Zn}^{2+}$  in a mixture of ethanol solvent at pH 7.2. Under the same experimental conditions, other competing metal ions had no effect on the fluorescence. By this project work, a wide horizon is therefore open for further investigation and developments in the field of fluorescent chemosensors.

## Study on Synthesis, Growth, Structural and Optical properties of Diisopropylammonium Oxalate Single Crystal

**Manju Kumari<sup>1,2\*</sup>, N.Vijayan<sup>2</sup>, Debabrata Nayak<sup>1,2</sup>, Kiran<sup>1,2</sup>, Sudha Yadav<sup>1,2</sup>and  
R.P.Pant<sup>1,2</sup>**

*<sup>1,2</sup>Academy of Scientific and Innovative Research, CSIR – National Physical Laboratory,  
New Delhi 110012, India*

*<sup>2</sup>CSIR – National Physical Laboratory, Dr K.S. Krishnan Road, New Delhi 110012, India*

**\*Email:** manjukumari1794@gmail.com

### ABSTRACT

The innovative technologies like optical data processing, optical limiting, electro-optic modulation, data computation, optical switching and telecommunication rely on the nonlinear optical (NLO) behaviour of a material. The NLO materials regulate the efficiency of these applications and thus, the development of NLO materials leads to the evolution of these various technologies. A diisopropylammonium oxalate single crystal has been harvested using slow evaporation solution growth technique. The structural information and lattice parameters have been evaluated by powder X-ray diffraction. The optical properties of grown crystal were evaluated by UV-visible, Photoluminescence analysis. The structure perfection of harvested crystal has been evaluated by high resolution X-ray diffraction (HRXRD) rocking curve measurements. The band gap was evaluated by Tauc's plot. The surface morphological pattern was thoroughly studied by Scanning electron microscopy (SEM) method. The observed results will be presented in detail.

## Quantum Chemical calculations of NLO Active Di isopropyl ammonium 4-aminobenzenesulfonate

**Adlin D Steffy<sup>1</sup>, D.Aruldhas<sup>2</sup>**

*<sup>1,2</sup>Department of Physics &Research Centre, Nesamony Memorial Christian College,*

*Manonmaniam Sundaranar University, Tirunelveli, India*

*E mail:* steffy909090@gmail.com

### Abstract

The main objective of the study was based on the quantum chemical computation methodology performed on the structural activity study in order to find the NLO activity of Diisopropylammonium 4-aminobenzenesulfonate molecule. The optimized structural parameter of the title compound were computationally obtained at DFT/ B3LYP level of theory using 6-31G(d,p) basis set using Gaussian 09 program and compared with the crystal data. Stability of the molecule that arises due to intra and intermolecular hydrogen bonding and hyperconjugative interaction were also analyzed by using NBO analysis. The Mulliken charge analysis, HOMO - LUMO energy gap, softness and electrophilicity indices were also analysed by this method. The molecular electrostatic potential was calculated to identify the electrophilic and nucleophilic sites which favour the formation of hydrogen bonds. In addition, Hirshfeld surface analysis was evaluated in order to discern the interactions in the crystal structure. The non-linear character of the compound was also determined by computing non-linear optical parameters like dipole moment, polarizability and hyperpolarizability.

**Keywords:** DFT, NBO, HOMO-LUMO, Hirshfeld, NLO

## Modifications of the band gap of CdSe nanocrystals by SHI irradiation: A supported theoretical DFT based analysis

Ratan Das<sup>1\*</sup>

<sup>1</sup>*Nano-Physics & Nanotechnology Research Laboratory,*

*Department of Physics, Tripura University, Suryamaninagar 799 022, India*

\*Email- dasratanphy@gmail.com

### ABSTRACT

CdSe nanocrystals have been prepared by wet chemical method, where selenium precursor, and cadmium chloride ( $\text{CdCl}_2$ ) are used. Then SHI irradiation experiment has been performed with 120 MeV  $\text{Ag}^{7+}$  ions at IUAC, New Delhi. XRD analysis confirms that this irradiated samples have structural changes along with the modifications in the lattice geometry. Such changes finally manifest in the modification of band structure as confirmed from the UV-Visible spectroscopic study and PL spectral study. Further, DFT based study on Quantum espresso Code supports the experimental results.

## Studies of MnO<sub>2</sub>/g- C<sub>3</sub>N<sub>4</sub> hetro structure efficient of visible light photo catalyst for pollutants degradation by sol-gel technique

S.Panimalar

*Ph.D Research scholar, Deapartment of Physics, Periyar University, Salem-5.*

E-mail address: cvesta19@yahoo.com (C. Inmozhi)

### ABSTRACT

MnO<sub>2</sub> and g -C<sub>3</sub>N<sub>4</sub> Hetero structure were constructed by simple sol-gel technique combined with annealing process were characterized different variety of techniques to understand the structural, morphological, optical and elemental composition were using XRD, TEM, Raman, UV, PL, BET and EDAX analysis. In fact, XRD and FESEM results shows that  $\alpha$ -phase MnO<sub>2</sub> Structure Were individually spherical shaped - like morphology nanostructures the average diameter 25 nm to 40 nm was observed apparently. In order to understand, the optical band gap properties and specific surface area of MnO<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> Na no composites were ranging from 2.55eV- 2.78eV & 67.23 -105.21 m<sup>2</sup>/g, which is confirmed through UV- vis DRS and N<sub>2</sub> nitrogen absorption desorption study. Therefore, the Photo catalytic activity of the Photo catalysts were estimated by degradation effect of methyl orange (MO) and toxic phenol pollutants. Among the results reveal that the MnO<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> hybrid catalyst have showed to owing the degradation Effect 98% and high stability (only loss 3.5%) towards phenol dye concentration. This can be attributed to the separation of photo generated electron- hole (e<sup>-</sup>/h<sup>+</sup>) Overwhelms the recombination of free charges were reported in detail.

### Keywords:

MnO<sub>2</sub>,g- C<sub>3</sub>N<sub>4</sub>,Sol-gel,Electron microscopy studies, Phenol, Degradation dye.

## Synthesis, growth and characterization of organic nonlinear optical material: morpholinium 2-chloro-4nitrobenzoate

A. Santha<sup>1</sup>, S. Karthick<sup>2</sup>, S. Ganesamoorthy<sup>3</sup>, S. Brahadeeswaran<sup>1\*</sup>

<sup>1</sup>Department of Physics, University College of Engineering (BIT campus), Anna University, Tiruchirappalli – 620024, India.

<sup>2</sup> Department of Physics, Muthayammal Engineering College, Rasipuram, Namakkal – 637408,

<sup>3</sup>Materials Science Division, IGCAR, Kalpakkam – 603102, India.

### ABSTRACT

Morpholinium 2-chloro-4-nitrobenzoate (M2C4N), a new nonlinear optical crystal was grown successfully by slow evaporation technique using acetonitrile as solvent at room temperature. The simulated and experimental powder XRD patterns confirmed the crystalline phase of M2C4N and it was found to crystallize in the noncentrosymmetric space group of P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>. Fourier Transform Infrared (FTIR) spectral analysis confirmed the presence of functional groups in the synthesized compound. The UV-Vis Spectrum showed that the grown crystal is transparent in the entire visible region. Second harmonic efficiency was determined using Kurtz power method in comparison with KDP to confirm the nonlinearity of the material.

**Keywords:** Slow Evaporation method, Nonlinear optics, XRD, FTIR

**Acknowledgement:** A.S, S.G and S.B would like to acknowledge UGC-DAE CSR through Grant number: CSR-KN/CRS-112/2018-19/1051

## Structural and Photoresponse Studies of Hafnium Doped Tin Diselenide Crystal

**Megha Patela<sup>\*</sup> , G. K. Solankia , Mohit Tannaranab , Chetan K Zankatb , Paratik Pataniyac , Abhishek Patelb , Sanjay Bhakhara , Anand patela , V. M. Pathaka , and K. D. Patel**

<sup>a</sup>*Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Anand-388120, Gujarat,*

<sup>b</sup>*Shri. Alpesh. N. Patel P. G. Institute of Science & Research, Anand 388001, Gujarat, India.*

<sup>c</sup>*Department of Physical Science, P. D. Patel Institute of Applied sciences, CHARUSAT, Changa 388421, Gujarat, India.*

*E mail:* meghapatel0802@gmail.com

### **ABSTRACT**

Recently, transition metal dichalcogenides (TMDCs) fascinate great attention due to their earth-abundant, low cost, chemical inertness and stable environmental characteristics. Recently hafnium based transition metal dichalcogenides are presumed to own high room temperature mobility and increasing interest of researcher. Though, only few experimental investigations are reported hitherto. In this work, the Hafnium doped tin diselenide ( $Hf_{0.05}Sn_{0.95}Se_2$ ) crystal was grown by direct vapour transport(DVT) technique using dual zone horizontal furnace. The stoichiometric proportion of elements was confirmed by Electron dispersive analysis of X-ray (EDAX). The Hexagonal crystal structure with most prominent peak (001) of grown material is determined by Powder X-ray Diffraction (XRD) analysis. The crystalline nature of grown material is confirmed by High resolution transmission electron microscopy (HRTEM). The selected area electron diffraction (SAED) pattern represents the material is highly crystalline in nature. Here we also demonstrate the photoresponse study of  $Hf_{0.05}Sn_{0.95}Se_2$  crystal. Ag/  $Hf_{0.05}Sn_{0.95}Se_2$ /Ag photodetector illustrated remarkable photocurrent under illumination of polychromatic light. The highest photocurrent 1.072 mA is measured under 120mW/cm<sup>2</sup> intensity of white light. The photocurrent increases with increasing intensity of polychromatic light. This excellent results obtained here shows the promising application of  $Hf_{0.05}Sn_{0.95}Se_2$  crystal as high performance photodetector.

## Synthesis and crystallite phase analysis of CdS, TiO<sub>2</sub> powders, CdS Thin-film for optoelectronic application

N.Gopinathan, A.Monica, S.Sathik Basha\*,

<sup>1</sup>Department of Physics, B.S.Abdur Rahman Crescent Institute of Science and Technology, Chennai

E mail: [sathiknoushin@gmail.com](mailto:sathiknoushin@gmail.com)

### ABSTRACT

Cadmium sulfide (CdS) is considered one of the most widely used II-VI semiconductors in optoelectronic device applications. In this report, cadmium sulfide (CdS) quantum dots (QD's) and TiO<sub>2</sub> powder are successfully synthesized by the Sol-gel method. The thin film of CdS QD's on TiO<sub>2</sub> was prepared by the drop-casting method. The XRD patterns were used to confirm the crystalline phases of CdS QD's and TiO<sub>2</sub>. These materials can be used in many optoelectronic device applications.

## Novel Fluorescent Carbon Quantum Dots and its Sensing Applications – A Review

Rajnee Yadav\*, V. Lahariya

Department of Physics, Amity School of Applied Sciences, Amity University Haryana-122413

Email: yadav.rajnee307@gmail.com

### ABSTRACT

Carbon Quantum Dots are highly fluorescence, chemical stable and non-toxic carbon nanoparticles. Due to its size dependent properties below 10nm size range, it has been widely used in diversify applications such as bio sensor, optical sensors, photocatalytic etc. Among various synthesis methods, hydrothermal and microwave irradiation are the most reliable, cost effective and quick methods for Carbon Dot synthesis. Further, surface passivation, doping, synthesis method is seen to be affecting the size and optical propertyof the dots. Recently, use of green precursors such as bio-waste, fruits, vegetables, plants as carbon source have been drawn much attention. Due to its chemically inert behaviour, CQDs have been used in metal ion and organic molecule sensing and detection. Metal ions such as  $Hg^{2+}$ ,  $Fe^{2+}$ ,  $Cu^{2+}$  etc. present in consumable items are toxic in nature. They have acquired health and environment hazardous issues. In this regard, results on carbon quantum dots have shown promising results for sensing and detection applications. This paper presents the comprehensive review on detection of contamination, metal ions, pesticides and organic molecules in various media. A brief study on biological sensing is also discussed and reviewed.

## Mechanical and thermal properties of glycine - phthalic acid single crystals

K. Rajesh<sup>1\*</sup>

<sup>1</sup> Department of Physics, AMET University, Kanathur, Chennai - 603112, India.

Email: [\\*krishjayarajesh@gmail.com](mailto:krishjayarajesh@gmail.com)

### ABSTRACT

Good quality Glycine - Phthalic acid (GPA) single crystals were grown by slow evaporation solution growth technique at room temperature. Powder X-Ray diffraction, thermal studies, dielectrical properties and Mechanical characterizations of GPA single crystals are analyzed in this article. Coats and Redfern method was used to determine kinetic parameters of GPA. The dielectric study was carried out by determining dielectric constant, dielectric loss and ac conductivity using LCR meter and the variation of these parameters with frequency and temperature was analyzed. Mechanical properties such as Vicker's microhardness number, work hardening index, standard hardness values, Yield strength, fracture toughness, brittleness index, and elastic Stiffness constant values were determined and analyzed using Vicker's microhardness tester.

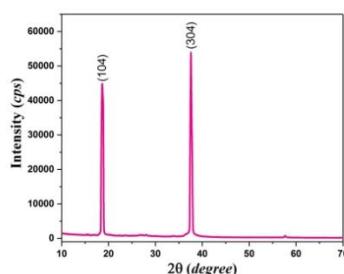


Figure : X-Ray diffraction pattern of GPA

## Red emission by samarium doped Zinc Aluminate synthesized by green combustion

R. Venkatesh<sup>a\*</sup>, L.N.Dhananjaya<sup>a</sup>, L.S. Reddy Yadav<sup>b</sup>, A. Jayasheela<sup>c</sup>

<sup>a\*,a</sup> Department of Physics, B.M.S. Institute of Technology and Management, Bangalore- 560 064, Karnataka, India.

<sup>b</sup>Department of Chemistry B.M.S. Institute of Technology and Management, Bangalore- 560 064, Karnataka, India.

<sup>c</sup>Department of Physics, Maharani Cluster University, Bangalore-560 003, Karnataka, India

E mail: [venki75.phy@gmail.com](mailto:venki75.phy@gmail.com)

### ABSTRACT

The Samarium doped Zinc aluminate ( $ZnAl_2O_4$ ) nanoparticles were prepared by green biogenic technique using Resinifera *E-tirucallilate*x. Nitrates of all precursors were used as starting materials. Naturally available Resinifera latex of Euphorbia family was used as a combustion agent. The samples prepared were calcined at  $900^{\circ}C$  for three hours. The final calcined powders were analysed for X-ray diffraction to study the structural analysis and an average crystallite size was calculated to be around 16 nm using Scherrer's and Williamson hall equation. Fourier Transform Infrared spectroscopy confirms the purity of the sample. The optical properties were determined by UV-Visible spectra. At an excitation wavelength of 408 nm, a high intense peak of emission was observed at 608 nm for transitions ( ${}^4G_{5/2} \rightarrow {}^6H_{7/2}$ ) of Sm<sup>3+</sup> ions in the PL spectra.  $ZnAl_2O_4$  phosphor doped with samarium can be used on the screens of optical electronic systems and also is suitable for emission of reddish orange colour.

**Keywords:** Green combustion; Luminescence; XRD; FTIR Spectra;

**Supercapacitive behaviour of CeO<sub>2</sub> nanoparticles in organic electrolyte****N. Maheswari\*, S. Kalpana, S. Rafi Ahamed**

*Department of Physics, Academy of Maritime Education and Training- Deemed to be University,  
Chennai.*

**E mail:** maheswari.n@ametuniv.ac.in

**ABSTRACT**

The nanostructured CeO<sub>2</sub> has been synthesized via hydrothermal method. Ce(NO)<sub>3</sub> was used as the precursor and CTAB act as a capping agent. The structural and morphological features of the samples were characterized by XRD, FTIR and SEM. The electrochemical performance of the CeO<sub>2</sub> electrodes has been studied through electrochemical studies like cyclic voltammetry, charge discharge studies and ac-impedance technique. Propylene carbonate was employed as an organic electrolyte in three electrode system. The highest specific capacitance of 370 F g<sup>-1</sup> at a scan rate of 2 mV s<sup>-1</sup> obtained for 1 M organic electrolyte. The same behaviour was confirmed by charge discharge studies. Further this electrode exhibits 100 % capacitance retention after 2000 continuous charge discharge cycles. This good cyclic stability and excellent charge storage behaviour reveals that the prepared CeO<sub>2</sub> electrode to be appropriate material for energy storage applications.

## Triple Bond Effect on Spacer and Acceptor of Phenothiazine Organic Dye Sensitizer for DSSCs: Quantum Chemical Investigation

R. Govindarasu, M. K. Subramanian

*PG & Research Department of Physics, Thiruvalluvar Government Arts College,  
Rasipuram-637401, Namakkal, India.*

*Email:* govindras80@gmail.com

### ABSTRACT

In this work, a series of phenothiazine based organic dye sensitizers for dye - sensitized solar cells (DSSCs) have been designed and screened. The electron - donor as a phenothiazine, cyanoacrylic acid as an electron acceptor based on donor - acceptor (D - A) as reference dye SB. So as to enhance the triple bond effect on spacer and acceptor moieties has been investigated based on SB dye. The substituent effect of the spacer and electron acceptor on the absorption spectra and photovoltaic (PV) properties have been investigated by the combination of density functional theory (DFT) and time - dependent DFT (TD - DFT) method approaches. Different exchange - correlation functional have been initially evaluated in order to establish an accurate methodology for calculating the excited state energy of the SB dye. Consequently, TD - CAM - B3LYP method and 6-311++G (d, p) basis set have used been the comparison of experimental value. From the calculated results, concluded that the phenothiazine - 4 - ((7- ethynylbenzo [c] [1, 2, 5] thiadiazol - 4 - yl) ethynyl) benzoic acid (PT - EBTEBA) dye was strongly grouped for more red - shift and electrons injected into semiconductors effectively. It is expected to provide some theoretical guidance on designing photosensitive with new metal - free organic dyes for application in DSSCs yielding highly efficient performance.

**Keywords:** Organic Dye; DFT and TD-DFT; Exchange-Correlational Functional; Electronic and Absorption Spectra.

## Design and Synthesis of SubstitutedImidazole-Phenothiazine based Organic Materialsfor Dye Sensitized Solar Cells

S. Sambathkumar, G. R. Divya Praba\*

Vivekanandha College of Arts and Sciences for Women (Autonomous), Elayampalayam,  
Tiruchengode, Namakkal 637 205, Tamil Nadu, India

E-Mail: sambathtacw@gmail.com

### ABSTRACT

Over the past decade, dye sensitized solar cells (DSC's) based on nanocrystalline mesoporous metal oxides (typically TiO<sub>2</sub>) have been intensively studied and developed as a promising, low-cost alternative to conventional silicon photovoltaic devices<sup>1</sup>. As a critical component in DSC's, the sensitizer plays a vital role in the light harvesting efficiency providing electron injection in to the conduction band of the semiconductor upon light excitation and they usually possess the structure<sup>2</sup> of Donor - π Bridge -Acceptor (D- π-A). In the present case, special consideration has given to the design of the molecular structure to determine its correlation to the performance of DSC's, a series of novel organic materials, whose structures has slightly different from one to another has been synthesized based on phenothiazine with an additional donor and characterized with various spectroscopic techniques. The Optical, and electrochemical performances of the synthesized organic dyes were analyzed systematically. This contribution brings further credit to these molecular designs as efficient sensitizers for DSCs, *en route* for a cheap and less toxic substitute to ruthenium based sensitizers and silicon based photovoltaics as potential eco-friendly energy candidates for the development of sustainable materials and technologies.

**Key Words:** Dye sensitized solar cells, electron injection, sustainable materials, carbazole, TiO<sub>2</sub>

## Importance of ZnO nanoparticles in solar cell application

Manjula R<sup>1</sup>, Daruka Prasad B<sup>2\*</sup>, Y. S. Vidya<sup>3\*</sup>

<sup>1</sup> Department of Physics, Government Science College (Autonomous), NT Road, Bangalore-560001, India

<sup>2</sup> Department of Physics, BMS Institute of Technology and Management, Bangalore, 560064

<sup>3</sup> Department of Physics, Lal Bahadur Shastri Govrnment First Grade College, RT Nagar, Bangalore – 560032, India

E-mail:darukap@bmsit.in and vidays.phy@gmail.com

### ABSTRACT

ZnO is an n-type semiconductor with a wide optical band gap and has high optical transmittance low electrical resistivity. It is also an environmental friendly material. Zinc Oxide nanoparticles (NP's) prepared by *using modified combustion method*. Prepared samples were characterized for structural, morphological and compositional details using Powder X-Ray diffractometer (PXRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDX) and UV-Vis Spectroscopic respectively. PXRD pattern confirmed the hexagonal quartzite structure of the product with the average crystallite sizes of about ~20 nm. The SEM images shows non-uniformity, agglomeration morphology. EDX spectra confirms the perfect purity of the ZnO NP's. Estimated energy band gap was found to be 3.34 eV, which correlates with the reported literature. Gas chromatography Mass spectrometer was used to know the possible polysaccharides and their compositions. ZnO serves as electron acceptor material. ZnO has important role in solar cells as it may enhance the absorption of light in to the device and improve the electrical transportation. Unique property of ZnO which makes them suitable for dye -sensitized solar cell applications, organic solar cell and hybrid solar cell, solar cell photodiode and transistor applications, due to the silent characteristics such as low cost, easy synthesis, non-toxicity, high stability and good optical properties.

**Keywords:** ZnO Nanoparticles; solar cell

## Nanosilicates doped Polymer Nanocomposites for the effective Electromagnetic Shielding

Nasreen Taj M<sup>1</sup>, Daruka Prasad B<sup>2,a</sup>, N Rama Rao<sup>3</sup>, Nagabhushana H<sup>4,b</sup>

<sup>1</sup>Department of Electrical and Electronics Engineering, HMS Institute of Technology,  
Tumakuru-572104, India

<sup>2</sup>Department of Physics, BMS Institute of Technology and Management, Avalahalli,  
Bangalore-560064, India

<sup>3</sup>Department of Electrical and Electronics Engineering, BMS Institute of Technology and  
Management, Bangalore-560064, India

<sup>4</sup>Prof. C.N.R. Rao Centre for Advanced Materials Research, Tumkur University,  
Tumakuru-572 103, India

\* E-mail: <sup>a</sup>darukap@bmsit.in; <sup>b</sup>bhushanvlc@gmail.com

### ABSTRACT

Innovative technologies such as advanced navigation, satellite communication, electronic devices, and wireless communications radiate powerful electromagnetic waves. This leads to electromagnetic interference which affects the human health and also the malfunctioning of equipment. Hence, to protect from these, EMI shielding materials with high electrical conductivity, high absorption capacity, light weight, good thermal stability and anti oxidation capability are in need. In this paper, we reported the thin film preparation by spin coating method. The prepared samples were the weight percentage of polymers and the doped strontium silicate nanopowders (NP's). For the prepared samples, characterization was done to know the crystal composition of NPs and also the morphological nature of the samples. The samples were subjected to electrical and EMI shielding studies. Results showed that the prepared samples have the crystallite size in the range of 22-29 nm and falls in the category of monoclinic crystal structure. Particles of NP's were almost spherical in shape shows the better adhesion between the silica substrate and the NP's. Polymer matrix provides the platform for the NP's to disperse and to have firmed bonding with the NP's, so that the film can be lifted off from the substrate. Results indicate that the prepared NPS achieves excellent electromagnetic shielding effectiveness of 38.1 dB at X band with only 1 mm of sample thickness. This study provided an idea for the structural design of high-performance electromagnetic shielding materials in the GHz frequency range (X band).

## Spectroscopic characteristics of Holmium impurities doped lead fluoroborate glasses.

Susheela K. Lenkennavar<sup>1</sup>

<sup>1</sup>Department of physics, Bangalore University, Bangalore -56, India

E mail: sushhh10@gmail.com

### ABSTRACT

The lead fluoroborate glasses doped with Ho<sup>3+</sup> ions were prepared by using melt quenching technique. The prepared glasses were characterized optical properties by using CIE diagram, absorption, and photoluminescence (PL) spectral measurements and Structural properties by X-ray diffraction (XRD) and infrared spectrophotometer (FTIR). The objective is to report detailed studies of glass matrix. Since Ho<sup>3+</sup> ion has been used as an excellent optical activator. Using proper optimization method we can make use of these lasers for photonic applications. From the luminescence spectra it's clear that synthesized glass offers red colour and can be an auspicious laser candidate.. The physical parameters have been evaluated. The densities ( $\rho$ ) of the glass samples were measured using Archimede's principle with toluene as an immersion liquid. Refractive indices (n) of samples were measured at 589.3 nm using an Abbe's refractometer and few physical parameters of the glasses like, molar volume ( $V_m$ ), molar refractivity ( $R_m$ ), polarizabilities ( $\alpha_m$ ), concentration of rare earth ion ( $N_i$ ), polaron radius ( $r_p$ ), inter ionic distance ( $r_i$ ), field strength(F), reflection loss ( $R_L\%$ ) and dielectric constant ( $\epsilon$ ). Using proper optimization method we can make use of these lasers for photonic applications. The detailed studies of them have been reported for the better understanding.

**Keywords:** X-Ray Diffraction, physical parameters, UV/Visible Spectroscopy, photoluminescence, FTIR.

## Study on preparation and characterization of polycarbonate composites for light diffuser application

**Kameshwari Devi S.H. and Arpitha C**

*Department of Polymer Science and Technology,, Sri Jayachamarajendra College of Engineering,  
JSS Science & Technology University, Mysuru, India.*

**Email:**shkdevi@sjce.ac.in

### **ABSTRACT**

Light emitting diodes (LED's) are long lasting, energy saving efficient light sources and also challenging for the lighting designers since these can create hot spots of focused light that can detract from the visual appeal of a fixture. To provide glare-free LED lighting, or to create wider angle viewing angles, designers choose diffusers to diffuse the light emitted by the LEDs. The study was to develop the polycarbonate composites for light diffuser application. Here in this work films are prepared using polycarbonate filled with different inorganic fillers like barium sulphate, magnesium oxide and titanium dioxide. The polycarbonate composites films were prepared using solvent casting method. The films prepared are evaluated in terms of mechanical, optical and thermal properties. According to the tensile properties observation tensile strength and elongation at break decreases with addition of the fillers. But modulus is increased with addition of fillers. But the film containing polycarbonate filled with barium sulphate retains all the three parameters compare to neat polycarbonate film. According to the optical properties observation the haze increases along with the retaining of transmittance with the addition of diffusing agents. But polycarbonate filled with titanium dioxide showed increased haze with decrease in transmittance compare to all other compositions. Differential scanning calorimetry results shows that there is no much changes occurs in the glass transition temperature with the addition of inorganic fillers. From the above results it can be concluded that the film containing barium sulphate content of 1% have optimum properties when compared to the other formulations and promising material for light emitting diode light diffuser application.

**Key words :** polycarbonate, barium sulphate, magnesium oxide , titanium dioxide

## Effect of rare-earth substitution on the dielectric and conductivity studies of $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ ceramics

**<sup>1</sup>S. Tanuja, <sup>1</sup>S Behera\***

<sup>1</sup> Department of Physics, Centurion University of Technology and Management,  
Odisha, 751050, India

E-mail: [saubhagyalaxmi.behera@cutm.ac.in](mailto:saubhagyalaxmi.behera@cutm.ac.in), [mamisana1410@gmail.com](mailto:mamisana1410@gmail.com)

### ABSTRACT

Structural, micro structural and dielectric properties of Gadolinium -modified sodium bismuth titanate ( $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ ) (NBT) ceramics were investigated. X-ray diffraction (XRD) analysis of the prepared materials confirmed the formation of the compounds with rhombohedral crystal system. The nature of scanning electron micrographs of the compounds showed the uniform distribution of grains throughout the samples. The temperature dependent dielectric parameters at various frequencies describe the improved dielectric properties on addition of trivalent Gd ions at A site. The dielectric constant at transition temperature was found to be decreased with increase of broadening of the dielectric peak on increasing Gd content in the sample. The transition temperature ( $T_m$ ) shifted to higher temperature side on addition of Gd (up to 2%), whereas the reverse trend was observed for higher concentration of Gd (i.e. 3 to 4%). The tangent loss was also found to be decreased on the incorporation of Gd into NBT. The ac conductivity of the Gd-modified NBT obeyed the Jonscher's power law behaviour.

**Keywords:** X-ray diffraction, SEM micrographs, Dielectric properties, Jonschers Power law

## Synthesis, Structural and DNA binding studies of 4-aminoantipyrine based Schiff base metal complexes

**M.Muthumariammal and R.Paulpandiany \***

*Research Department of Chemistry, VHNSN College, Virudhunagar-626 001, Tamil Nadu.*

\* E-mail:paulpandiansrs@gmail.com

### **ABSTRACT**

Schiff bases form an important division of organic compounds in chemistry due to their constructive physical and chemical properties and large number of reactions they undergo. Schiff bases, derived from substituted aliphatic amines and aromatic aldehydes have a wide variety of applications in many fields, *e.g.* biological, inorganic and analytical chemistry [1,2]. Complex combinations of Cu(II), Ni(II), Co(II) and Zn(II) were synthesized with the condensation of 4-aminoantipyrine with cinnamaldehyde. The synthesized metal complexes were characterized by various physico-chemical techniques and they were found to be stable in air and moisture. The complexes have been characterized by the micro analytical data, IR, UV-Vis., <sup>1</sup>H NMR, <sup>13</sup>C NMR and ESI mass spectra. Their magnetic susceptibility values of the complexes at room temperature are consistent with octahedral geometry around the central metal ions. These complexes show lower conductance values, supporting their non-electrolytic nature. The data show that the complexes have composition of [ML<sub>2</sub>] type. *In vitro* CT DNA binding studies were performed by employing UV-vis. absorption titration, viscometry and cyclic voltammetry methods. These techniques indicate that all the metal complexes bind to DNA *via* intercalation mode. Fascinatingly, copper complex are found to exhibit greater binding affinity than other complexes.

**Keywords:** Physico-chemical techniques; non-electrolytic nature; octahedral geometry; intercalation mode; binding affinity

## Physicochemical properties of metal ion embedded nanocomposite glass materials for bio sensing application.

**S. Rafi Ahamed<sup>1</sup>, P.Manikandan<sup>2\*</sup>,S.Kalpana<sup>1</sup>, N.Maheswari<sup>1</sup>**

<sup>1</sup>. Department of Physics, Academy of Maritime Education and Training, Kanathur -603112, Chennai, Tamil Nadu India

<sup>2</sup> Department of Physics, Krishnasamyi College of Engineering & Technology, S Kumarapuram 607109 Cuddalore Tamil Nadu India

Email: rafiahamed81@ametuniv.ac.in

### ABSTRACT

The optical, electronic, magnetic and chemical properties of these nano clusters are found to be very different from those of the bulk form and they also depend sensitively on their size, shape and chemical composition. Thus, the clusters of transitional metals are found to have reactivities that are considerably larger than those of the bulk by orders of magnitude with size. Optical absorption spectroscopic analysis was done on the metal nanocluster composite glasses, and the spectra are well studied as a function of various post ion-exchange treatments and different sizes. The noble metal nanoclusters play an important role for nanobiomedical and modern optical devices. Raman scattering is a non destructive tool for probing the composition and symmetry of nanocrystalline semiconductors and insulators. It has been prominently exploited well in biological applications, where it is able to detect and analyze DNA and RNA molecules. Generally, there are four main types of Raman spectroscopy, but the most feasible in biological field is the SERS. The present paper explored the single and bi-metallic nanoclusters embedded in soda-lime glass that is prepared by ion-exchange method. The ion-exchanged glasses are annealed by different methods. These samples exhibit surface plasmon and surface enhancement effect. As size effects are an essential aspect of nanomaterials, the effect of size on the optical absorption metal nanoclusters shall be studied through optical absorption, SERS, TEM, and X-ray diffraction. From this study we find optimized SERS substrate for single and different molecule detection.

**Key words:** Metal Cluster, Optical Absorption, SERS, FESEM, XRD, Hardness.

## Thermoacoustical Parameters and Excess Properties of Binary liquid Mixtures at Various Temperature

Duraivathi C.<sup>1\*</sup>, Jeya Priya J.<sup>1#</sup> & Poongodi J.<sup>1</sup>, Johnson JeyakumarH.<sup>2</sup>

<sup>1\*,2</sup>Pope's College, (Physics), Sawyerpuram, (Tamil Nadu), India

<sup>1#</sup>V.O. Chidambaram College, Thoothukudi, (Tamil Nadu), India

<sup>1</sup>Kamaraj College, (Physics), Thoothukudi, (Tamil Nadu), India

Affiliated to Manonmaniam Sundaranar University, Tirunelveli

\*E-mail: cduraivathikamali@gmail.com, jayapriyaj9610@gmail.com

### ABSTRACT

An endeavor has been made to report the ultrasonic velocity ( $U$ ), density ( $\rho$ ) and viscosity ( $\eta$ ) of the binary liquid mixtures of lactic acid with acetone and methanol of the various compositions at different temperature. Thermo dynamical parameters such as adiabatic compressibility, free length, free volume, internal pressure, etc., have been calculated using these measured data. The excess values of the above parameters are also computed and the results are utilized to dispute the nature of interaction taking place among the component of liquid mixtures in the binary system.

**Keywords:** ultrasonic velocity, density, free length, free volume, excess values.

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## Growth, Structural and Morphological Studies of V Doped WSe<sub>2</sub> Compound

**Badal L. Chauhan, G. K. Solanki, Sanjay A. Bhakhar , Nashreen F. Patel, Anand Patel,  
Pratik Pataniya, K. D. Patel and V. M. Pathak**

<sup>1</sup>*Department of Physics, Sardar Patel University, Vallabh Vidyanagar Anand-388120*

<sup>2</sup>*Department of Physics, P.D. Patel Institute of Applied Science, Charotar University of Science  
and Technology, Changa388421, India*

**Email:** b.chauhan389@gmail.com

### ABSTRACT

Transition metal Dichalcogenides (TMDCs), provides significant advantages in electronics and optoelectronics devices modelling and engineering to enhance devices performance. Additionally, these TMDC materials show a good ability to bear different surroundings in terms of temperature, low and high pressure, electric and magnetic field. Here in the present investigation, we report the growth and characterizations of pure and Vanadium doped Tungsten Di-Selenide (V-WSe<sub>2</sub>) compound grown by Direct Vapour Transport technique. The elemental conformation was done by energy dispersive analysis of X-ray (EDAX). The structural analysis of the grown material was carried out by powder X-ray diffraction. The scanning electron micrographs show the surface morphology through which the morphological effect of dopant material can be estimated. Energy band gap plays an important role for the device applications of the grown materials. From the UV-Vis analysis, bandgap comparison of pure and doped materials was carried out.

**Keywords:** TMDC material, Crystal Growth, Doping, XRD

## Molecular docking studies and anticancer activity of (E)-2-((2-chlorophenylimino)methyl)phenol

T. Beena<sup>a</sup>, L. Sudha<sup>a</sup>, S. Shobana<sup>b</sup>,

<sup>a</sup>Department of Physics, SRM IST, Ramapuram, Chennai 600089, Tamil Nadu.

<sup>b</sup>Department of Bioinformatics, School of Bioengineering, SRM IST, Kattankulathur,

E mail: beenat@srmist.edu.in

### ABSTRACT

Molecular docking studies for the synthesized (E)-2-((2-chlorophenylimino)methyl)phenol (CMP) into ATP-binding site of EGFR-TK's was performed and the ability of the compound to inhibit the tumorogenic agents and the binding mode in the active site of EGFR- TK's was investigated. The epidermal growth factor receptor (EGFR) is highly expressed in many types of cancers, especially colon, breast and bladder cancers. Targeting this EGFR receptor represents a good strategy for the design of new anticancer drugs. In CMP, three hydrogen bond interactions were prominently noted; one is formed between hydrogen atom of SER 787 and oxygen atom of CMP. The remaining two hydrogen bonds were formed between the hydrogen atom of ASP 960 and the oxygen atom of CMP and between GLN 788 hydrogen atom of ASP 960 and the oxygen atom of CMP. Key residues involved in interactions are ASN784, GLY786, GLN 788,SER 787 ,GLU 961,ILE 957,PRO 951,LEU 790, LEU791, GLU 961, TYR 789 and exhibited the highest dock score of -8.97 kcal/mol in comparison to the standard erlotinib inhibitor which exhibited a glide score of -10.54. Anticancer activity of the compound CMP was screened using tumor cell lines. Measurements were performed and the concentration required for a 50% inhibition (IC<sub>50</sub>) was determined graphically. The analysis of the data reveals that, in CMP compound, the % cell viability on MCF-7 cell line IC<sub>50</sub> value is 54.71% and for the cell line HT-29 IC<sub>50</sub> value is 50.79% for the concentration of 31.2 g/mL which shows the ant proliferative activity against tested cell line.

## Investigations on performance of traffic sign recognition system under improved VGG 16 network

**R.Vijay**

*Department of Electronics and Instrumentation Engg., SRM Institute of Science and Technology,  
SRM University, Kattankulathur, Chennai.  
Email: vijayrajendran2012@gmail.com*

### **ABSTRACT**

Traffic signs are crucial for keeping our roads safe and efficient. We must carefully evaluate the capabilities and limitations of automated traffic sign systems for detection. The number of traffic signs in existing datasets is restricted in terms of the type and severity of difficult circumstances because of the lack of metadata relating to these conditions, it is impossible to analyse the effect of a single element. Several climatic conditions are changing at the same time. In order to overcome the existing dataset's flaws, we take a different approach. An improved convolution neural network (CNN) technique to address the entire detection and recognition process. End-to-end learning is automated. We offer a number of enhancements that are tested on traffic sign detection and lead to improved overall performance. This method is used to recognise 300 traffic-sign categories are included in our new dataset. The findings are presented for some of the most difficult traffic sign categories that have yet to be addressed in earlier research. We present a detailed investigation of the deep learning strategy for detecting traffic signs with considerable intra-category appearance variation, demonstrating error rates of less than 3% the proposed method. We needed to look at the average performance of a traffic sign recognition system employing upgraded CNN architecture, and we discovered that detection performance can drop dramatically under difficult conditions. To enhance precision and accuracy in difficult weather conditions such as snow, haze, rain, darkness, noise, and blur. Our frequency domain analysis revealed that the simulated difficult conditions of detector performance.

## Studies on Copper Bismuth Selenide Nanoflakes for Photovoltaic applications.

C. Bhagya lakshmi<sup>1</sup>, K. Thangakavila, S. Jayalakshmi, S. Annavenus

<sup>1</sup> Physics Research Centre, St. Xavier's college (Autonomous), Palayamkottai-627002, India.

Email id: [annavenus\\_physics@yahoo.co.in](mailto:annavenus_physics@yahoo.co.in), [bhagya.jey@gmail.com](mailto:bhagya.jey@gmail.com)

### ABSTRACT

Copper bismuth selenide (CBSe) nanoflakes have successfully been synthesized via solvothermal method using Copper oxide and bismuth oxide as a major precursors. The formation of CBSe nanostructure and its secondary phases were also clearly evinced in phase characterization studies. The morphology of CBSe were revealed through SEM studies. The optical bandgap value were estimated as 1.3 eV using Tauc's plot. The vibrational bonding of Se in CBSe were shown in FTIR spectrum. The photoluminescence spectra shows the excitation peaks at nm. Cyclic voltammetry performance in CBSe results that the cathodic peaks are at 0.45v and anodic peaks shown at 0,01A. Thus the prepared CBSe nanoflakes using CuO and BiO as starting materials have betterment in the results and suggested for photovoltaic applications.

**Keywords:** Copper Bismuth Selenide, Cyclic Voltammetry, Solvothermal Method, Nanoflakes.

## Spectroscopic Studies and physic-chemical properties on Red soil samples in Thiruvannamalai, Tamilnadu, India.

**S. Manigandan, A. Chandrasekaran, A. Lakshmi**

*Sri SivasubramaniyaNadar College of Engineering (Autonomous), Chennai-603110, Tamilnadu*

Email: [chandrasekarana@ssn.edu.in](mailto:chandrasekarana@ssn.edu.in)

### **ABSTRACT**

In this present investigation, we measured the physico-chemical and mineralogical characteristics of red soil samples collected from 8 different locations in Na. Pudhoor to Velanandhal situated in Thiruvannamalai, Tamil Nadu, India. In, soil characterization, % of sand, silt, clay and pH and electrical conductivity (EC) of red soil samples were performed to identify its level of quality. In addition to that, major and minor minerals were identified by FT-IR technique using their observed frequencies by comparing available literatures, resulting of quartz and clay minerals like kaolinite and montmorillonite are majorly present in the samples and also feldspar minerals (orthoclase, microcline, and albite) and carbonate minerals (aragonite and calcite) are present in the samples and confirmed by X-ray diffraction technique. In addition to that, extinction co-efficient were used to measure the relative distribution of minerals in soil samples. So that this study proves the spectroscopic investigation on red soils is found to be an ideal tool for mineral analysis in soil samples.

**Keywords:** Red soil, FT-IR, XRD, Minerals, Extinction co-efficient,

## Molecular Interactions of Aqueous Glycine with Butyltriglycol System at 303.15 K

K.Karpagavalli<sup>1</sup> and K.Raju<sup>2</sup>

<sup>1</sup>AVC College of Arts and Science (autonomous), Mannampandal, Mayiladuthurai.

<sup>2</sup>Easwari Engineering College (autonomous), Ramapuram, Chennai

Email: karpagam2abi@gmail.com

### ABSTRACT

Density, viscosity and ultrasonic velocity have been measured for aqueous glycine with butyl triglycol system at 0.1 to 1 mole fractions and at 303.15 K. With the concentration increases of BTG, the density, viscosity and ultrasonic velocity decreases as interactions becomes weak, it indicate decrease in solute-solvent and solvent- solvent interactions which results structure-breaking of the solvent. Thus it is clear from the above parameters that there is a weak association between present systems showing hydrophobic nature.

**Keywords:** Adiabatic compressibility, Relaxation time, Wadas constant

**Spectroscopic and molecular docking studies of Benzhydrylpiperazine****N.R. Sheela<sup>a</sup>***<sup>a</sup>Department of Physics, Sri Venkateswara College of Engineering, Sriperumbudur, 602 117,*

E mail: nrsheela@svce.ac.in

**ABSTRACT**

The quantum level theoretical studies by density functional theory have been carried out on the compound benzhydrylpiperazine. The optimized geometry and the vibrational frequencies are computed by the density functional theory with the B3LYP method and 6-311++G(d,p) basis set. The stability of the compound is determined by natural bond orbital analysis. By Time Dependant density functional theory mechanism the maximum absorption wavelength is obtained and compared with the UV-Vis experimental spectrum. By using the frontier molecular orbitals, the energy values and all other important parameters are elucidated. The Non-Linear Optical characteristics like dipole moment, polarizability, and hyper polarizability of benzhydrylpiperazine were analyzed by changing the keyword on the same basis set. The reactive areas around the molecule are found by molecular electrostatic potential studies. ADME studies have been carried out.

**Keywords:** DFT; NLO; TD-DFT; NBO; MEP

## Preparation and characterization of CuO modified MoS<sub>2</sub> thin films for solar selective absorbers

J.Selvi<sup>1\*</sup>, V.Prasanna Venkatesh<sup>2</sup>, N. Murugesan<sup>3</sup>, and S. Karthick Kumar<sup>3</sup>

<sup>1</sup>*Department of Physics, Hindustan Institute of Technology and Science, Chennai*

<sup>2</sup>*Department of Physics, Velammal College Of Engineering and Technology, Madurai*

<sup>3</sup>*Department of Physics, Sethu Institute of Technology, Virudhunagar*

\*corresponding author: angelinselvi11@gmail.com

### ABSTRACT

A thin cupric oxide film (CuO) was straddled with MoS<sub>2</sub> nanoparticles are proposed as a promising solar absorber layer in the solar collectors. The CuO nanoparticles were incorporated with the MoS<sub>2</sub> (MoS<sub>2</sub>/CuO) thin films, grown via solvothermal followed by dipcoating technique on the aluminium (Al) substrate. The surface morphology of the pure CuO and MoS<sub>2</sub>/CuO thin films were carried out by scanning electron microscopy (SEM). The structural properties were analyzed by the X-ray diffraction (XRD). The energy dispersive spectroscopy (EDAX) studies were used to analyze the present chemical composition in the prepared samples. The influence of the optical properties of the MoS<sub>2</sub>/CuO nanocomposite thin films were investigated in details by the UV-vis NIR data, which showed the reduction in optical reflectance, and an enhancement in its solar absorptance after the composition. The significant improvement in optimization of the MoS<sub>2</sub>/CuO solar absorbers was attributed to enhancing the absorption of visible region and increasing its solar selectivity.

**Keywords:** MoS<sub>2</sub>/CuOnanocomposite, thin films, dipcoating and solar absorbers

## Growth, Optical, Nonlinear optical and Dielectric properties of a Semi-Organic Single Crystal: 1,4 Oxazinanium dihydrogen phosphate

**H. Arul<sup>1\*</sup>, M. Lakshmipriya<sup>2</sup> and M. Gowrishankar<sup>3</sup>**

<sup>a</sup>*Department of Physics, School of Foundational Sciences, Kumaraguru College of Technology, Coimbatore*

<sup>b</sup>*Department of Physics, School of Basic Sciences, Vels Institute of Science Technology and Advanced Studies, Chennai*

<sup>c</sup>*Department of Science and Humanities, Sri Venkateshwara College of Engineering and Technology, Chitoor*

**E mail:** arul.h.sci@kct.ac.in

### ABSTRACT

Engineering of new nonlinear optical materials, structures, and devices with the enhanced figure of merit has developed a major force to drive nonlinear optics from the laboratory to real time applications. Incorporation of an inorganic additive with an organic molecule provides high optical nonlinearity, chemical flexibility, thermal stability, and excellent transmittance in the visible region. Oxazinanine is a strong alkali, which can be considered as a kind of secondary aliphatic amine. The incorporation of dihydrogen phosphate ion into six-member ring of morpholine makes the molecule a good nucleophile. Morpholinium dihydrogen phosphate single crystals were synthesized and subsequently grown by slow evaporation technique at room temperature for nonlinear optical applications. The grown crystal has been subjected to single crystal X-ray diffraction to confirm the structure. The crystal belongs to the monoclinic system with the space group P2<sub>1</sub>. The UV-Vis-NIR spectroscopic study was carried out on the grown crystal, and it shows good optical transparency in the entire visible region with a minimum cut-off wavelength of 289 nm. Optical band gap was computed as function of photon energy using Tauc's plot as 4.32eV. Refractive index of the grown crystal was determined using Metricon Prism Coupler. Dielectric studies were carried out for various frequencies at different temperatures. Dielectric constant, dielectric loss and AC conductivity were calculated and plotted as a function of frequency at different temperatures. The value of activation energy for ionic migration was calculated using Arrhenius plot. The second harmonic conversion efficiency was determined using Kurtz-Perry powder technique and the efficiency was found to be 1.4 times greater than that of standard KDP.

## Copper (II) - Schiff Base- Chlorine / 1, 10-Phenanthroline Complexes: Synthesis and Characterization

**Dr. Addla Shilpa**

*Department of Chemistry Mahatma Gandhi Institute of Technology (MGIT), Kokapet, Hyderabad,  
Telangana 500075, India.*

Email : addlashilpa\_chem@mgit.ac.in

### ABSTRACT

NN donor bidentate schiff base (SB) was synthesized by condensation of aromatic planar ligand with Phenylene diammine in methanolic medium. Yellow coloured formed schiff base was isolated and characterized by spectroscopy techniques like IR, Proton NMR, ESI-MS. Copper (II) complexes of schiff base ligand were synthesized with and without heterocyclic base 1, 10 Phenanthroline i.e.  $[\text{Cu}(\text{SB})(\text{Phen})]$  and  $[\text{Cu}(\text{SB})\text{Cl}_2]$ . Complexes formed were characterized by Magnetic moment, Conductivity measurements, Elemental Analysis, ESI-MS, IR, UV-Vis spectroscopy. Analytical data for complexes agree well with the molecular formulae proposed for complexes. Characterization data for complexes indicate a square planar geometry around Cu(II) with the schiff base and 1,10 phenanthroline coordinating through N,N donor atoms. Molecular modelling studies were performed to get energy minimized and stable structures for complexes. Complexes display a band at around 530-570nm region in the UV-Vis spectroscopy confirming distorted square planar geometry of complexes. In future it is planned to study their DNA binding and Cleavage Ability.

**Keywords:** Aromatic schiff base, Phenylene Diammine, Cu(II) Complexes, 1, 10 phenanthroline, Molecular Modelling studies.

**Structural, optical, and elastic properties of oleic acid coated  $Zn_xFe_{3-x}O_4$   
( $0.4 \leq x \leq 0$ ) mixed ferrite nanofluids**

**Prashant Kumar<sup>1,2,\*</sup>, Saurabh Pathak<sup>4,5</sup>, Arjun Singh<sup>2,3</sup>, Kuldeep<sup>1,2</sup>, H. Khanduri<sup>1</sup>,  
G.A.Basheed,<sup>1,2</sup> R.P.Pant<sup>1,2,\*</sup>**

<sup>1</sup>*Indian Reference Materials Division, CSIR-National Physical Laboratory, New Delhi-110012*

<sup>2</sup>*Academy of Scientific and Innovative Research, CSIR-NPL Campus, New Delhi-110012*

<sup>3</sup>*Department of physics, Indian Institution of Technology, Jammu-181221*

<sup>4</sup>*School of Engineering, RMIT University, VIC 3000 Australia*

<sup>5</sup>*Department of Mechanical Engineering, University of Melbourne, Parkville, VIC, 3010 Australia*

\*Corresponding Authors- prashantkhichi92@gmail.com, rppant@nplindia.org

## ABSTRACT

A series of zinc doped  $Fe_3O_4$  magnetic nano-fluids with different Zn concentrations represented as  $Zn_xFe_{3-x}O_4$  ( $x=0, 0.1, 0.2, 0.3$  &  $0.4$ ) were synthesized by the wet chemical co-precipitated technique and oleic acid used as surfactant to prevent the agglomeration of magnetic nanoparticles. Structural, morphological, optical and elastic properties of these ferrofluids have been investigated using different sophisticated characterization techniques. The structural and Rietveld refinement was carried out by the XRD data and the result confirms that single cubic spinel phase belongs to  $Fd\bar{3}m$  (227) space group and the average crystallite size calculated from the XRD data varies from 12 to 15 nm. The Transmission Electron Microscopy (TEM) studies revealed that the particles are spherical in nature and mean particle size varies from 15 to 20 nm and all samples are polycrystalline in nature. The SEM result was also demonstrated the surface morphology of magnetic particle is spherical in shape nanoparticle with least agglomeration. FTIR spectroscopy showed the molecular dynamics and the formation of cubic spinel phase of frequency bands at  $560\text{ cm}^{-1}$  and  $420\text{ cm}^{-1}$  respectively and also gives the evidences of oleic acid are present on the surface of MNPs. The UV-Visible measurement we have estimate the band gap of the materials lies between (2.2 to 2.8, 3.1 & 3.8 e V) of the all the sample form optical absorption spectra fitting by Tauc plot method. Therefore, the synthesized magnetic nanofluids have a potential candidature in the biomedical filed like magnetic fluid hyperthermia, MRI and targeted drug delivery.

**Keywords:** HRTEM, Polycrystalline, SEM, Ferrofluids, Magnetite, MNP's, FTIR.

## Screening and Molecular Docking the Bioactive Constituents of Solanum nigrum For Inhibiting Gastric Acid Secretion

**S. Veni Sri Ambika and S. Gunasekaran**

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

**Email :** venisriambika@rediffmail.com

### **ABSTRACT**

Oral route is the direct path way for both nutrients and pathogens. Gastric acid plays an important role in digesting food and destroying pathogens. But excess secretion of gastric acid will lead to the disease Peptic ulcer. So, like other bodily functions, secretion of gastric acid has to be regulated. Acid -suppression therapy is an effective treatment for Peptic Ulcer. Gastric acid is secreted by a special cell called Parietal cell. The final target in the parietal cell for neutralizing the acid is gastric H<sup>+</sup>/K<sup>+</sup> - ATPase (Proton Pump). For the secretion of gastric acid, H<sup>+</sup> and K<sup>+</sup> ions are exchanged between the cytoplasm and lumen of the stomach. Recently, Potassium acid blockers (PCABs) are prescribed for acid suppression therapy. K<sup>+</sup> ions present on the apical membrane of the Parietal cell are the logical targets for PCABs. PCAB's competes with the potassium ion and prevents it in reaching the binding site of proton pump from the apical side.

Nowadays, some of the secondary metabolites and vitamins present in the plants act as ligands for biological targets and perform as drugs. Solanum nigrum is one such plant considered for the study. GC-MS study has been carried out to identify the bioactive constituents present in the leaves of solanum nigrum. Vitamin E is one of the bioactive constituents identified from the GC-MS study.

Molecular docking is a powerful tool in the field of drug discovery. Using Vitamin E as a ligand molecular docking has been carried out for inhibiting proton pump from the apical side of the Parietal cell. Similarly, molecular docking has been carried out for the standard PCAB Vonoprazan. The docking score and glide energy of Vitamin E and Vonoprazan are compared.

**Molecular structure and vibrational analysis of N-Allyl-N-ethylformamide  
by FT-IR &UV-Vis spectroscopies combined with DFT calculations**

**P.Rajesh<sup>1\*</sup>, C.Prabhu<sup>1</sup> and K.Pratheebha<sup>2</sup>**

*<sup>1</sup>Department of Physics ,School of Basic Sciences, Vels Institute of Science Technology & Advanced Studies(VISTAS), Pallavaram, Chennai, 600 117, Tamilnadu, India.*

*<sup>2</sup> Easwari Engineering College (autonomous), Ramapuram, Chennai*

**E mail :**

**ABSTRACT**

The complete vibrational assignment and analysis of the fundamental vibrational modes of N-Allyl-N-ethylformamide was carried out using the experimental FT-IR, and UV-Vis data and quantum chemical studies. The observed vibrational data were compared with the wavenumbers derived theoretically for the optimized geometry of the compound from the DFT-B3LYP gradient calculations employing 6-311G (d,p) basis set. The HOMO-LUMO energy gap has been calculated. The intramolecular contacts have been interpreted using natural bond orbital (NBO) analysis. Important non-linear properties such as first hyperpolarizability of N-Allyl-N-ethylformamide have been computed using B3LYP quantum chemical calculation.

**Keywords:** FT-IR, FT-Raman, UV-Vis, NBO

**Study of various Boride crystal derivatives- Hardness properties****R.Raja\*, S. Venkatesh**

Department of Physics, SCSVMV UNIVERSITY ,Kancheepuram 631561.

E mail: sridev.raja@gmail.com

**ABSTRACT**

Crystals, since way back, have been experimented with to discover the hardest substance in existence. The hardest substance currently known is Diamond which is scarcely available in nature and can also be produced artificially, but with extreme environmental conditions. To limit the expenditure in producing a hard material that has many industrial and scientific uses, researchers all over the world have endeavoured to fabricate a substitute for the Diamond. This article consists of a collection of such samples (specifically, the derivatives of Borides) that have been produced as a potential material in terms of crystals with high hardness. The article also discusses their crystal structure as analyzed by the process of X-Ray Diffraction and their hardness as given by the Micro Vickers Hardness Test. A comparative study has been put forth to better understand the importance of the family of Boride crystals as one of the major proxies for the expensive Diamond.

**Synthesis of 2,2'-[<sup>1Z,11Z</sup>-2,5,8,11-Tetraazadodeca-1,11-diene-1,12-diyldiphenol and its Vibrational Spectroscopic characterization**

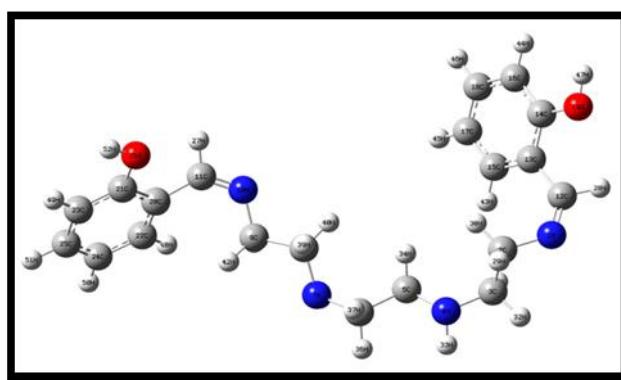
**<sup>a</sup>V.Ragavendran\***

*<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Enathur, Kanchipuram, Tamilnadu, India - 631 561*

**Corresponding Author:** [ragav910@gmail.com](mailto:ragav910@gmail.com)

**ABSTRACT:**

In the present study, the title compound was synthesized by choosing 1,4,7,10-Tetraazadecane and 2-hydroxy benzaldehyde as base compounds. The resulting complex was characterized by FT-IR Spectroscopy and NMR (<sup>13</sup>C and <sup>1</sup>H) Spectroscopy. The vibrational picture of the title molecule has been investigated using Density Functional Theory (DFT) at B3LYP level with 6-31G\*\* basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50cm<sup>-1</sup> respectively. The optimized geometry, intensity and vibrational wavenumbers of the title compound were obtained using DFT calculations. During optimization procedure all the parameters were allowed to relax. The HOMO, LUMO energies and energy gap of the title molecule was calculated by B3LYP/6-31G\*\* method. The intramolecular interactions, delocalization of electrons and stabilization energy of the title compound was investigated by performing Natural Bond Orbital (NBO) analysis.



Optimized Structure of 2,2'-[<sup>1Z,11Z</sup>-2,5,8,11-Tetraazadodeca-1,11-diene-1,12-diyldiphenol

**Keywords:** DFT, FT-IR, FT-Raman, NMR, HOMO-LUMO, NBO.

## An insight into the Vibrational behaviour of a Salen base Schiff based ligand

<sup>a</sup>V.Ragavendran\*

<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Enathur,  
Kanchipuram, Tamilnadu, India - 631 561

Corresponding Author: [ragav910@gmail.com](mailto:ragav910@gmail.com)

### ABSTRACT:

In the present study, the title compound was synthesized by refluxing the Ethylene diamine and Salicylaldehyde in proper mole ratio. The resulting complex was characterized by FT-IR Spectroscopy and NMR (<sup>13</sup>C and <sup>1</sup>H) Spectroscopy. Density Functional Theory (DFT) has been utilized by choosing proper methodology and basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50cm<sup>-1</sup>respectively. In order to obtain a close agreement between predicted and observed frequencies and hence to perform a reliable assignment, the theoretically obtained frequencies were scaled empirically. The global minimum energy obtained for the title compound was ascertained and the title compound belongs to C<sub>1</sub> symmetry. In addition to the vibrational assignment, the Mulliken chargeanalysis for the title compound was predicted and thermodynamic analysis has also been carried out.

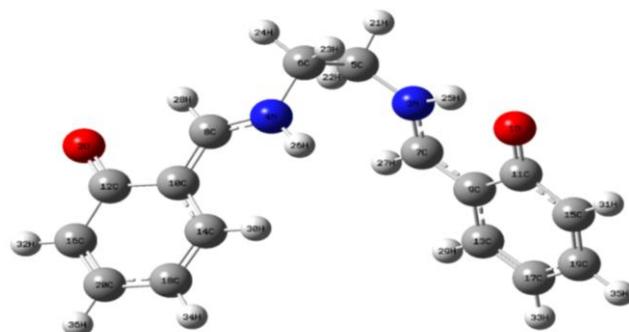


Figure shows Optimized Structure of the title compound

**Keywords:**DFT, FT-IR, FT-Raman, NMR, HOMO-LUMO, NBO.

## Density Functional Theory studies of N,N'-Bis(2-hydroxy-benzylidene)-3-azapentane-1,5-diamine

<sup>a</sup>V.Ragavendran\*

<sup>a</sup>*Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Enathur, Kanchipuram, Tamilnadu, India - 631 561*

**Corresponding Author:** ragav910@gmail.com

### **ABSTRACT:**

In the present study, the title compound was synthesized by choosing DETA and Salicylaldehyde as base compounds. The resulting complex was characterized by FT-IR Spectroscopy and NMR (<sup>13</sup>C and <sup>1</sup>H) Spectroscopy. In the present work DFT based vibrational Spectroscopic characterization of N,N'-Bis(2-hydroxy-benzylidene)-3-azapentane-1,5-diamine have been studied. The predicted wavelengths using DFT are comparable to the experimentally observed FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup> respectively. Thus the observed and the calculated frequencies are found to be in good agreement. The Geometrical parameters and the electronic properties, such as HOMO and LUMO energies, were obtained by DFT approach. The HOMO and LUMO shows that charge transfer occurs within the molecule. NBO analysis shows the anti-bonding orbitals ( $\sigma^*$ ,  $\pi^*$ ), the electron density (ED) changes and their energies E(2) as a clean evidence for stabilization of energy emerging from molecular interactions. Thermodynamic properties such as the zero point vibrational energy, entropy, heat capacity have been computed out.

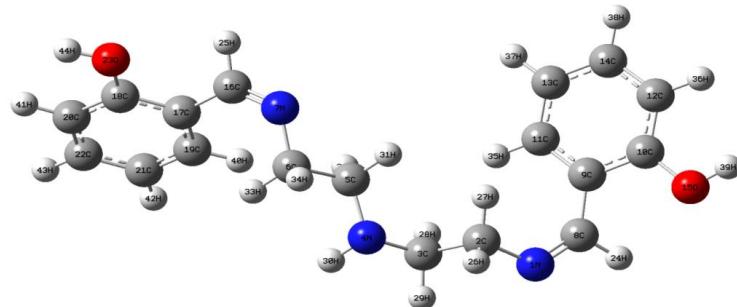


Figure. Optimized Structure of N,N'-Bis(2-hydroxy-benzylidene)-3-azapentane-1,5-diamine

**Keywords:** DFT, FT-IR, FT-Raman, NMR, HOMO-LUMO, NBO.

**Synthesis, Characterization and MOF studies of  
2,2'-(**(1Z,14E)-2,5,8,11,14-pentaazapentadeca-1,14-diene-1,15-**  
**diyl)diphenol****

**<sup>a</sup>V.Ragavendran\***

*<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi ViswaMahavidyalaya, Enathur,  
Kanchipuram, Tamilnadu, India - 631 561*

**Corresponding Author:** ragav910@gmail.com

**ABSTRACT:**

In the present study, the title compound was synthesized by refluxing (Tetraethylenepentamine)TEPA with Salicylaldehyde taken in proper ratio. The resulting complex was characterized by FT-IR Spectroscopy and NMR (<sup>13</sup>C and <sup>1</sup>H) Spectroscopy. The Fourier transform infrared spectra and FT-RAMAN of the titled compounds was recorded in the region ranging from 4000-400cm<sup>-1</sup> and 4000-50cm<sup>-1</sup> respectively. In addition, the fluorescence spectrum has also been recorded. The geometrical optimization and calculation of vibrational frequencies were performed using Gaussian 09W program within DFT approach. The gradient-corrected correlation functional of Lee, Yang and Parr as proposed and parameterized by Becke and Lee et al. was used along with the double Zeta split valence basis set 6-311G\*\*[2,3]. The optimized structural parameters were used in the vibrational frequency calculations at DFT levels to characterize all stationary points as minima. The HOMO and LUMO shows that charge transfer occurs within these molecules. In addition to the above, the mulliken charges and thermo dynamical parameters were also calculated in the present study.

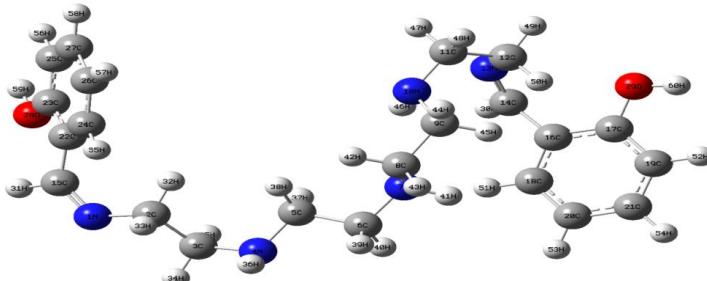


Figure. Optimized Structure of 2,2'-(**(1Z,14E)-2,5,8,11,14-pentaazapentadeca-1,14-diene-1,15-**  
**diyl)diphenol**

## Synthesis of (*3E,5E*)-6-phenyl-3,5-hexadien-2-one via extended conjugation

<sup>a</sup>V Ragavendran\*

*<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi ViswaMahavidyalaya,  
Kanchipuram - 631561, Tamilnadu, India*

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

The title molecule (*3E,5E*)-6-phenyl-3,5-hexadien-2-one was synthesized through a single step base catalyzed aldol type condensation between acetone and cinnamaldehyde. The prepared molecule has been characterized using <sup>1</sup>H and <sup>13</sup>C NMR spectra. The complete vibrational characterization of the molecule was performed using experimental (FTIR and FT-Raman) spectra and calculations at DFT level. In order to carry out a detailed vibrational spectroscopic analysis of CA, Fourier Transform Infrared and Fourier Transform Raman spectra recorded in condensed phase were used. To determine the optimized geometry and vibrational wavenumbers, Density functional theory calculations in the B3LYP/6-31G\*\* level have been carried out followed by scaling using the scaled quantum mechanical methodology. Full normal coordinate analysis was performed on the title compound in order to make the complete assignments. A root mean square deviation of 6.53 cm<sup>-1</sup> has resulted from the scaled quantum mechanical treatment.

**Keywords:** Synthesis, FTIR & FT-Raman, DFT, SQM.

## Vibrational Spectroscopic characterizations of buphedrone

<sup>a</sup>V Ragavendran\*

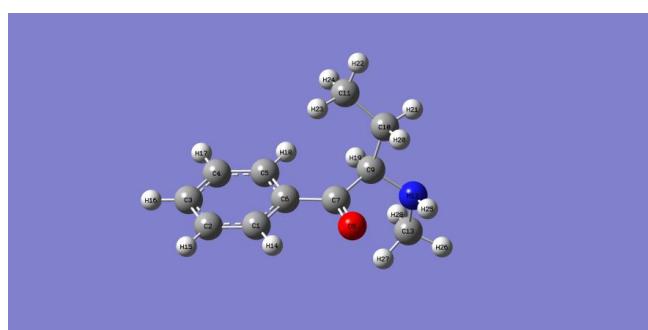
<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi ViswaMahavidyalaya,

Kanchipuram - 631561, Tamilnadu, India

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

The structure of the title molecule buphedrone was taken from the spectral database and used for performing DFT calculations. The complete vibrational characterization of the molecule was performed using experimental (FTIR and FT-Raman) spectra and calculations at DFT level. In order to carry out a detailed vibrational spectroscopic analysis, Fourier Transform Infrared and Fourier Transform Raman spectra recorded in condensed phase were used. To determine the optimized geometry and vibrational wavenumbers, Density functional theory calculations in the B3LYP/6-31G\*\* level have been carried out followed by scaling using the scaled quantum mechanical methodology. Full normal coordinate analysis was performed on the title compound in order to make the complete assignments. The energy gap of the title compound was calculated.



Optimized structure of buphedrone

**Keywords:** FTIR & FT-Raman, DFT, Energy gap.

## A study on the inter and intramolecular charge transfer mechanism of 3,4,5-trimethoxy benzaldehyde

<sup>a</sup>V Ragavendran\* and <sup>a</sup>B.Gayathri

<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya,  
Kanchipuram - 631561, Tamilnadu, India

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

In the present study, the title compound 3,4,5 Trimethoxybenzaldehyde was investigated using Density Functional Theory as an investigating tool. The experimental FT-IR and FT-Raman Spectra were taken from SDDBS spectral database. The vibrational picture of the title molecule has been investigated using Density Functional Theory (DFT) at B3LYP level with 6-31G(d,p) basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup> respectively. The optimized geometry, intensity and vibrational wavenumbers of the title compound were obtained using DFT calculations. During optimization procedure all the parameters were allowed to relax. The HOMO and LUMO energies shows that charge transfer within the molecule. The stability of the molecule arising from hyper conjugative interactions and the charge delocalization has been analyzed using natural bond orbital (NBO) analysis Mulliken population analysis and thermodynamic parameters of the title compound has been calculated.

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

## Analyzing the charge transfer mechanisms of 4-hydroxy-3-methoxy-5-nitrobenzaldehyde

<sup>a</sup>VRagavendran\* and <sup>a</sup>V.R.Kumanan

<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya,  
Kanchipuram - 631561, Tamilnadu, India

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

In the present study, the title compound 4-hydroxy-3-methoxy-5-nitrobenzaldehyde was investigated using Density Functional Theory as an investigating tool. The experimental FT-IR and FT-Raman Spectra were taken from SDDBS spectral database. The vibrational picture of the title molecule has been investigated using Density Functional Theory (DFT) at B3LYP level with 6-31G(d,p) basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup> respectively. The optimized geometry, intensity and vibrational wavenumbers of the title compound were obtained using DFT calculations. During optimization procedure all the parameters were allowed to relax. The HOMO and LUMO energies shows that charge transfer within the molecule. The stability of the molecule arising from hyper conjugative interactions and the charge delocalization has been analyzed using natural bond orbital (NBO) analysis Mulliken population analysis and thermodynamic parameters of the title compound has been calculated.

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

## Molecular geometric investigations of 1,2,4-Trimethyl benzene using Density functional theory

<sup>a</sup>V Ragavendran\* and <sup>a</sup>K. Priyadarshini

<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya,  
Kanchipuram - 631561, Tamilnadu, India

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

In the present study, the title compound 1,2,4-Trimethyl Benzene was investigated using Density Functional Theory as an investigating tool. The experimental FT-IR and FT-Raman Spectra were taken from SDBS spectral database. The vibrational picture of the title molecule has been investigated using Density Functional Theory (DFT) at B3LYP level with 6-31G(d) basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup> respectively. The optimized geometry, intensity and vibrational wavenumbers of the title compound were obtained using DFT calculations. During optimization procedure all the parameters were allowed to relax. The HOMO and LUMO energies shows that charge transfer within the molecule. The stability of the molecule arising from hyper conjugative interactions and the charge delocalization has been analyzed using natural bond orbital (NBO) analysis and Mulliken population analysis of the title compound has been calculated.

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

## Theoretical studies of 2-Hydroxy-3-Methoxy-5-Nitrobenzaldehyde using Density functional theory

<sup>a</sup>VRagavendran\* and <sup>a</sup>S.Vasantha

<sup>a</sup>Department of Physics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya,  
Kanchipuram - 631561, Tamilnadu, India

**Corresponding Author:** ragav910@gmail.com

### ABSTRACT

In the present study, the title compound 2-hydroxy-3-methoxy-5-nitrobenzaldehyde was investigated using Density Functional Theory as an investigating tool. The experimental FT-IR and FT-Raman Spectra were taken from SDDBS spectral database. The vibrational picture of the title molecule has been investigated using Density Functional Theory (DFT) at B3LYP level with 6-31G(d) basis set and experimentally recorded FT-IR and FT-Raman spectra ranging from 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup> respectively. The optimized geometry, intensity and vibrational wavenumbers of the title compound were obtained using DFT calculations. During optimization procedure all the parameters were allowed to relax. The HOMO and LUMO energies shows that charge transfer within the molecule. The stability of the molecule arising from hyper conjugative interactions and the charge delocalization has been analyzed using natural bond orbital (NBO) analysis and Mulliken population analysis of the title compound has been calculated.

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

**Studies of Polymer Compound – PET thin films with Electrical Conductivity****R. Sivakumar\* and V.Balajivijayan<sup>2</sup>**

\*Associate Professor, Department of Physics, Easwari Engineering College, Ramapuram,  
Chennai-600 089.

<sup>2</sup>Assistant Professor, Dept of Computer Science & Engineering, Vignan foundation for Science  
Technology and Research, Vadlamudi, Guntur, Andhra Pradesh - 522213

\*Corresponding author: sivakumar.r@eec.srmrmp.edu.in

**ABSTRACT**

The electrical conductivity of commercially available electrical conductive polymer-compounds like polyethylene terephthalate (PET) thin films is usually between 2.4 S/m and 3.2 S/m what means that they are already 10 to 50 times higher than the other polymer materials. During the studies the values for thermal conductivity of PET polymer-compounds could be increased to more than 5 S/m. In this study the thermal conducting properties of polymer polyethylene terephthalate has been investigated by using a four-probe apparatus because of its importance in industrial applications. The dependence of DC (direct current) surface resistance on thickness was measured using this method. The surface resistance exhibits the size effect in accordance with the sample of thickness of the order of 100 to 250 microns (PET) material. The readings are taken with different combination materials such as copper, aluminum carbon strips etc. According to this study suggests that possibility of using PET thin films in electronic components (capacitors, resistors, etc.) that operate at temperature dependence applications and this classification not only for polyethylene terephthalate (PET) thin films but also for the other polymer materials.

**Key words:** High Thermal Conductivity, Resistivity, Four-Probe method, PET thin films

## Effect of Sulphur Doping on the Structural and Optical Properties of ZnO Nanorods

**U.K. Panigrahi<sup>1</sup>, Shamima Hussain<sup>2</sup> and P. Mallick<sup>1,\*</sup>**

<sup>1</sup> Department of Physics, Maharaja Sriram Chandra Bhanja Deo University, Baripada 757003,

<sup>2</sup> UGC-DAE Consortium for Scientific Research, Kalpakkam Node, Kokilamedu 603104, India

\*E-mail: pravanjanphy@gmail.com

### ABSTRACT

We report the synthesis of ZnO nanorods doped with sulphur by a low cost wet chemical method. XRD characterization indicated the samples crystallized in wurtzite structure of ZnO along with the appearance of an additional peak at  $\sim 29.19^\circ$  corresponding to ZnS. The intensity of the ZnS peak increased with increasing molar doping concentration of sulphur in ZnO. Morphological characterization revealed the nanorod features in all the samples. The size of the nanorods, initially decreased with increasing sulphur doping concentration to 10%, showed a peak at a sulphur doping concentration of 20% and decreased again at 30% sulphur doping concentration. The optical band gap of ZnO decreased from 3.211 to 3.007 eV and the emitted colour shifted from blue to green region with increasing sulphur doping concentration from 0 to 30%. The suppression of UV emission band intensity and enhancement of green emission band in PL spectra indicates that our samples could be useful for UV blocking agent or optoelectronics devices which work in visible spectrum.

**Keywords:** ZnO nanorods, Sulphur doping, Optoelectronics devices.

**Growth and Characterization of L-Valine Hydrobromide Single crystal for nonlinear optical applications****Naghma Khan<sup>1,2</sup>, N. Vijayan<sup>2\*</sup>, Ravinder Kumar<sup>1,2</sup>**

*1Academy of Scientific and Innovative Research (AcSIR), CSIR HRDC Campus, Ghaziabad, Uttar Pradesh-201002*

*2CSIR –National Physical Laboratory, Dr K. S. Krishnan Road, New Delhi 110 012, India*

E-mail: [aayat22@gmail.com](mailto:aayat22@gmail.com)

**ABSTRACT**

The single Crystal of L- Valine Hydrobromide (LVHBR) was grown from aqueous solution by slow evaporation solution technique (SEST). The grown crystal was subjected to Powder X-ray diffraction for the sake of plane indexing and match phase analysis was also carried out along with the inbuilt rietveld refinement to get the refine lattice parameter. The transmission spectrum was examined by UV-Vis spectroscopy in the entire visible region which reflects that the titled crystal has good optical transparency in the entire visible region and its direct band gap was also evaluated with the help of tauc plot. The grown crystals were characterized by Fourier Transform Infrared (FTIR) spectroscopic analysis to find the different modes of vibration due to various functional groups present in the grown crystal emission spectra was also examined with the photoluminescence spectroscopy. All these studies indicate that the LVHBR crystal can be considered as a potential candidate for the fabrication of optoelectronic devices.

**Keywords:** NLO material, PXRD, Rietveld, UV-Vis and Photoluminescence.

## Investigation on growth kinetics of potassium hydrogen phthalate single crystals doped with Na<sup>+</sup> ions.

S.K. Geetha<sup>1,\*</sup>, G. Chandrasekar<sup>2</sup>

<sup>1</sup>PG and Research Department of Physics, Government Arts College for men (A), Nandanam, Chennai – 600 035, Tamil Nadu, India

<sup>2</sup>Department of Chemistry, M.P.B. Government Girls Higher Secondary School, East Tambaram, Chennai – 600 059, Tamil Nadu, India

E mail: skgeetha@yahoo.com

### ABSTRACT:

Induction period were measured at various super saturations for pure and sodium doped KAP solutions and hence the interfacial energies were calculated as 0.5329mJ/m<sup>2</sup> and 0.4348mJ/m<sup>2</sup> respectively. Nucleation parameters such as critical free energy change, radius of critical nucleus and nucleation rate have been evaluated for pure and sodium doped KAP solutions. The determined interfacial energy is found to be comparable with theoretical values. Pure and Sodium doped KAP single crystals were grown using solution technique. The influence of impurities on the growth kinetics, surface morphology, structural, optical and mechanical properties has been studied. Optical observations reveal no surface features on (010) planes of sodium doped crystal. Large shift towards higher energy (1565 cm<sup>-1</sup>) for the peaks due to carboxylate group in the FTIR spectra of all sodium doped crystals confirms the replacement of high atomic mass potassium with low atomic mass sodium. The percentage of transmission increases from 71.12% to 74.31% due to sodium addition. The microhardness value was found to decrease with the applied load for all concentration of the dopant.

**Keywords:** crystal growth, FTIR, hardness, optical properties, Functional, solidification

**Structural and dielectric properties of  $(\text{BFO})_{0.75} - (\text{NBT})_{0.25}$  solid solution**

<sup>1</sup> B N Parida, <sup>2</sup>S Behera

<sup>1</sup>Department of Physics, Central Institute of Technology Kokrajhar, (Deemed to be University, MHRD, Govt. of India), Assam-783370

<sup>2</sup> Department of Physics, Centurion University of Technology and Management, Odisha, India, 751050.

E-mail: [saubhagyalaxmi.behera@cutm.ac.in](mailto:saubhagyalaxmi.behera@cutm.ac.in)

**ABSTRACT**

The polycrystalline sample of NBT-BFO was synthesized by solid-state reaction method. The temperature required for synthesis of the desired material is 940°C. The formation of a single-phase compound was confirmed by preliminary X-ray structural studies of the material. The SEM micrograph of the compound showed uniform growth of grains. SEM also shows that the material has less porosity. Detailed studies of dielectric and electrical impedance (impedance, electric modulus and conductivity) properties of the system in a range of frequency (1 kHz - 1 MHz) and temperature (27- 450°C) showed that these properties are strongly dependent on temperature and frequency. The nature of frequency dependence of ac conductivity follows the Jonscher's power law.

**Keywords:** X-ray diffraction, SEM micrographs, Dielectric properties, Electrical impedance

## Effect of lone pair doping on the multiferroic properties of orthorhombic LuMnO<sub>3</sub>: A first Principle study

Sathya Sheela Subramanian<sup>1</sup>, N. Baskaran<sup>2</sup>

<sup>1</sup>*RV Institute of Technology and Management, Bangalore*

<sup>2</sup>*National Institute of Technology, Tiruchirappalli.*

*E mail:*

### ABSTRACT:

Multiferroics are compounds that are found to possess at least two of the ferro (electric, magnetic, toroidic and elastic) properties in the same compound. Among them, Type I multiferroics exhibit high electric polarization but no coupling between the magnetic and electric order parameters. Type II multiferroics have strong coupling between the magnetic and electric order parameters but they exhibit low electric polarization. Orthorhombic LuMnO<sub>3</sub> is a Type II multiferroic which exhibits ferroelectricity even in the centrosymmetric Pbnm space group, due to the symmetry breaking effects of its E-type antiferromagnetic behaviour. Consequently, this special type of antiferromagnetism results in ferroelectricity but the electric polarization is not very high. Motivated by this, we carry out first principles density functional theory studies to analyze the effect of lone pair doping i.e. substituting 50% of Bi at the A-site of o-LuMnO<sub>3</sub>, in an effort to induce a Type -I multiferroic behaviour in the new compound. We report the most stable ground state structure of Lu<sub>0.5</sub>Bi<sub>0.5</sub>MnO<sub>3</sub>, in addition to studying its electric and magnetic properties. We also analyse the effect of Bi 6s<sup>2</sup> lone pairs on the structure and properties of Lu<sub>0.5</sub>Bi<sub>0.5</sub>MnO<sub>3</sub>.

**Keywords:** Multi ferroics, Rare earth manganite, DFT, Electronic structure, First Principle

**Intermolecular interaction studies of methyl formte, 1-propanol and benzene at various temperatures by using ultrasonic technique.****Sampandam Elangovan**

*Department of Physics, College of Natural and Computational Science, Wollega University,  
Ethiopia*

*E-mail: [elangovan.physics@rediffmail.com](mailto:elangovan.physics@rediffmail.com)*

**ABSTRACT**

Density ( $\rho$ ), viscosity ( $\eta$ ) and ultrasonic velocity (U) have been measured for a ternary mixture of methyl formate, 1-propanol and benzene at 303K, 308K and 313K. From the experimental values, adiabatic compressibility ( $\beta$ ), free length (Lf), free volume (Vf), viscous relaxation time ( $\tau$ ) and Gibbs free energy ( $\Delta G$ ) have been determined. The excess values of various parameters ( $\beta_E$ ,  $Lf_E$ ,  $Vf_E$ ,  $\tau_E$  and  $\Delta G_E$ ) have also been deduced and interpreted in terms of molecular interactions. The deviations in the sign and values of these excess parameters from the ideal mixing reveal that intermolecular interactions decreased with increasing the 1-propanol concentrations.

**Keywords:** Methylformate ; 1-propanol; benzene; ultrasonic velocity; hydrogen bonding.

## Bio-Synthesis of $\text{Co}_3\text{O}_4/\text{SiO}_2$ Core Shell using *Aristolochia Indica* Bark Extract and Its Opto – Structural and Morphological Analysis

S. Thangewari<sup>a</sup>, Dr. K. Amudhavalli <sup>b\*</sup> and Dr. T. Daniel<sup>c</sup>

<sup>a</sup> Research Scholar, Department of Physics, V.O.Chidambaram College, Thoothukudi- 628 008.

Affiliated to Manonmaniam Sundaranar University, Abishekappatti, Tirunelveli- 627 012.

<sup>b</sup> Associate Professor of Physics, V.O.Chidambaram College, Thoothukudi- 628 008.

<sup>c</sup> Department of Physics, Manonmaniam Sundaranar University, Abishekappatti, Tirunelveli- 627 012. Tamil Nadu, India.

[thangam8991@gmail.com](mailto:thangam8991@gmail.com) \* amub2@yahoo.com

### ABSTRACT

This research work reports on the green synthesis of  $\text{Co}_3\text{O}_4/\text{SiO}_2$  core shells using *Aristolochia Indica* natural extract as an effective chelating agent. The crystalline structure, surface, morphology and optical properties of  $\text{Co}_3\text{O}_4/\text{SiO}_2$  core shell were studied using various characterization techniques. The X-ray diffraction (XRD) analysis confirmed the formation of spherical shaped  $\text{Co}_3\text{O}_4/\text{SiO}_2$ . The Fourier Transform Infrared Spectroscopy (FTIR) explored the stretching vibration of Co–O and Si–O core shells. The average grain size of the  $\text{Co}_3\text{O}_4/\text{SiO}_2$  core shells were observed from scanning electron microscopy (SEM) and it is found to be 21 nm. The optical characterization clearly revealed the information about direct band gap of 1.9 eV for core and 2.3 eV for core shell.

**Key words:** bio synthesis, *Aristolochia Indica*,  $\text{Co}_3\text{O}_4/\text{SiO}_2$  core shells, FTIR and Bandgap.

**Discrimination of Acne Vulgaris with Human Scalp Hair tissues and Efficacy of Adapalene 0.1% and Benzoyl peroxide 2.5% gel using FTIR-ATR Spectroscopic technique**

**Padmavathi R<sup>1\*</sup>, Rajamannan B<sup>2</sup>, Gunasekaran S<sup>3</sup>, Ramkumar G.R<sup>4</sup>, Sankari G<sup>5</sup>, Muthu S<sup>6</sup>**

<sup>1</sup> Department of Physics, Meenakshi Sundararajan Engineering College, Kodambakkam, Chennai

<sup>2</sup> Department of Engineering physics, FEAT Annamalai University, Annamalai Nagar, 608002,

<sup>3</sup> Research and Development, St. Peter's University, Avadi, Chennai

<sup>4</sup> Department of Physics, C. Kandaswaminaidu College for Men, Anna Nagar East, Chennai-600102

<sup>5</sup> Department of Physics, Meenakshi College for Womens, Kodambakkam, Chennai-600024

<sup>6</sup>Department of physics, Govt. Thirumagal Mills College, Gudiyatham-632602, Vellore

E mail: [pathmavati@gmail.com](mailto:pathmavati@gmail.com)

## ABSTRACT

Acne is a multifactorial disease characterized by pathological alteration in pilosebaceous units of the neck and upper trunk. Acne is a chronic inflammatory skin disease and occurs in adolescence. The present study focuses mainly on qualitative and quantitative studies on healthy and acne vulgaris human scalp hair tissues and efficacy of the gel Adapalene 0.1% and Benzoyl Peroxide 2.5% using FTIR-ATR spectroscopy. The main objectives are to analyze human scalp hair tissues using FTIR-ATR spectroscopy to compare and discriminate the spectral signatures of acne vulgaris and healthy scalp hair samples through acne biomarkers Protein, Amide I, Amide II and Squalene (LDL), using the method of internal ratio parameters. To evaluate the safety and efficacy of the (ADP+BPO) fixed-dose combination, in a few human (both male and female) for the treatment of Acne vulgaris 60 scalp hair tissues were collected, 20 healthy subjects, 20 acne patients hair samples, 20 after medication hair tissues were collected and used to evaluate the efficacy of gel ADP+BPO. After the medication, FTIR spectra of the Acne vulgaris, hair samples (Post-treatment) were recorded in the mid-infrared region, and the biomarkers for the acne vulgaris samples with specific peaks during the before treatment (Pre-treatment) were analyzed and compared with, hair samples of healthy subjects. Some of the biomarkers such as  $R_1 = I_{3264}/I_{2864}$ ,  $R_2 = I_{1633}/I_{2864}$ ,  $R_3 = I_{1516}/I_{2864}$ , and  $R_4 = I_{1454}/I_{2864}$  were used as diagnostic parameters, the significance of the intensity ratio results was estimated using dependent t-test statistic method. For the statistical interpretation, low p-value ( $p < 0.05$ ) is taken as statistically significant. Hence the efficacy of Adapalene 0.1% and Benzoyl Peroxide 2.5% is estimated.

## Progressive Development in the solar cell research and its applications.

Munirajappa N N<sup>1</sup>, Devaraj P B<sup>2</sup>, Daruka Prasad B<sup>3</sup>

<sup>1</sup> Department of Physics, Nrupathunga University (Government Science College Autonomous) (A), N.T Road, Bangalore-560001, India.

<sup>2</sup> Department of Physics, Kalpatharu College of Engineering, Tipaturu – 572201, India

<sup>3</sup> Department of Physics, BMS Institute of Technology and Management, Bangalore, 560064, India

\*Corresponding author E-mail: munirajappann.leo@gmail.com

### ABSTRACT

The light from the sun is not only a non-vanishing resource of energy but also it is an Eco-Friendly resource of energy. It can easily compensate for the energy requirements fulfilled by the other resources, which are depleting and environment challenges, such as Fossil Fuel and petroleum deposits. The electronic device which receives solar energy from the sun in the form of sunlight and it converted into electric energy using solar cell by the principle of Photovoltaic effect. The major challenges in obverse of the development and implementation of solar cells are cost and efficiency. Discontinuous supply is also a problem while using solar energy. The fabrication of solar cells has passed through a large number of improvement steps from one generation to another. Silicon based solar cells were the first generation solar cells grown on Si wafers, mainly single crystals. Further development to thin films, dye sensitized solar cells and organic solar cells enhanced the cell efficiency. In this article, we have reviewed a progressive development in the solar cell research from the effect of MoO<sub>3</sub> anode buffer layer on power conversion efficiency and stability of small molecular photovoltaic devices and their applications.

**Keywords:** solar cells, semiconductor materials, sustainable energy, absorption, photovoltaic energy.

## Physico-Chemical Properties of Strontium Containing Bioactive Glasses

C.Manjula<sup>1,\*</sup>, V. Dhivya<sup>1</sup>, G. Rajkumar<sup>1</sup> and K. Sakthipandi<sup>2</sup>

<sup>1</sup>Department of Physics, Easwari Engineering College, Chennai - 600 089, Tamil Nadu, India

<sup>2</sup>Department of Physics, SRM TRP Engineering College, Tiruchirappalli 621 105, Tamil Nadu, India

\*Corresponding author Email: [dr.g.raajkumar@gmail.com](mailto:dr.g.raajkumar@gmail.com)

### ABSTRACT

Phosphate based glasses  $48\text{P}_2\text{O}_5 - 32\text{CaO} - (20-x)\text{Na}_2\text{O} - 3\text{CaF}_2 - x\text{SrO}$  ( $x = 0, 2, 4$ , and  $6$  mol%, henceforth, termed as SrF0, SrF2, SrF4 and SrF6 respectively) with varying different SrO content were prepared using melt quenching technique. To study the influence of strontium on the physicochemical properties and bioactivity of phosphate based glasses, various experimental analysis such as density, elastic moduli, and microhardness as a function of SrO concentration were carried out to examine the impact of strontium on the physicochemical characteristics and bioactivity of phosphate-based glasses. It is interested to explore that SrO serves as a network modifier in the prepared phosphate-based glasses, weakening the glass network, as seen by the declining trend in shear and Young's modulus when SrO was added. The anisotropic nature of all the prepared fluorophosphate glass samples was showed the variation in elastic moduli. Further, Fourier Transform Infra-Red spectra and X-ray diffraction pattern also revealed showed the structural changes in the glass samples and formation of crystalline apatite on glass surface during 21 days *in vitro* studies during the addition of SrO content.

**Keywords:** elastic moduli, Ultrasonic velocity, Micro Hardness, Strontium

## Electrical, Structural, Dielectric and Ultrasonic studies on Isovalent La-Gd-Cr perovskites

**K. Sakthipandi<sup>1\*</sup>, G. Rajkumar<sup>2</sup>, A. Joseph Sagaya Kennedy<sup>1</sup>, B.Sethuraman<sup>1</sup>**

<sup>1</sup>*Department of Physics, SRM TRP Engineering College, Tiruchirappalli 621 105, Tamil Nadu, India*

<sup>2</sup>*Department of Physics, Easwari Engineering College, Chennai 600089, Tamil Nadu, India*

\*Corresponding author Email: [sakthipandi@gmail.com](mailto:sakthipandi@gmail.com); [sakthipandi.k@trp.srmtrichy.edu.in](mailto:sakthipandi.k@trp.srmtrichy.edu.in)

### ABSTRACT

In recent years, Lanthanum chromite ( $\text{LaCrO}_3$ ) doped perovskites presently a nickel-free anode material for high-temperature solid oxide fuel cells (SOFC). Currently, Ni/Yttria-stabilised zirconia (YSZ) cermets and Fe/Co-based perovskites were most often used anode materials for SOFC. Ni/YSZ cermets expose outstanding catalytic properties and stability for hydrogen oxidation at/under SOFC operating conditions. However, these nickel cermets have drawbacks such as limited tolerance to sulphur, thermal mismatch with YSZ, and carbon deposition when using hydrocarbon fuels. Ceramic perovskite could be used to replace to Ni/YSZ cermets as an anode material for SOFC.

In this study, the solid-state reaction technique was used to make gadolinium doped lanthanum chromate ( $\text{La}_{1-x}\text{Gd}_x\text{CrO}_3$ ) with different compositions of  $x=0.00, 0.01, 0.05, 0.10, 0.15$  and  $2.0$ . The XRD pattern of all compositions shows single-phase formation with a crystal structure similar to undoped  $\text{LaCrO}_3$ . The average crystallite size of prepared perovskites was found to be  $35$  nm. At room temperature, the observed XRD pattern shows an orthorhombic structure with a space group Pnma. The different structural modes of vibrations are visible in the FTIR spectra of the investigated compositions. SEM micrographs of all compositions reveal spherical, oval, and irregular morphology with high density. In the frequency range  $20$  Hz to  $1$  MHz, the real part of electrical conductivity exhibits frequency independent behaviour over a wide range of temperature from  $310$  to  $675$  K.

Up to  $573$  K, the d.c. conductivity of the perovskites exhibits the Arrhenius behaviour. The d.c. conductivity of perovskites increases when the composition changes from  $x=0.0$  to  $x = 0.01$ . The conductivity falls after  $x = 0.01$  composition until it reaches  $x= 0.10$ . Further, an increase in conductivity is observed up to  $x = 0.20$ . The defects created by the size and concentration of the dopant ions were used to explain the temperature and composition dependent conduction mechanism. Temperature-dependent ultrasonic velocities and

attenuation measurement was made employing indigenous experimental set-up over a wide range of temperature from 300 to 700 K. Anomalies in temperature-dependent ultrasonic parameters were used to investigate the metal-insulator transition of produced  $\text{La}_{1-x}\text{Gd}_x\text{CrO}_3$  perovskites.

**Keywords:** Perovskites, Dielectric response, Ultrasonic measurements, Phase Transition

## Fabrication and testing of electrochemical gas sensor for detecting ammonia and hydrogen sulphide

**R. Sharan**

*Department of Physics, Easwari Engineering College, Ramapuram, Chennai – 600089.*

*E mail:* sharan.r@eec.srmrmp.edu.in

### ABSTRACT

Electrochemical gas sensors were developed in amperometric mode for sensing very low concentration (3-40 ppm) of ammonia ( $\text{NH}_3$ ) and hydrogen sulphide ( $\text{H}_2\text{S}$ ) with lanthanum gallate ( $\text{LaGaO}_3$ ) based electrolyte materials such as  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Ga}_{0.8}\text{Mg}_{0.2-x}\text{Ni}_x\text{O}_3$  (LSGMN) and  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Ga}_{1-y}\text{Fe}_y\text{O}_3$  (LSGF). For sensing  $\text{NH}_3$  and  $\text{H}_2\text{S}$ ;  $\text{Ce}_{1-p}\text{Zr}_p\text{O}_2$  and  $\text{CoCr}_{2-q}\text{M}_q\text{O}_4$  solid solutions were optimized as active electrode (predominantly supports sensing gas oxidation) (AE) respectively. The inactive electrode (which promotes oxygen reduction) (IE) was optimized among the compositions e.g.,  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$ (LSC),  $\text{La}_{0.5}\text{Sr}_{0.5}\text{FeO}_3$ (LSF),  $\text{La}_{0.5}\text{Sr}_{0.5}\text{NiO}_3$ (LSN),  $\text{La}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Ni}_{0.2}\text{O}_3$ (LSCN)and  $\text{La}_{0.5}\text{Sr}_{0.5}\text{Mn}_{0.8}\text{Ni}_{0.2}\text{O}_3$ (LSMN).All the materials were synthesized by solution combustion technique and nanopowder characterizations were done for basic properties. To achieve highest sensing performance compositions of AE, IE and electrolytes were systematically studied. By applying +1V at AE, oxygen pumping current through lanthanum gallate based electrolyte (oxygen ion conductor) was evaluated in 5%  $\text{O}_2$  added to  $\text{N}_2$  (base gas) and ppm level of sensing gas in base gas (3-40 ppm) as target gas from 200-550°C.

The AE with composition  $\text{Ce}_{0.7}\text{Zr}_{0.3}\text{O}_2$  (CZ73) produced highest  $\text{NH}_3$  sensitivity when  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Ga}_{0.8}\text{Mg}_{0.1}\text{Ni}_{0.1}\text{O}_3$  (LSGMN10) and  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$  (LSC) were used as fixed electrolyte and IE. It was observed in micro-raman and x-ray analysis, 30 mol% Zr in  $\text{CeO}_2$  is the limit of doping and beyond which  $\text{ZrO}_2$  segregates; thus reducing sensitivity. Subsequently,  $\text{La}_{0.5}\text{Sr}_{0.5}\text{Mn}_{0.8}\text{Ni}_{0.2}\text{O}_3$  was found as best IE with optimized AE and LSGMN10 electrolyte. With these optimized electrodes, composition of both LSGMN and LSGF were optimized and performance was correlated with the temperature dependent electrical conductivity of electrolytes. LSGMN10 with 10 mol% Ni doping showed highest sensitivity of 29  $\mu\text{A}/\text{decade}$  at 400°C. On the other hand, LSGF5 with 5 mol% Fe doping produced highest sensitivity of 43  $\mu\text{A}/\text{decade}$  at 450°C. Incidentally, experiments proved that these two compositions posses highest total electrical conductivity.

With the both optimized electrolyte (LSFG5) and optimized IE, AE for H<sub>2</sub>S detection was optimized. A composition CoCr<sub>2-q</sub>Fe<sub>q</sub>O<sub>4</sub> (q: 0-0.2) was optimized and 15 mol% Fe doping produced exceptionally high performance of 41 mA/decade at 400°C. Further, Fe was replaced by Ni and Mn and overall Fe (15 mol%) doping showed the best performance to H<sub>2</sub>S sensing. Sensing mechanism in both the gas sensors were proposed and verified. Selectivity of the sensors were also examined for suitability of exhaust gas monitoring applications.

**Keywords:** Electrochemical Gas Sensor, Active Electrode, Inactive Electrode, Ammonia, Hydrogen Sulphide.

## Synthesis of Ag Nanoparticles for the Removal of Heavy Metal Analysis and Antimicrobial Study

D Saravanakkumar<sup>1</sup>, A. Ayeshamariam<sup>2</sup>,

<sup>1</sup>PG & Research Department of Physics, Thiagarajar College, Madurai, Tamil Nadu, India

<sup>2</sup>Department of Physics, Khadir Mohideen College, Adirampattinam, Tamil Nadu, India, 614 701

Email: dsktca@gmail.com

### ABSTRACT

Silver nanoparticles have been synthesized by using Sonochemical approaches in the presence of urea and studied the effect of crystal size on the bacterial studies of Ag nanoparticles was analyzed by X-ray diffractometer, Raman Spectrum, Fourier transform infrared spectroscopy and UV-Vis Spectroscopy which divulged that the prepared product is well crystalline cubic phase optically active nanoparticles. Additionally Ag was exploited as redox mediator for the development of Ag nanoparticles.



**Keywords:** Ag nanoparticles, Scanning Electron Microscopy, redox reaction and antibacterial activity

**Excess Debye Temperature and Excess Surface Tension Variations with  
Excess Acoustical factors in Aniline with Amines at T = 303.15K, 308.15K,  
313.15K & 318.15K.**

**TimmeswaraSarma Nori<sup>1\*</sup>, Sk.FakruddinBabavali<sup>2</sup> and Ch.Srinivasu<sup>3</sup>**

<sup>1</sup> Dept. of Physics, Lakireddy Bali Reddy College of Engineering, Mylavaram, Andhra Pradesh,

<sup>2</sup> Dept. of Physics, V.R.Siddhartha Engineering College, Vijayawada, Andhra Pradesh, India,

<sup>3</sup> Dept. of Physics, Andhra Loyola College, Vijayawada, Andhra Pradesh, India, 520008.

E mail: ts.nori95@gmail.com

## ABSTRACT

In the present perspective, the variation of acoustical and their allied factors with a variation in the Debye temperature and surface tension in Aniline with + Toluene, + o-Xylene & + Mesitylene liquid mixtures is studied at T = 303.15 K 308.15 K, 313.15K & 318.15 K. The work is progressed in the study of the excess acoustical variations as well as excess Debye Temperature along with excess surface tension at ratio of different mole fractions. Excess acoustical factors such as excess adiabatic compressibility ( $\beta^E$ ), excess intermolecular free length ( $L_f^E$ ), excess Gibb's free energy ( $G^E$ ) and excess acoustic impedance ( $Z^E$ ) have been computed from basic experimental data. It is observed that the component molecules in the liquid mixture are supposed to be a cause of variation in their acoustical and their excess factors. The results are given with reference to the standard values from the literature data and tried to establish a connection for the excess acoustical values with excess Debye temperature and excess surface tension in the liquid mixtures at the experimental range of temperatures.

## Nitrogen-Incorporated Boron-doped Diamond Nanowires for Microplasma Illumination

Salila Kumar Sethy,<sup>1</sup>M. Ficek,<sup>2</sup>R. Bogdanowicz,<sup>2</sup>K. J. Sankaran<sup>1,\*</sup>

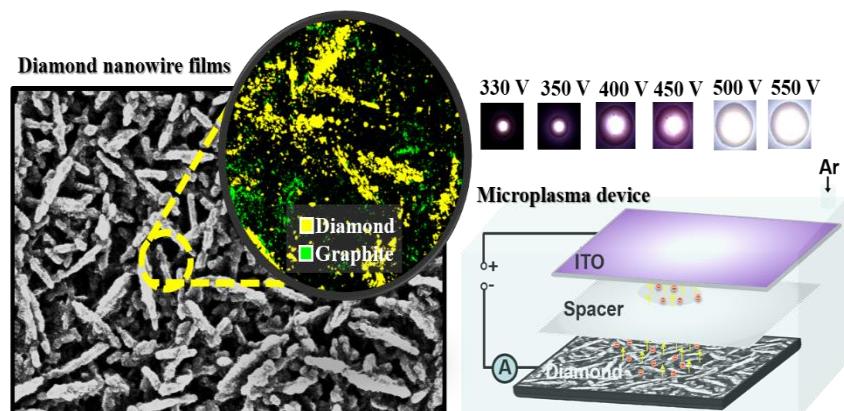
<sup>1</sup>*CSIR- Institute of Minerals and Materials Technology, Bhubaneswar, Odisha-751013, India.*

<sup>2</sup>*Faculty of Electronics, Telecommunications and Informatics, Gdańsk University of Technology, 80-233 Gdańsk, Poland.*

\*Corresponding author: kjsankaran@immt.res.in

### ABSTRACT

Low-temperature microplasmashave gained huge recognition from the plasma community because of their wide-range of applications in the development of nanomaterials and devices. But luminous efficiency of the current microplasma devices is insufficient. Aiming towards the development of an efficient microplasma device, nitrogen incorporated boron doped electrically conducting nanocrystalline diamond (NCD) films have been deposited by varying the substrate temperatures (Ts) between 400°C and 850°Cusing H<sub>2</sub>/CH<sub>4</sub>/B<sub>2</sub>H<sub>6</sub>/N<sub>2</sub>-based microwaveplasma-enhanced chemical vapor deposition system. Ts causes a drastic change in morphology and



microstructure and thereby the various properties of the NCD films. The NCD films grown at low Ts (400°C) contain faceted diamond grains. The morphology changes to nano-sized diamond grains for NCD films grown at 550°C (or 700°C). Interestingly, the NCD films grown at 850°C possess one-dimensional nanowire-like morphological grains. These nanowire-like NCD films possess the co-existence of sp<sup>3</sup> diamond and sp<sup>2</sup> graphitic phases, in which the sp<sup>2</sup> graphitic phases are at the grain boundaries surrounding the diamond nanowires. While boron doping increased the electrical conductivity of the diamond grains, the incorporation of N<sub>2</sub> facilitated the formation of nanographitic grain boundary phases that provide conductingpathways for the electrons, thereby achieved a high electrical conductivity for the

NCD films grown at 850°C. The microplasma devices using these nanowire-like NCD films as cathode show superior plasma illumination characteristics of low threshold field of 3300 V/ $\mu$ m, high plasma current density of 1.04 mA/cm<sup>2</sup> at an applied voltage of 520 V and stable emission current of 490 min. The outstanding plasma illumination characteristics of these conducting nanowire-like NCD films make them appropriate as cathodes paves the way for the utilization of these materials in various microplasma device applications.

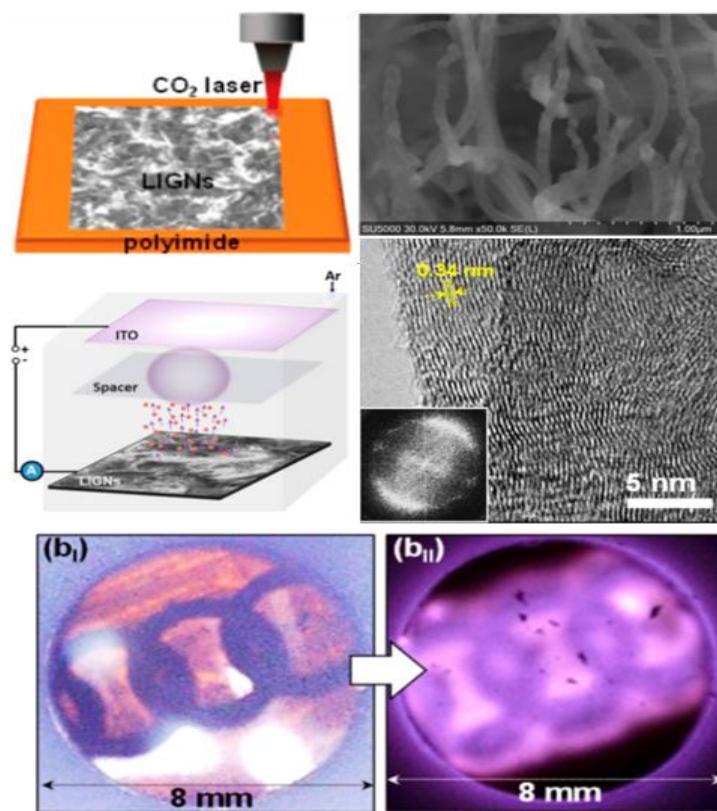
## Enhanced Field Electron Emission and Plasma Illumination Characteristics of Laser Induced Graphene Nanoribbons

**Shradha Suman, K. J. Sankaran**

*Advanced Materials Technology Department, CSIR- Institute of Minerals and Materials  
Technology, Bhubaneswar  
shradha.2021@immt.res.in*

### **ABSTRACT**

Displays are an essential interface in machine-based communication. There have been major developments in display technology, with the potential to enable television, handheld computers, and mobile phones to be more functional and user-friendly. In this regard, plasma display devices (PDDs) are very attractive for display technology. However, their relatively high operating voltage and poor plasma stability have limited their widespread use. To mitigate these issues, several studies have been conducted to find a suitable cathode material, which possesses a high proficiency in producing secondary electrons through plasma ion bombardment for a longer duration.



In this work graphene nanoribbons are synthesized using laser induction process on commercially available polyimide sheets, which are utilized as cathode for making field emitters andthus, in plasma display devices. The laser induced graphene nanoribbons (LIGNs) possess prominent, vertically aligned sharp-edged graphene materials with high aspect ratio providing more individual field emission sites. These nanoribbons have homogeneous interconnected morphology with anaverage width of  $\sim$ 100 nm and thickness  $\sim$ 120 nm. The presence of graphene phase in the material is confirmed by TEM, Raman and XRD analysis, which showed a multilayered graphene with interlayered spacing of 0.34nm and higher degree of  $sp^2$  network. The field electron emission (FEE) properties of LIGNs showed a low turn-on field of 0.44 V/ $\mu$ m, a high FEE current density of 49.7 mA/cm<sup>2</sup> at an applied field of 2.33 V/ $\mu$ m and a large enhancement factor of 4578. The plasma illumination (PI) measurements reveals that the brightness of the plasma increases with the increase in applied voltage. The plasma image at an applied voltage of 350V shows the uniform lighting pattern of the LIGN-based plasma devices indicating that they are directly patternable.



For further details, contact

**DEPARTMENT OF PHYSICS  
EASWARI ENGINEERING COLLEGE  
(AUTONOMOUS)  
BHARATHI SALAI, RAMAPURAM  
CHENNAI - 600089  
PHONE - 044 4392 3208  
hod.phy@eec.srmrmp.edu.in**

A background graphic featuring a repeating pattern of blue spheres connected by yellow rods, resembling a molecular lattice or crystal structure. The text is overlaid on this graphic.