International Conference
On
Material Science And Technology (ICMAST- 2017)

August 28 -29, 2017

Organised by

PG & RESEARCH DEPARTMENT OF PHYSICS

PACHAMUTHU COLLEGE OF ARTS & SCIENCE FOR WOMEN, Dharmapuri

In Collaboration With

ELAVENIL SCIENCE ASSOCIATION, Chennai

A Warm Welcome To All

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Message

I am extremely glad to know that the Department of Physics is organizing an International Conference on Material Science and Technology on 28-29 August 2017. This Women's college, is a trend setter and a bench marker, in this district for many innovative practices, in the field of Education, Science and Technology.

I hope that this conference would certainly help everyone to experience a panoramic view of the latest updates in the field of Material Science and Technology and thereby encourage the scientific community to contribute fruitfully to the current social needs.

On behalf of Pachamuthu College of Arts and Science for Women, I heartily welcome the honorable dignitaries keynote speakers, eminent scientists, Professors, International and National Delegates and the participants to our conference.

I express in advance my whole hearted wishes to the Department of Physics for the success of ICMAST-2017.

Vice Chairman
Dr. B. Sangeeth Kumar

Message

I am immensely happy to know that the Department of Physics has initiated in a big way to organize an International Conference on Material Science and Technology on 28-29 August 2017.

I hope that this conference would certainly induce innovative ideas and fruitful interactions among the participants paving way for inventive ideas and new technologies in the material science field.

I extend my warm wishes to the Faculty members and students of Physics Department who has worked for the grand success of the conference.

Principal
Dr.R.PhilomeneAlisa Phyllis

Message

It is a great pleasure for me that our PG and Research Department of Physics is conducting an International Conference on Material Science and Technology on 28-29 August 2017.

The conference is a confluence of information exchange between the conceiver, designer and implementer or the end user. The development of a nation can be seen from the advancements made by scientific and research communities. I hope this conference ICMAST-2017 will be intuitive, informative, scintillating and memorable for the participants.

"Success will never lower its standards to accommodate anyone.

One has to raise one's standard in order to achieve it"

I wish all the faculty members, students and all those who worked for this conference a grand success of ICMAST- 2017.

Convener message

It gives me great sense of pride and satisfaction to convene this esteemed international conference **"International Conference on Material Science and Technology(ICMAST – 2017)"** which is being held in the prestigious campus of Pachamuthu Arts and Science for women, Dharmapuri.

The conference ICMAST-2017 aims to bring researchers from various fields of material science and technology to share their thoughts, findings and applications.

The primary objectives of the conference are to provide scientists, students, research scholars and other professionals with a forum to actively engage in research discussions and professional development and create opportunities for the next generation workforce to develop their professional skills. I hope this interaction between delegates attending the conference has led to new ideas and exciting research directions.

ICMAST-2017 will cover a wide range of interdisciplinary and current research topics related to Material Science and Technology includes nano materials, composites, bio-nano materials, etc. These materials have numerous applications in electronics, bio technology, energy harvesting and medicine.

The response from the academic community has been enthusiastic, with almost 170 submissions received. I am very grateful to all the contributors and presenters who have shared their view, findings and their latest developments in their respective fields.

I am very much thankful to our Management and Principal for their full hearted support. Finally, my special thanks to the conference organizing team who have coordinated all the activities.

I hope this conference is of high quality and will be a thoroughly enjoyable gathering.

M. Anitha
Convener, ICMAST-2017
Head of Physics Department
Pachamuthu College of Arts and Science for women
Dharmapuri

KEY NOTE

1. Dr. R.K. Sumathi

Dr. R. Radhakrishnan Sumathi is a well-known crystal growth expert for III-Nitride Semi conductor Materials, Specifically Aluminium Nitride (AIN) presently Dr. Sumathi is a faculty at Materials Science and Applied Crystallography Institute, University of Munich, Germany. There she is leading a research group in wide bandgab Semi conductors and functional materials. She has obtained her Ph.D., degree in Physics from Anna university, Chennai, and has excellent academic track of records with many distinctions. She had been of records with many distinctions. She had been working as a senior research Scientist in 5 different German Universities in the field of material science/solid state physics. Dr. Sumathi has also received many awards and honour.

To name few: “young Scientist” awards by both Indian Physical Society and Wuropean Physical Society, “Young promising researcher” award given by German crystal growth Asoociation. Dr. Sumathi has more than 75 papers in peer reviewed journal publications/International or National level conference presentations. She is acting as a reviewer for several international journals, and also acting as National/International “Thesis evaluator”, doctoral committee member & Ph.D., examiner.

2) Dr. P. Kumaradhas:-

Dr.P.Kumaradhas, Professor, Department of Physics, Periyar University, Salem. He received his Doctoral Degree from Dangalore University, Bangalore in the field of X-ray Crystallography in 1997. He is a well known expert in X-ray crystallography, Quantum Chemistry Calculations. Charge density analysis of molecules via High resolution X-ray diffraction, Molecular electronics (Nano devices).

His post doctoral Reseach fellowships were, 1) Post-Doctoral Research at University of Texas, Houston,USA. 2) Post-Doctoral Research at University of Toledo, Ohio USA, 2000-2002. 3)Post-Doctoral Research at University of Witwatersrand, Johannesburg (Prestigious Fellowship) 1999-2000. 4) Post-Doctoral Research at Jawaharlal Nehru centre for Advanced Scientific Research, Bangalore, India (1997-1999).

He has published more than 73 Research publications. He has organized 7 Seminar/conference/workshops.

His current research interest were, Design of molecular Nano-wires, Swithes and Diodes. X-ray Crystal Structure determination of small and macromolecules.

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IT 01 CURRENT TRENDS AND FUTURE SCENARIO OF PV TECHNOLOGY

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Among all the renewable energy sources, PV solar cell plays a main role [1]. Single crystal and multi- crystalline solar cells are considered as first generation solar cells. Thin film based solar cells (a-Si, micromorph, CdTe/CdS and CIGS) are considered as second generation solar cells. Nano-crystalline based dye-sensitized solar cells (DSSCs), polymer-based solar cells and concentrated solar cells are considered as third generation solar cells. There is lot of crystal growth in several of these solar cells.

We have been working on the following three type of solar cells which involves plenty of crystal growth:

1. mc-Si by DS method.
2. TiO_2 nano-crystals for DSSCs
3. Micromorph& Nano-wire based a-Si solar cells by PECVD.

The majority of PV solar cells are fabricated from bulk silicon crystals, which may be either single-crystalline or multi-crystalline. A market share ofmono- and multi-crystalline silicon (mc-Si) are more than 90% at present and will be so in the foreseeable future [2]. Single-crystalline wafers typically have better material parameters but are also more expensive which are grown by Czochralski (Cz) growth process. CZ wafers contain a large amount of oxygen in the silicon wafer. Oxygen impurities reduce the minority carrier lifetime in the solar cell, thus reducing the voltage, current and efficiency. In addition, the oxygen and complexes of the oxygen with other elements may become active at higher temperatures, making the wafers sensitive to high temperature processing. To overcome these problems, Float Zone (FZ) wafers may be used. Due to the difficulty in growing large diameter ingots and the often higher cost, FZ wafers are typically only used for laboratory cells and are less common in commercial production. Multi-crystalline silicon (mc-Si) is an important material with advantages of low-production cost and high conversion efficiency. It has a market share of more than 60% in all photovoltaic materials. Directional solidification (DS) method has become the leading technique for producing mc-Si because of its better feedstock tolerance, higher throughput and easier operation.Solar cell efficiency is decreased by impurities, precipitates, and structural defects in the mc-Si ingots. The generation and distribution of these are investigated using numerical analyses in this paper. Simulation of heat and mass transfer in bulk growth has become an indispensable tool for an efficient, time and cost saving optimization procedure. A global modelling of heat transfer was performed to study the generation of creep stress and formation of dislocations in multi-crystalline silicon at the various growth stages for the various modified DS systems. The aim is to increase average grain size in silicon multi-crystals and reduce the impurities distribution and dislocation density.

Nano-crystalline based dye sensitized solar cells have reached 14.3 % of conversion efficiency. This is most attracted area in the field of photovoltaic technology due its low cost. These cells are expected to be produced easily in the labs as well as in industries without using any complex technologies. In DSSCs, TiO_2nano-crystalline particles are widely used as photoanodes. In order to enhance the electron transport in the TiO_2 network, one-dimensional crystalline TiO_2 nanostructures such as nanorods, nanotubes, and nanowires have been estimated to increase the electron diffusion length. In this study, different crystalline TiO_2 nanostructures were prepared by chemical methods. The synthesized materials were subjected to powder x-ray diffraction, electron microscopy and nitrogen adsorption-desorption isotherm analysis. Finally, the prepared nanostructures were integrated into DSSCs and their performances were analysed under simulated solar light (100 mW/cm^2). High conversion efficiency of 9.7 % has been achieved with crystalline TiO_2nanorods based photoanode. To solve the stability problem with liquid electrolytes, new solid polymer electrolytes (PVDF/KI/I_2 and 4, 4'-bypyridine in PVDF/KI/I_2) are being developed.

In recent days, the micromorph and nanowire solar cell research have become hot topics. The tandem solar cells of microcrystalline and amorphous silicon known as "micromorph" solar cell represents a promising way of overcoming the efficiency limits of single junction silicon solar cells and reducing the light induced degradation associated with amorphous silicon single junction solar cell. Oerlikon Solar Lab and Corning Incorporated demonstrated 11.9% stable efficiency micromorph tandem cell without any anti-reflection coating, as independently measured by NREL . Silicon nanowires are grown by PECVD for radial junction solar cells using thin gold and tin metal catalyst layers which are subjected to Raman study. Raman peak around 510 cm^{-1} confirms the crystalline nature of grown nanowires.

Graphene, the crystalline allotrope of carbon with 2D properties, has attracted immense research interest recently. Possible applications of graphene as a transparent conducting electrode in solar cells, as a diffusion barrier layer in P-N junction solar cells, as a counter electrode in DSSCs and as an intermediate layer in tandem solar cells are being explored. We synthesize graphene using CVD technique and Hummer method. We are exploring its applications as a transparent conducting electrode in amorphous silicon solar cells and DSSCs and as counter electrode in DSSCs.

IT 02 GENESIS OF SILICONINTEGRATED-CHIPS DEVELOPMENT, ITS PRESENT TRENDS AND ITS IMPACT IN OUR MODERN LIFE STYLE

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Rapid developments in electronics and its penetration in various fields representsan important emerging niche market, and entails the operation of electronic components in almost all domains such as conventional commercial, or even military usefulness. Examples of modern applications include: 1) High Definition-TeleVisions, Flexiblelectronics, Organic Light Emitting Diodes, New generation Smart Phones; 2) Drones; and 3) Automated car driving. All such applications are mainly build upon Integrated circuit devices (ICs) and these ICs, particularly Silicon (Si) technology based onesoffer great potential to simultaneously satisfy, both, with an ease of simple processing and also ultimately providing compelling cost advantages, including extreme environment applications. In this context, Si complementary metal oxide semiconductors (CMOS) technology is presently being used as an IC design platform to support the development of electronic components carefully designed to operate power efficiently, including under the harsh ambient conditions. In this presentation, we'll the review the history of IC developments starting from the invention of 1st transistor in 1945-47. Even the use of conventional electronics ranges into other areas like sensing, actuation, control and communications, the attraction of students into the "hardware" subject is rather less as compared to "software". This clearly must change, if India wants to be leading the hardware segment like our south-east Asianneighbours namely Japan, South Korea. One of the aims of this talk is to motivate and to draw the interestof students to take their career path in hardware field like semiconductor materials and devices. Like automotive, textile industries, the conventional commercial electronics industry was moving at a reasonable phase to offer unparalleled contribution to all walk of our day-to-day life. In this keynote address, we'll discuss the present status and trends in Si IC technology. The opportunities and challenges associated with utilizing Si technology in the general context of electronics applications will also be addressed in this talk.

IT 03 GRAPHENE-METAL OXIDE BASED NANOCOMPOSITESFORENERGY AND ENVIRONMENTAL APPLICATIONS

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Two dimensional graphene-based nanocomposites are emerging as a new class of materials with excellent properties, leading to their potential application in different areas. The study of decorating the graphene sheets with inorganic functional materials is now becoming a promising and challenging area of research. In this study, reduced graphene metal-oxide composites with SnO_2, CeO_2, MoS_2, V_2O_5 and CdS have been synthesized by homogeneous co-precipitation method[1,2]. Multi-layered composite structures with 1 D carbon nanotubes integrated with 2 D graphene structures with the addition of 3 D bulk nanoparticles were prepared with improved properties [3]. The structural propertiesofthegraphene oxide, graphene-metal oxide composites have been systematically studied. The prepared composite structure has been subjected to structural, optical, electrical property studies. The photocatalytic properties of the composites were studied for the degradation of organic dyes from industrial waste water [4]. The electrochemical properties of Graphene-metal oxide composites reveal that these materials can be effectively used as electrodes for supercapacitor application with improved specific capacitance, higher power density and cyclic stability [5,6]. Flexible free standing rGOpapers have been fabricated by evaporation induced self assembly process and their electrical, mechanical, optical and electrochemical properties have also been studied [7,8].

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IT 04 CHEMICAL BONDING AND ELECTROSTATICPROPERTIES OF MOLECULES FROMHIGH RESOLUTION X-RAY DIFFRACTION AND AIM THEORY

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Crystallography made paradigm shift in the areas of physical, chemical and life sciences. Conventional crystallography method enables to understand the structure of molecules at atomic resolution, which reveals the geometry of molecules and intermolecular interactions. Such information is limited to the geometry of molecules and not the chemical bonding and electrostatic properties molecules as it is necessary to understand the properties of materials. Experimental charge density analysis from high resolution X-ray diffraction gives the information about the nature of chemical bonding and the electrostatic properties of molecules. Such information allows to understand the structure-property relation of materials. Recent years, extensive experimental and theoretical charge density analysis of molecules has been performed to understand the drug-receptor interactions and high energy molecules. The detailed charge density analysis of some of the novel molecules will be presented.

IT 05 MODELLING MOLECULES, MATERIALS ANDROCESSES: BASICS & APPLICATIONS

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Several major scientific innovations appearedin the beginning of last century. Atomic structure was revealed, atomic spectra were explained, dualism of light was understood, quantum physics was born and many things followed. An important and notable development was the formulation of Schrodinger wave equation. Ever since this equation was published (1924) efforts were on to apply this equation to understand various physical, chemical and biological phenomena purely from theory. First such an effort was taken by Heitler and London (1927) who applied quantum mechanics to a chemical bond. This eventually led to the development of valence bond theory and molecular orbital theory, the two major approaches in Wave Function Theory (WFT) to explain bonding, structure and reactivity. Almost whole gamut of physics, chemistry and biology was brought under theory scanner. Of course the advent of computers have made the things much simpler and stretched the limits of the domains from physics to chemistry, biology and materials. From physics to biology or materials the system size increases manifold and complexity of interactions becomes very high. Consequently several approximations have to be invoked to numerically solve the formally exact Schrodinger equation and this has led to many types of errors and inaccuracies. So validation of the model against experimental results becomes mandatory before proceeding with the chosen model. Exactly forty years later Hohenberg and Kohn (1964) published two existential theorems that founded Density Functional Theory (DFT) that was widely applied in solid state physics and now it takes big strides in chemistry as a cheap alternative to WFT. Development of newer concepts and computer hardware and software have brought solutions of many complex problems into computing domain and particularly the development of graphical user interface (GUI) has made modelling very easy and attracted many non-specialists to use theory as a tool. In the early days designing molecules of a reasonable size was a formidable task but now with arrival of parallel architectures, materials or enzyme complexes or multi step reactions could be handled comfortably. Computational chemistry has sufficiently progressed and diversified into computational material science and computational biology and is still growing! The applications are ever expanding and newer basics are eventually introduced. Time dependant phenomena and relativistic effects are increasingly studied in recent years. Such complex developments have necessitated understanding of the underlying theory before use as one must understand the fact that a wrong application will lead to wrong results. Computational chemistry methods will always have to be used with scruples and caution to get meaningful results.Welcome to the domain of computational chemistry!

IT 06 MECHANISM AND DRUG INHIBITION OF INFLUENZA A (H1N1) VIRUS

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Swine influenza is a highly contagious respiratory disease, infecting people worldwide. There are many subtypes like H1N1, H2N2, H3N2, H5N1, H7N7 that have been confirmed both in humans and animals. The most common subtype, which affect human is influenza type A H1N1. Due to the high mutation rate of the virus, it is hard to find a vaccine. The influenza virus comprises three major target proteins, namely, Hemagglutinin (HA), Neuraminidase (NA) and M2-ion channel. The HA is responsible for binding terminal sialic acid on the host cell surface. The NA cleaves the terminal sialic from the cellular receptor, releases the newly formed progeny virions from the infected cell and permits them to infect other cells. The HA comprises the binding regions (130 loop, 190 helices, 220 loop and conserved residues 145, 153-155). The NA has two binding cavity 150 and 430 cavities.The M2-ion channel transfer protons into enodsomes of the infecting virus for the unpacking of the viral genome. The virus still continues to circulate in human populations, lead to millions of infections with many deaths and threatening people worldwide. There are two classes of anti-influenza drugs currently approved are M2-ion channel inhibitors (amantadine and rimantadine) and NA inhibitors (oseltamivir, zanamivir, peramivir and leninamivir). Though these drugs are powerful against influenza virus, it shows resistance to currently circulating influenza virus strains. Therefore, it is important to develop an improved novel anti-flu drugs which can limit the level of drug resistance. We have investigated the role of HA and NA viral proteins and how to target these proteins using suitable drugs by molecular docking and molecular dynamics simulations.

IT 07 NANOSTRUCTURED SEMICONDUCTOR MATERIALS FOR THERMOELECTRIC APPLICATIONS

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Thermoelectric nanomaterials have received much attention because of its high performance compared to bulk material due to increased phonon scattering at grain boundaries. Bismuth telluride (Bi_2Te_3) is a well-known low temperature TE material, and is commercially available for practical applications. Despite of huge efforts made by the researchers for the preparation of Bi_2Te_3 material, the large scale synthesis using conventional processes such as directional crystallization, is quite complicated as it requires sophisticated systems, due to the volatile nature and high vapour pressure of tellurium. Cobalt antimony ($CoSb_3$) is one of the skutterudite material for moderate temperature thermoelectric applications. In the present work, Bi_2Te_3 and $CoSb_3$ nanocrystals were synthesized by sol-gel method and pellets of nanocrystals were made by high pressure and high temperature sintering (HPHTS) process. The pellets were sinterred at different temperatures. The impact of sinterring temperature on phase transformation and morphological evolutions of pelletized nanocrystals were studied. Thermoelectric properties of as-prepared and sintered pellets were measured. Seebeck coefficient of Bi_2Te_3 and $CoSb_3$ nanocrystals has increased and the electrical resistivity decreased with sintering temperature. The variations of Seebeck coefficient and power factor are explained by a proposed model.

IT 08 SINGLE CRYSTAL XRD FOR PRECISE DRUG DESIGNING

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Drug development is evolved almost 'trial and error' over many centuries. Chemistry, biochemistry and spectroscopy advancements aid to identify causes of diseases and roles of protein and other biomolecules (putative drug targets) in such disease conditions.

By advancements in molecular biology, recombinant DNA technology and parallel developments of new physical methods such as flourimetry, calorimetry, microscopy and imaging techniques enriched our understanding about the disease mechanisms and role of particular biomolecule, whether small or macro, in such diseases.

Designing chemical compounds (ab initio or from traditional medicines) is the bottle neck in effective drug development efforts. The binding or recognition of these molecules with proteins (drug target) is primarily based on structural complementarity between target and drug. Hence it is easy to perceive that structural (3D) information about target and drug is necessary to establish the mechanism of action of the drug. More interesting fact is that if the target structure is known then library of structures (chemical space) can be screened against the target and identify new lead molecules. This is a virtual lab situation. If needed, leads can be optimized with desired characteristics to make them approvable drugs. Structure determination becomes essential to work with a small or macromolecule for effective and rational drug designing. X-ray crystallography, the only tool to establish the 3D structure and thereby it is the premier step in structure based drug design. Aiming PG students and Research scholars, appreciation of single crystal XRD will be made.

IT 09 COMPATIBILITY OF FERRITE MAGNETICNANOPARTICLES AND ZNOSEMICONDUCTORMETALOXIDE NANOPARTICLES IN CO GAS SENSORS

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The nanomaterial based gas sensors contain good sensitivity in the gas atmosphere, because nanomaterials of its high surface to volume ratio. The exact fundamental mechanisms that cause a gas response are still controversial, but essentially trapping of electrons at adsorbed molecules and band bending induced by these charged molecules are responsible for a change in conductivity. Grain size reduction is another main factor for enhancing the gas sensing properties of nanomaterials. On tailoring the advantages of the nanomaterials, a better response for different gases are brought out. A comparison is made in the present analysis on testing the gas sensing ability by two categories of nanomaterials such as spinel ferrites magnetic nanoparticles and zinc oxide semiconductor nanomaterials. Mn substituted $CoFe_2O_4$, $NiFe_2O_4$, $CuFe_2O_4$, $ZnFe_2O_4$ are considered for gas sensing study. Similarly, ZnO is formed under different morphology which is subjected to gas sensing analysis. Especially ZnO response is tested only for CO gas and these ferrites are also subjected to CO gas as well as other gases such as LPG, H_2 , NH_3 , Ethanol and methanol. The response time and recovery time are predicted and compared. In the first case, the ferrites materials generally possess high resistance and good magnetic property. Also, this material supported well to sense the LPG gas. But at the same time the response of CO gas is also observed for these ferrites. In the second case the morphological influence plays a dominant role in the sensing ability of CO gas. The sensitivity of CO is more in the case of ZnO nanoparticles than the ferrites. The higher sensitivity in the ferrites is also observed due to the presence of Zn^{2+} ions for sensing the gases. Moreover presence of Zn leads to good sensing ability of gases as it becomes metal oxide or a part in the ferrites.

IT 10 MANGANESE BASED CATHODE MATERIALS FORRECHARGEABLE LI-ION BATTERIES

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Rechargeable lithium-ion batteries (RLIBs) have emerged as themost dominant power sources for portable electronics andelectric vehicles and will remain so for many years to come. Manganese-based electrodematerials have become more attractive due to their inherentadvantageous properties such as earth-abundance, low-cost,environmental benignity and satisfactory thermal stability.Lithium manganese oxide, $LiMn_2O_4$ (LMO), a spinel for RLIBs is a cathode material that drives someelectric vehicle. However, the manganese based electrode materials have yet to meet the stringent requirement for electric vehicles due to problems arising from metal dissolution and capacity fading which limitslonger cycle life of battery. This talk will describe an overview of lithium -ion batteries, importance of electrode materials for electric vehicles and the strategies implemented to increase the cycle life of the cathode materials will also be discussed.

IT 11 IMPROVEMENT IN CRYSTALLINITY IF UNIDIRECTIONAL METHOD GROWNNONLINEAR OPTICAL (NLO) AND FERROELECTRIC SINGLE CRYSTALS FORSECOND HARMONIC GENERATION AND INFRARED (IR) DETECTOR APPLICATIONS

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Gravity driven concentration gradient is used in the uniaxially solution-crystallization method of Sankaranarayanan-Ramasamy (SR). TGS, GPI, KAP, SSDH, DGZCD, DGBCM, benzophenone and many more crystals have been successfully grown by SR method. Longest benzophenone crystal having dimension of 1350 mm length and 55 mm diameter was grown for the first time in solution growth by SR method. Starting with a thin plate as seed a large size crystal can be grown. Facets can be generated after cylindrical growth which may have its own added advantage in device making effort. Crystals with different crystallographic faces can be grown from conventional method and for practical applications where the specimen should have more size along a particular direction, therefore after the studies, the conventional method grown crystals with unique properties are collected and the chosen seeds are mounted in the SR method set up to get very high quality large size single crystals with minimum duration. Using slotted ampoule it was possible to avoid the accumulation of the segregated impurities while using not so very pure crystal ingredients. The experimental parameters involved in the present study were investigated in detail and a constant growth rate was achieved by compensating the loss of growth units in the solution. Using conventional and SR methods crystals have been grown and they were subjected to various studies like HRXRD, laser damage threshold, chemical etching, Vickers microhardness, birefringence, UV-Vis NIR, dielectrics and piezoelectrics. The SR method grown crystals show excellent optical, mechanical, dielectric and piezoelectric behavior and higher laser damage threshold capability compared to the conventional method grown crystals. HRXRD and etching studies showed that the quality of the SR method grown crystal is better than conventional method grown crystal. Similar enhanced performance was discovered in all the crystals studied. 100% solute-crystal conversion efficiency of SR method is an added advantage. We have performed real time and in-situ optical imaging of concentration and convection fields during unidirectional growth of benzophenone crystal. The shadowgraph technique is used to visualize convection, to quantify the thickness of the solutal boundary layer and the crystal growth rate. The Mach-Zehnder interferometry is used to quantify the gravity driven concentration profiles during growth. Special growth apparatus was designed and fabricated for performing the imaging experiments.

IT 12 COMPUTATIONAL MODELLING ON SILICON GROWTH PROCESS FOR ENHANCING SOLAR CELL EFFICIENCY

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Numerical simulation is a comprehensive tool in modern process development which is extensively used for promotion of crystal growth processes. Multi-crystalline silicon is an important material with advantages of low-production cost and moderately conversion efficiency of PV solar cells[1]. The control of grains as well as the grain boundaries is particularly important to the crystal quality and thus the solar cell efficiency. Flow in the molten phase is indispensable for transport of heat and mass convection in bulk crystal growth systems. Understanding transport of heat, mass and momentum is especially essential in bulk crystal growth processes. To grow high quality bulk crystals, i.e. the crystals with acceptable defect density and good dopant uniformity, understanding of transport processes coupled with the melt and gas chemistry is crucial[2]. Direct experimental investigation and in-situ observation of species transport are quite difficult due to the high-temperature environment. Therefore, crystal growth modelling attracts much attention in developing the technology and in finding an effective way to control mass transport during crystal growth. The work is broadly categorized into following:

- To study the melt flow properties ofsmall-scale molten silicon based on the dimensionless numbers such as Marangoni, Pecletand Reynolds numbers.
- To investigate the melt flow properties for large scale molten silicon based on the dimensionless numbers like Rayleigh, Reynolds and Prandtl numbers.
- To study the non-metallic impurities such as carbon, oxygen, nitrogen and their inclusions based on Schmidt number during directional solidification and its effect on the solar cell efficiencies.
- To analyse the generation of stress and dislocation densities in grown mc-silicon at various growth stages in industrial scale DS system.
- To introduce the bottom groove DS furnace and investigate some of the thermo-mechanical properties in grown mc-silicon ingot.

Also, many modifications are made on DS system for developing high performance of mc-silicon ingots such as heater modification, varying insulation movement, crucible rotation, crucible vibration and magnetic field application.

IT 13 TRANSITION METAL DOPED ZNO NANOROD ARRAYS FOR ENVIRONMENTAL APPLICATIONS

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In the present scenario“green life” has been inspiring people to pay more attention to eradicate hazardous substances in the environment especially in wastewater. The photocatalytic reaction has become a desirable method to covert the hazardous pollutants into simple and harmless compounds to remove the environmental pollution. Zinc oxide (ZnO) is a nontoxic wide band gap semiconductor photocatalyst, having unique properties such as high mobility, excellent chemical and thermal stability, high transparency and biocompatibility. To enhance its photocatalytic activity in the visible region and to utilize more solar energy, ZnO can be doped with metals and non-metals. In the present work, transition metals (TM) doped ZnOnanorod arrays on thin films have been prepared by hydrothermal method. Morphology, phase structure and optical properties of the thin films have been characterized by field-emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), and UV–Vis Spectroscopy. Formation of hexagonal wurtzite phase of ZnO was confirmed by XRD analysis. FESEM images showed the well-defined hexagonal shapeZnOnanorods. UV-Vis transmission spectra show that the substitution of TM in ZnO leads to band gap narrowing which was attributed to the formation of more defects in the nanorods. Photocatalytic properties were studied by the photodegradation of different organic dyes under visible light irradiation and the results reveal that the organic dyes were fully degraded within a minimum interval of time under visible light. The TM doped ZnO films were found to exhibit improved photocatalytic activity for the degradation of organic dyes under visible light in comparison with the undopedZnO film. The bactericidal efficiency of TM doped ZnO films were investigated against a Gram negative (Escherichia coli) and a Gram positive (Staphylococcus aureus) bacteria and the result showed that TM doped ZnO films enhances the antibacterial activity of pure ZnO.

IT 14 SUPERCONTINUUM GENERATION IN PHOTONIC CRYSTAL FIBERS

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We design a solid hexagonal photonic crystal fiber (PCF) with air holes of different diameters in the cladding region using the finite element method. We achieve a low group velocity dispersion of −5.483 ps2⁄km and a high nonlinearity of 111.4 W−1 km−1 at 450 nm with d1⁄Λ being 0.345, which could ensure single-mode propagation. The low dispersion and high nonlinearity form the crucial requirements to generate the supercontinuum (SC) pulse. The designed PCF exhibits a broad SC spectrum of bandwidth 600 nm at an operating wavelength of 450 nm which might find a great relevance in optical sensing applications.

IT 15 FABRICATION OF SN:CEO_2/ TIO_2 HYBRIDPHOTOANODEWITH HIGH PHOTO CURRENTCONVERSION EFFICIENCY OF DSSC

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CeO_2 and Sn:CeO_2 nanocrystals were successfully synthesized by Simple SonochemicalTechniue. Their photo voltaic performance were investigated doping with TiO_2 nanostructure in an effort to enhance the light conversion efficiency of DSSCs. The highest short circuit current was measured among them, which was proved to be related to the fast electrons transferred in the hybrid electrodes. CeO_2 has high band gap energy and conduction band of both stable Ce^{3+} ($4f^15d^0$) and Ce^{4+} ($4f^05d^0$) oxide states, owing to the remarkable redox property and oxygen storage capacity. The Ceria changes in the conduction band of TiO_2, due to the unoccupied Ce-4f trap states in the band gap, and reduction of Ce^{4+} to Ce^{3+} when electrons are injected in the photo anode. The cerium oxide doped photoanodes with special electrochemical properties which strongly influence the performance of DSSCs. The PCE of the Sn:CeO_2-TiO_2anode cell was conspicuously improved by loading the Sn:CeO_2 and the maximum PCE was 5.4 %. The overall solar to electric energy conversion efficiency was about 24 % for Sn:CeO_2/TiO_2 (AM-1.5, 100 mW/cm^2) compared with pristine anode.

IT 16 TRANSITION METAL DOPED ZNO NANOROD ARRAYS FORREMOVAL OF ENVIRONMENTAL POLLUTION

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In the present scenario,"Green Life" inspires researchers to pay more attention to eradicate hazardous substances in the environment especially in wastewater. The photocatalytic reaction has become a desirable method to covert the hazardous pollutants into simple and harmless compounds to remove the environmental pollution. Zinc oxide (ZnO) is a nontoxic wide band gap semiconductor photocatalyst, having unique properties such as high mobility, excellent chemical and thermal stability, high transparency and biocompatibility. To enhance its photocatalytic activity in the visible region and to utilize more solar energy, ZnO can be doped with metals and non-metals. In the present work, transition metals (TM) doped ZnOnanorod arrays on thin films have been prepared by hydrothermal method. Morphology, structure and optical properties of the thin films have been characterized by XRD, FESEM, and UV–Vis spectral studies. Formation of hexagonal wurtzite phase of ZnO was confirmed by XRD analysis. FESEM images showed the well-defined hexagonal shapeZnOnanorods. UV-Vis transmission spectra show that the substitution of TM in ZnO leads to band gap narrowing which is attributed to the formation of defects in the nanorods. Photocatalytic properties were studied by the photodegradation of different organic dyes under visible light irradiation and the results reveal that the organic dyes are fully degraded within a minimum interval of time under visible light. TM doped ZnO films were found to exhibit improved photocatalytic activity for the degradation of organic dyes under visible light in comparison with the undopedZnO film. The bactericidal efficiency of TM doped ZnO films were investigated against a Gram negative (Escherichia coli) and a Gram positive (Staphylococcus aureus) bacteria and the result shows that TM dopant in ZnO films enhances the antibacterial activity.

IT 17 RECENTLY DEVELOPED UNIDIRECTIONAL ORGANIC SINGLE CRYSTAL CYLINDERS FOR SCINTILLATOR APPLICATION

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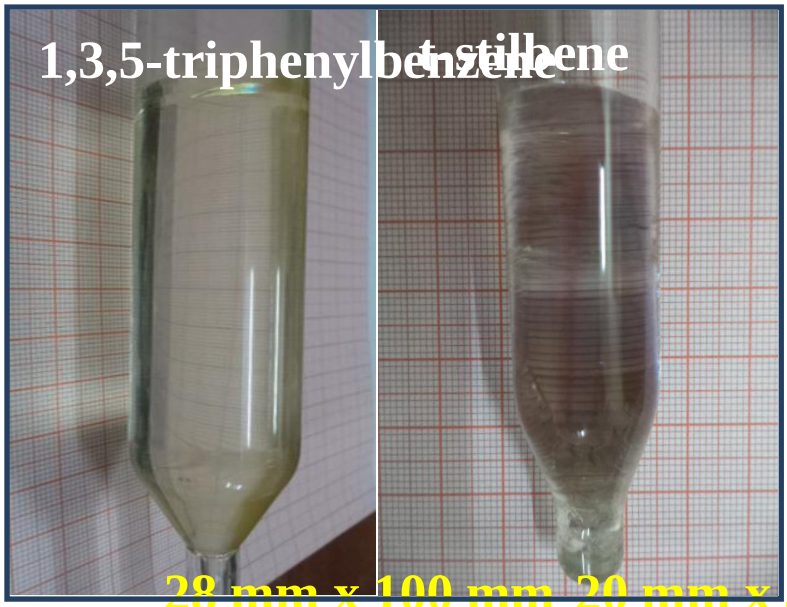
The well known organic scintillation materials namely t-stilbene and 1,3,5-triphenylbene were successfully grown unidirectionally with cylindrical dimension of 5cm x 2cm for t-stilbene and 10cm x 2.5cm for 1,3,5-triphenylbenzene. The growth along <001> in the case of t-stilbene and <110> for 1,3,5-triphenylbenzene and the obtained cylindrically morphology without any post growth machine lathing processes are the main features of the present study which may find commercial application as scintillation detectors. The selection of growth container facilitates the required cylindrical morphology and the temperature gradient assisted Sankaranarayanan-Ramasamy method offers crystals with acceptable merit. The grown crystals are investigated with PXRD, HRXRD, FT-IR, Micro-Raman, UV-Visible and Photoluminescence studies in order to establish phase purity, crystalline perfection, functional group identification, optical transparency and luminescence. The mechanical and thermal properties were also revealed by Vickers micro hardness test and TG/DTA analysis. The scintillation characteristics of the grown crystals under Gamma and Beta radiation sources resulted radioluminescence emissions at 365nm (t-stibene) and 355nm (1,3,5-triphenylbenzene). It is observed that the radioluminescence emission peaks are similar to that of their photoluminescence emission when t-stilbene was excited with 285nm and 1,3,5triphenylbenzene by 275nm. The functionality of scintillation characteristics for both the materials on their crystallographic direction and on the absence of boundary between planes is in progress.



IT 18 SINGLE CRYSTAL GROWTH OF HUMAN TISSUE-EQUIVALENT MATERIALS – EU AND DY DOPED BORATE SINGLE CRYSTALS AND THEIR CHARACTERIZATION

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Tissue-equivalent thermoluminescence (TL) dosimetry single crystals of dysprosium doped lithium potassium tetraborate (Dy:LKBO), and europium doped lithium potassium tetra borate (Eu:LKBO), were grown by Czochralski technique.

i. The Eu: LiKB4O7 polycrystalline compound was synthesized by standard solid-state reaction method. Phase purity of the samples were confirmed by powder X-ray diffraction technique. UV-Vis-NIR spectral analysis was carried out to study the optical characteristics of the grown crystal. The presence of functional groups, the existence of BO_3 and BO_4 bonding structure and the molecular associations was analyzed by FTIR spectroscopy. Europium ion in the trivalent state in the host $LiKB_4O_7$ was confirmed by its characteristic emission at 613 nm due to the $^5D_0 \rightarrow {}^7F_2$ transition. The (x, y) color chromaticity coordinates of Eu: $LiKB_4O_7$ was found to occur in the orange region of CIE 1931 diagram. The Eu: $LiKB_4O_7$ single crystalline sample was γ- irradiated by a Co-60 source with different doses and their thermoluminescence (TL) properties was analyzed. The prominent TL glow peak of the grown crystal appears around 184 °C. The TL intensity increases linearly up to 156 Gy and the fading was calculated for tenure of 60 days.
ii. Dysprosium doped lithium potassium tetraborate (Dy:LKBO) material with the effective atomic number (Z_{eff}) 8.07 was grown by the Czochralski technique in a platinum crucible. Preliminary characterization including XRD, UV-VIS-NIR, FTIR, and PL measurements were carried out on the samples. TL measurements were carried out at a heating rate of 4 K/s for γ-ray irradiated samples. TL glow curve consists of a dominant peak at (peak-maximum T_m) 454 K and another peak with weaker intensity at 618 K. The peak shape analysis of the glow peak (454 K) indicates the kinetics to be of the second order. The value of E is calculated using peak shape (PS) and computerized glow curve deconvolution (CGCD) methods. With an increase in the irradiation dose (from 26 to 156 Gy), the peak intensities of TL glow curves were found to increase linearly up to 156 Gy. The fading of TL signal was observed when the crystalline sample was stored in a dark box. The gamma irradiation storage stability was excellent for the grown crystal, with only 8% of the signal intensity being lost when the sample is stored in dark atmosphere over a period of 90 days.

The grown single crystals could act as potential materials in TL dosimetry applications.

AB 01 CUO/N-DOPED GRAPHENE NANOCOMPOSITE FOR ELECTROCHEMICALDETECTION OF GLUCOSE

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A new catalyst of N-doped Graphene CuO (NG-CuO) nanocomposite, for the electro catalytic oxidation of glucose. The nanocomposite was prepared by copper sulfate, cetyl ammonium bromide (CTAB) and graphite as starting materials. Crystalline phase and morphological structure of nanocomposite was studied with the techniques like X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and transmission electron microscope (TEM). Based on this composite a non-enzymatic glucose sensor was constructed. Electrochemical techniques were done to investigate the electro catalytic properties of glucose in alkaline medium. The fabricated sensor showed a linear response over a wide range of concentration from 3 to 1000 µM, with sensitivity of 2365.7 $\mu AmM^{-1}cm^{-2}$ and a fast response time of 5 s. The good analytical performance, low cost and simple fabrication procedure make this novel electrode material promising for the development of effective non-enzymatic glucose sensor.

AB 02 EXPERIMENTAL AND COMPUTATIONAL STUDIES OF TRIPHENYLAMINE BASEDORGANIC SENSITIZERS WITH DIFFERENT ANCHORING GROUP FOR DYE SENSITIZED SOLAR CELL (DSSC) APPLICATION

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Dye sensitized solar cells (DSSCs) represent a promising alternative to conventional silicon based photovoltaic technology, providing high photon-to-current conversion efficiency with possibly reduced fabrication cost. Metal free organic sensitizers have been synthesized for dye sensitized solar cell (DSSC) application. The dyes with D-π-A of two different dye structures are experimentally synthesized and theoretically analyzed by density functional theory (DFT) and time dependent density functional theory (TD-DFT).Two dyes TPA-1 and TPA-2 were investigated,

both dyes have triphenylamine group as donor part. TPA-1 and TPA-2 have acceptor groups are cyanoacrylic acid and melonic acid group respectively. The ground state geometries of the dye sensitizers are optimized in both the gas phase and N,N-dimethylformamide phase using Gaussian 09W [1] package, with Becke's three-parameter hybrid functional combined with the correlation functional of Lee, Yang and Parr (B3LYP) with 6-311G(d,p) [2] basis set. The various parameters of synthesized dyes such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), light harvesting efficiency (LHE) [3] and electronic absorption spectrum were analyzed and verified with experimental results. The free energy of dye regeneration and electron injection of the dyes are calculated by DFT and TD-DFT analysis. Dyes are synthesized and used as sensitizer in DSSC cell. The efficiency of the dye was measured by making the DSSC cell. The obtained results show that the TPA-1 is more efficient sensitizer compared to TPA-2. The results will be discussed in detail.

AB 03 DIRECTIONAL GROWTH, PHYSICOCHEMICAL PROPERTIES AND QUANTUM CHEMICAL INVESTIGATIONS ON 2-AMINO-5-NITROPYRIDINIUM P-PHENOLSULFONATE (2A5NPP) SINGLE CRYSTAL FOR NONLINEAR OPTICAL (NLO) APPLICATIONS

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Bulk single crystal and its distinctive property play an important role in nonlinear optics (NLO), electronics and photonics. In the past decades, extensive efforts have been made to grow crystal in bulk size with high quality for practical device applications. In this present work, an efficient organic nonlinear optical (NLO) 2-amino-5-nitropyridinium p-phenolsulfonate (2A5NPP) single crystal was grown by modified Sankaranarayanan-Ramasamy (SR) method in the period of 60 days. The grown single crystal has size 85 mm length and 15 mm diameter and it is observed that the growth rate of modified SR method grown crystal was found to be 10 times higher than the conventional method grown crystal. The unit cell parameters and morphology of the grown crystal were deduced by the Single crystal X-ray diffraction (SXRD) analysis. The molecular structure and the presence of functional groups were determined by NMR and FTIR spectroscopy analyses, respectively. The UV-vis-NIR analysis shows that the grown crystal possesses good optical transparency (85%) in the visible and NIR region. The title compound is thermally stable upto 200°C. The photoconductivity result reveals that the grown crystal possesses positive photoconductivity in nature. Frequency dependent dielectric constant, dielectric loss and AC conductivity of the grown crystal were analyzed. Photoluminescence spectral study evidence that the grown crystal has strong blue emission. Laser induced damage threshold study was carried out for the grown crystal. The Kurtz-Perry powder second harmonic generation (SHG) test has

been carried out for the 2A5NPP crystal and it exhibits 22 times that of standard KDP material. The theoretical calculations were performed by B3LYP/6-311++G (d,p) basis set. The structural parameters of 2A5NPP were studied using DFT method and the calculated results were compared with experimental values. The first order hyperpolarizability of the present molecule was calculated and it was found to be 2.9×10-29 e.s.u, which is 37 times higher than the standard urea molecule. The above results lead to conclude that the grown 2A5NPP crystal is a promising material for nonlinear optics (NLO) and optoelectronic device applications.

AB 04 THEORETICAL MODELLING ON CZ-SILICON GROWTH PROCESS FOR PV APPLICATIONS

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Numerical simulation is one of the important tools in the investigation and optimization of the single-crystal silicon growth by the Czochralski (Cz) method. In the present work, numerical simulation has been done for the growth of Cz-grown silicon single crystal during the initial stage of growth process at a certain crystal position of about 100mm. In Cz growth process, thermal stress is a major factor responsible for the dislocation generation. Therefore, in order to grow a good quality crystal, it is important to control thermal stress distribution. A 2D steady global heat transfer model was used to investigate the thermal stress distributions at particular crystal position during the Czochralski growth process.Thermal stress in Czochralski-grown silicon single-crystals is determined with a 2D axisymmetric approach taken from the global heat computations in which the temperature distribution in the crystal is axisymmetric due to axisymmetric boundary conditions. This 2D numerical simulation accounting for heat and mass transfer within the melt predicts physical phenomena inside the Cz furnace. The variation in thermal stress and comparative studies for with and without crystal and crucible rotations are done. A crystal growth simulation software CGSim (Crystal Growth Simulator) has been used for all computations. From the computational results, the thermal stress distribution along grown crystal and the possible reason for dislocation formation in the Czochralski-grown single-crystal silicon are determined.

AB 05 EFFECT OF CRUCIBLE DIMENSION IN THE DIRECTIONAL SOLIDIFICATION PROCESS

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Growth of world population is increasing day by day with energy requirement. Currently energy technology has been turning to the renewable energy side, because of long term requirement. In renewable energy sources solar energy is crucial one. Installed renewable power grids (excluding large hydro) in India (Up to Feb 2016): Wind power is 29,151 MW (59.8 %), Solar power is 9,566 MW (18.6 %), Bio mass power is 8,182 MW (15.9 %), Small hydro power is 4,346 MW (8.5 %) and Waste-to-power is 114 MW (0.2 %). Percentage of wind power in the renewable energy power production is very high but it has drawbacks compared to solar panels such as maintenance cost and lower efficiency after the life time of 20 years (wind energy is 66% and solar panel is 80 %). In the PV market 60 % of solar panels are occupied by the mc-Si solar cells, it is produced by DS process. Efficiency of mc-Si wafer is less than the mono-Si wafers but it has low cast, simple operating process and high mass production compared to mono-Si wafer production. During the mc-Si growth process stress and dislocation reduction is important because it will affect the conversion efficiency of mc-Si wafer solar cells.

We have numerically simulated two 6.90 Kg mc-Si ingot directional solidification (DS) systems (Different crucible dimension: DSS-1 and DSS-2) by using Finite Volume Method (FVM). The temperature distribution, melt-crystal (m-c) interface shape, vertical temperature gradient and melt flow velocity have been investigated. DSS-1 has convex m-c interface shape and DSS-2 has concave interface shape. Lower vertical temperature gradient and lower melt flow velocity are obtained for DSS-1 compared to DSS-2.

AB 06 SIMULATION OF INDUSTRIAL SCALE IRECTIONAL SOLIDIFICATION FURNACE WITH BOTTOM OPENING INSULATION TO GROW MC-SI INGOT FOR PV APPLICATIONS

Nagarajan S G, Srinivasan M, Aravinth K and Ramasamy P

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The modified DS furnace has been simulated by using appropriate software to analyze the effect of bottom opening insulation and the model is 2D axi-symmetric model. The laminar melt flow pattern and the convex melt-crystal interface which are more desirable for DS process can be obtained by employing effective temperature gradient with the help of bottom opening insulation furnace. Because of this the von mises stress in the mc-Si ingot was minimized compared with the conventional directional solidification furnace. In conventional furnace the heat loss occurs at both bottom and side wall of the crucible due to the side insulation movement but here the bottom opening insulation can prevent the side wall heat loss which leads to get a convex melt crystal interface. The controlled temperature gradient, convex m-c interface and reduced von mises stress may decrease the structural defects and the crystal quality is enhanced.

Growth of multi crystalline silicon has simpler experimental technique such as directional solidification process compared to growth methods of mono-crystalline silicon and it is low cost

too, so the PV industries prefer the mc-Si ingot for solar cells. Higher temperature gradient in the melt region causes more fluctuation in melt flow pattern due to convection which leads to turbulent flow pattern. The melt-crystal interface is another important factor to determine the quality of the ingot. The concave melt-crystal interface should minimize the ingot quality because some nucleations were formed near the crucible wall ahead of the melt-crystal interface and they are engulfed in the growing crystal which causes severe mechanical stress in the mc-Si ingot. The structural defects and the grain boundaries can reduce the quality of mc-Si ingot, those defects may be controlled by growing mc-Si ingot with low von mises stress. The modified furnace has bottom opening insulation. Here the total heat loss occurs only through the bottom of the crucible. By opening the bottom insulation the heat is extracted only through the bottom of the crucible so the crystal quality is improved. Fig.2a&b shows temperature gradient (left) and von mises stress (right) in grown ingot by conventional and modified furnace.

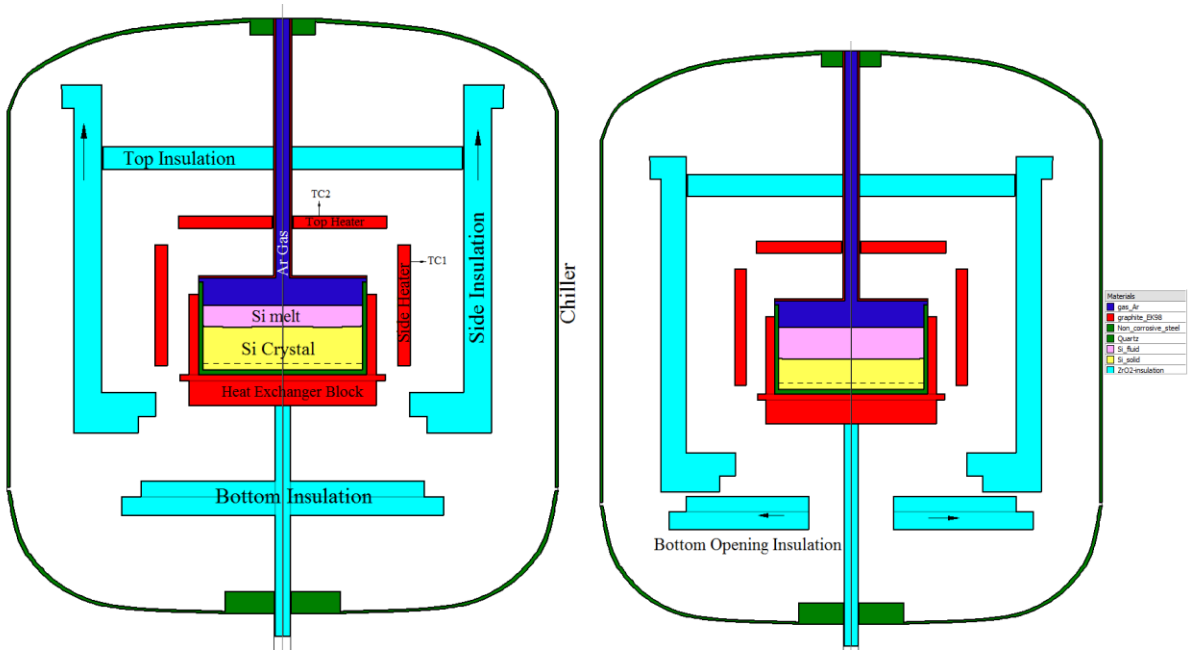

Figure 1, 2-D view of Conventional DS furnaceand Modified DS furnace (hole opening)

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AB 07 REDUCTION OF THERMAL STRESS AND DISLOCATION DENSITY BY ANNEALING THE DS GROWN MC-SI INGOT FOR PV APPLICATION

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90% of the solar industries are using crystalline silicon. Cost wise the multi-crystalline silicon solar cells are better compared to mono crystalline silicon. But because of the presence of grain boundaries, dislocations and impurities, the efficiency of the multi-crystalline silicon solar cells is lower than that of mono crystalline silicon solar cells. By reducing the defect and dislocation we can achieve high conversion efficiency. The velocity of dislocation motion increases with stress. By annealing the grown ingot at proper temperature we can decrease the stress and dislocation. Our simulation results show that the value of stress and dislocation density is decreased by annealing the grown ingot at 1400K and the input parameters can be implemented in real system to grow a better mc-Si ingot for energy harvesting applications.

AB 08 GROWTH OF 4-METHYLBENZOPHENONE (4MB) SINGLE CRYSTALS BY CZOCHRALSKI METHOD AND ITS STRUCTURAL, MECHANICAL AND OPTICAL CHARACTERIZATION

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4-Methyl Benzophenone (4MB) single crystal was successfully grown by Czochralski method. 4MB crystal belongs to monoclinic crystal system with the centrosymmetry space group of $P2_1/C$. The various functional groups present in the 4MB single crystal were identified by Fourier transform infrared (FTIR) spectrum analysis. The Vickers microhardness study was carried out for 4MB crystal. The nonlinear optical properties of 4MB crystal were carried out using Z-scan measurements.

AB 09 SYNTHESIS OF NANOCRYSTALLINE TIO_2ANORODS/NANOPARTICLES BY HYDROTHERMAL METHOD TO ENHANCE THE PERFORMANCE OF DYE SENSITIZED SOLAR CELLS (DSSC)

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Since notable breakthrough in 1991, the dye sensitized solar cell (DSSC) has been a more attracted candidate owing to its lower production cost and high energy conversion efficiency. In fabrication process, TiO_2 nanoparticles have been widely used. Even though, TiO_2 nanoparticles have high surface area for the attachment of the dye molecules, the grain boundaries reduce the

performance of the device due to the charge recombination. In recent times, one-dimensional (1D) nanomaterials have demonstrated significant advantage for the energy conversion applications. 1D nanostructure has been studied to improve the electron mobility and transport rate. However, 1D nanostructure suffers from inefficient dye loading owing to their low surface area, so that the additional work is needed to improve light harvesting efficiency. Therefore, a careful synthetic strategy is needed to fabricate TiO_2 materials, which is still a challenging task [1-2] for researchers. In this approach, novel TiO_2 nanorods/nanoparticles were prepared via hydrothermal process [3]. The structural information for prepared samples was confirmed with powder X-ray diffraction, which shows anatase phase with good crystalline behavior. The field emission scanning electron microscopy (FESEM) results indicate that the formed nanostructures are having porous structures. From the high resolution transmission electron microscopy (HRTEM) results, the images of nanorods/nanoparticles were clearly observed. Brunauer-Emmett-Teller (BET) analysis shows that the surface area of the sample is 93.08 m^2/g. The DSSCs were made using NR/NP based photoanode. The solar energy conversion efficiency (η) of the DSSC was about 8.5 % with J_{sc} of 19.58 mA/cm^2, V_{oc} of 0.704 V and FF of 0.62.

AB 10 THE EFFECT OF MULTIPLE-HEATERS ON THE REDUCTION OF IMPURITIES IN MC-SI INGOTS

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The purpose of this numerical study is to investigate the concentration of impurities during directional solidification (DS) of multi-crystalline silicon (mc-Si) with different modified heaters. . It has been suggested that the use of reduced heater area can reduced the carbon and oxygen impurity of mc-Si in a DS system. The simulation shows that the carbon impurities accumulate easily in the melt near the central region of the melt/crystal interface and oxygen impurities accumulate near the corner wall/crystal interface due to convection in the Directional solidification. A modified multiple-heater in the improved multiple-heaters show that the carbon impurities in the crystal can be reduced was designed to reduce the carbon and oxygen impurities. Global simulations of carbon transport to a value of 1.9×10^{17} atoms/cm^3 from 4.9×10^{17} atoms/cm^3. Oxygen impurities are reduced to a value of 7.4×10^{16} atoms/cm^3 from 5.12×10^{17} atoms/cm^3.

AB 11 INVESTIGATIONS ON SYNTHESIS, GROWTH AND PHYSICAL CHARACTERIZATION OF $CDGA_2SE_4$ SINGLE CRYSTAL BY MODIFIED VERTICAL BRIDGMAN METHOD

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$CdGa_2Se_4$ polycrystalline material was synthesized by melt oscillation method. Good quality $CdGa_2Se_4$ single crystal was grown by modified vertical Bridgman method. The crystalline phase and growth orientation were confirmed by powder X-ray diffraction pattern and unit cell parameters were confirmed by single crystal X-ray diffraction analysis. The stoichiometric compositions of $CdGa_2Se_4$ were measured using energy dispersive spectrometry (EDS). The structural uniformity of $CdGa_2Se_4$ was studied using Raman scattering spectroscopy at room temperature. The transmission spectrum of $CdGa_2Se_4$ single crystal was achieved in the near IR region and the absorption edge of the material is near 680 nm. The calculated optical band gap is 1.8 eV. Thermal property of $CdGa_2Se_4$ has been studied using differential thermal analysis (DTA). Thermal diffusivity, specific heat capacity and thermal conductivity were measured. Electrical property was measured using Hall Effect measurement and it confirms the n-type semiconducting nature. Photoconductivity measurements with different temperatures have confirmed the positive photo conducting behavior.

AB-12 SYNTHESIS OF PEROVSKITE TYPE DOPED-$SRMNO_3$ NANOPARTICLESFOR SOLAR CELL APPLICATIONS

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Titanium (Ti) doped Strontium Manganate with different Manganese contents has been synthesized by microwave assisted hydrothermal process. The structural, morphological and optical characteristics of obtained nanorodshas been characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) andultraviolet (UV) diffuse reflectance spectra analysis. The phase and crystallite structure of as-prepared strontium manganate depends on doped Ti content. SEM observations shows that the dopedstrontium manganate are composed with the diameter in range of nanoscale and length in micro scale range of about 10μm.SEM images reveals the nanorod like structure. The band gap energy of as-prepared material was estimatedto be 4.2eV from respective tauc plot.

AB 13 SYNTHESIS AND CHARACTERIZATION OF RARE-EARTH BASED DELAFOSSITE OXIDE MATERIALS FOR THERMOELECTRIC APPLICATIONS

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Thermoelectrics (TE) is a promising technology to convert the waste heat into electricity. By recycling the waste heat, CO_2 emission can be controlled up to some extent which leads to

green environment. The performance of the thermoelectric material is based on the Figure of merit of a material. Rare-earth based delafossite oxide ($CuLaO_2$) is one of a few materials available for high temperature thermoelectric applications. The SiGe materials are used in space in the SNAP-10, a nuclear reactor and have been the exculsive choice for radioisotope thermoelectric generator (RTG) launched by U.S. Since 1976. So, it is possible that Rare-earth based delafossite Copper oxide materials may replace Si-Ge alloys in future missions. On the other hand, Bismuth telluride is one of the commercially available thermoelectric material especially for low temperature applications. Therefore it is highly essential to develope a delafossite based thermoelectric materials for high temperature applications. Moreover, the nanostructuring is the promising way to enhance the thermoelectric properties of the material by controling the thermal conductivity. In the present work, Rare-earth based Copper oxide nanocomposite were prepared by mechanical ball milling method. The milling conditions were optimised by varying ball Size, milling time, Processing Control agent and Speed. The structural, morphological and thermoelectrical properties of the prepared materials were studied by XRD, SEM, TEM, Seebeck Coefficient, and Hall measurements. The thermoelectric properties of the prepared materials were studied as a functional of temperature. The results will be discussed in detail.

AB 14 STUDIES ON ZNO:YB NANOCRYSTALS FOR THERMOELECTRIC APPLICATIONS

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Zinc Oxide (ZnO) is one of the promising II-VI semiconductors with wide bandgap and useful for many applications include solar cells, biological labeling, optoelectronics. The thermoelectric properties of ZnO have been extensively investigated. The thermoelectric performance of a material can be determined by the dimensionless figure of merit (ZT). The problem with ZnO is its high thermal conductivity at elevated temperature which results low ZT of the material. Nanostructuring the material is an effective way to control the phonon transport thereby thermal conductivity of the material. In the present work, ZnO:Yb nanocrystals were synthesised by sol-gel method with various Yb concentration in the precursor solution. The structural properties of the material was studied by X-ray diffraction analysis and it confirms the crystal structure of the material. The functional groups of the nanocrystals were analysed by Raman spectra. The morphology of the synthesized nanocrystals was studied by FE-SEM analysis.

The thermoelectric properties of the nanostructured material was studied as a function of temperature and Yb concentration.

AB 15 INVESTIGATION OF OXIDE THERMOELECTRIC MATERIALS FOR ENERGY HARVESTING FROM WASTE HEAT

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High Temperature thermoelectric is a fascinating research field, that grows rapidly in current trends. This technique allows to harvest the electricity from waste heat and reduces CO_2 emission, which is beneficial for sustainable environmental. $SrTiO_3$, a promising peroveskite material suitable for thermoelectric application due to its superior physical and chemical properties, such as chemical and structural stability, great heat resistances, corrosion resistance and easy modification by other substances. In this work, a simple hydrothermal method is adopted to prepare the $SrTiO_3$ nanoparticles using Strontium Nitrate and TTIP as precursor. The structural, morphological and functional groups of prepared $SrTiO_3$ were analyzed using XRD, SEM, FTIR, RAMAN and UV-Vis Spectroscopic analysis. Thin transparent sheets of $SrTiO_3$ were formed during the lesser reaction time and their lateral dimensions are increased by increasing the reaction time in hydrothermal synthesis. The functional group and optical properties confirm the formation of $SrTiO_3$ nanomaterials. This material can be used as potential thermoelectric materials for high temperature thermoelectric applications.

AB 16 NOVEL METHOD FOR SYNTHESIS OF PEROVSKITE NANOMATERIALS FOR THERMOELECTRIC APPLICATIONS

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Thermoelectrics is one of the promising technologies for the conversion of an electricity from waste heat, which is coming out from industries and automobiles and etc. Thermoelectric technique is most suitable for efficiently utilizing the waste heat which leads to green environment. The performance of the thermoelectric materials can be analyzed by dimensionless Figure of Merit (ZT). Bismuth telluride is one of the well-known material for low temperature thermoelectric applications. Oxide materials are highly useful for high temperature thermoelectric applications because it has more stable and Thermal Conductivity. Metal oxides based perovskite have attracted high attentions as a novel thermoelectric material due to their excellent electrical conductivity. In the present work, $Ba_{1-x}RE_xSnO_3$(RE- La and Sr)materialwas prepared with different x=(0,0.02,0.04,0.06,0.08,0.1) values by polymerization complex method (PC) and pellets of the materials were made by high pressure and high temperature sintering (HPHTS) process. The

synthesized materials were characterized by XRD and TEM for structural and morphological analysis. Thermoelectric characteristics of the materials were studied by measuring the Seebeck coefficient (S) as a function of temperature. The La based sample shows high Seebeck coefficient compared to Sr based material. The substitution of La on the Ba site may resulted the variation in the carrier density and thereby the Fermi level which results high Seebeck coefficient compared to $BaSrSnO_3$.

AB 17 NANOSTRUCTURED COBALT OXIDE MATERIALS FOR THERMOELECTRIC APPLICATIONS

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World energy crises and the fast depleting energy resource stimulate the research on the alternate way of generating electricity. Thermoelectrics is a promising technology to convert waste heat into electricity. The performance of a thermoelectric material can be determined by its figure of merit which is directionally proportional to electrical conductivity and inversely proportional to thermal conductivity. Therefore a material should have high electrical conductivity and low thermal conductivity to be a best thermoelectric material. Nanostructuring is one of the promising way to control the thermal conductivity without degrading the electron transport. The oxide thermoelectric material shows the promising improvement in recent years. Moreover, the oxide materials are non-toxic and environmental friendly and ease to process as a devices. The cobalt oxide based thermoelectric materials are more reliable and hence we synthesized a series of $Bi_xCo_{1-x}O$ nanocrystals. Its basic characteristics such as structure, morphology and compositional variations were studied by XRD and SEM analysis. Thermoelectric properties of the synthesized materials were studied as a functional of temperature.

AB 18 SYNTHESIZE AND CHARACTERIZATION OF TI DOPED HEMATITE NANOPARTICLES BY HYDROTHERMAL METHOD

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The Ti doped hematite nanoparticles were prepared with various titanium weight levels (0, 5%, 10%, 15% and 20 at%) through hydrothermal method. The structural features of Ti doped iron oxide calcinated at 400 ^oC have been investigated by XRD, FT-IR, UV-DRS, PL, XPS and morphologies (SEM, TEM). The synthesis of Ti doped hematite at low temperature is helped to

form the small size of the particles. The pH value 8 has been considered for this approach to its excellent control of particle size, morphology, size distribution and properties. These results demonstrated that Ti-doped iron oxides could be acted as environmentally friendly catalysts for the deep oxidation of chlorinated volatile organic pollutants.Ti doping can also increase the electrical conductivity and decreases the Seebeck coefficient.

AB 19 PREPARATION AND CHARACTERIZATION OF CTAB REINFORCED SNO_2 NANOPARTICLES BYHYDROTHERMAL ROUTE

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The surfactant-mediated method is adopted to achieve tin dioxide nanoparticles with a high surface area which are generated within the template of the cationic surfactant (cetyltrimethylammonium bromide) micelle assembly. X-ray diffraction (XRD), field emission scanning electron microscopy, and transmission electron microscopy (TEM) were employed to characterize the annealed product, and optical property of the sample was studied by UV-visible diffuse reflectance spectroscopy (DRS). The XRD pattern of the sample is indexed to the tetragonal structure of SnO_2, and the calculated particle size is 22.4 nm, which is further confirmed by TEM. The selected area electron diffraction patterns showed continuous ring patterns without any additional diffraction spots and rings of secondary phases which is revealing their crystalline structure. Analysis of the DRS spectrum showed the bandgap of the synthesized SnO_2 to be 3.6 eV. The anionic surfactant CTAB plays a key role in the formation of the SnO_2 nanostructures.

AB 20 INCREASE IN EFFICIENCY OF THE SOLAR STILL DUE TO THE EFFECT OF DIFFERENT ABSORBING MATERIALS

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The most important factor that helps for the production of distilled water in solar still as the amount of solar radiation which is received on the glass cover. It is not assured that all the solar energy that falls on the surface of glass cover will be transmitted inside the solar still. It may get

reflected and absorbed by when it passes through. Part of the sunlight is reflected and observed by the glass, the water, and the basin surface. If the still is not perfectly sealed and insulated there will be heat losses to the surroundings. The different absorbing materials like charcoal, few selective coating materials, iron fillings etc., The performance of the still is studied by using these materials. The improvements in efficiency due to these absorbing materials are predicted.

AB 21 ROLE OF NARRATIVE ENGLISH LANGUAGE IN SCIENTIFIC CONTENT DEVELOPMENT

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Content development is the process of researching, writing, gathering, organizing, and editing information for publication either in print media or in mass media. Content development is basically about developing good content in a clear and presentable form. Hence, a content developer needs to have excellent command over written English. He/she should create web content based on analytical reports, press releases or survey reports and present them in a lucid, simple, easy to understand language. Content development could involve creative work, such as copy writing or graphics, or technical work. Content developers are essentially involved in the creation, development, and editing of content for various activities related to online marketing as well as front-end web development. There are a spectrum of content writing services for various sectors, including educational, product-related, medical, finance and art websites.

A content writer is responsible for creating original content for scientific publishing, websites, newsletters, press releases, blogs, articles and advertising and marketing materials based on the requirements. Content developers often use their skills, knowledge and experience in the mastery of English language coupled with softskills and information technology to develop the said content. Nowadays content developers also use web-based technology, to create and update content for websites.

Quite often, qualifications required for career as a content writer may vary. Hence, it is essential to keep yourselves updated with the latest technology trends to ensure on-going success. Self-employed content developers will have to attract and maintain a good client base to be successful in the long-term. Some of the basic skills required for a content developer are: Excellent communications and writing skills; Good observation, listening and converting skills; Multitasking abilities; Ability to work independently; Fairly good knowledge of current softwares like MS Doc, HTML, Photoshop, Dreamweaver, Macromedia flash, MS- FrontPage etc would be

of benefit in this profession. Before publishing the articles on the web, he or she should edit/proof read it.

Based on the requirements of the organization, a content writer needs to create new content, rewrite the existing content or edit and proofread content. He/she would also be responsible for managing content on print media, social media and develop unique ideas for web content. A content writer should clearly understand the objectives of the organization, his/ her target audience, and must develop simple, easy-to-understand, user friendly content while employing good search engine optimization (SEO) techniques. The content should be informative and engaging and should enable the visitors to get their information promptly and efficiently.

AB 22 QUANTUM CHEMICAL AND CHARGE DENSITY STUDIES ON GOLD SUBSTITUTED 8A,9,10,10A-TETRAHYDRO-2,6-BIS-(2-PHENYLETHYNYL) ANTHRACENE BASED NANO-MOLECULAR WIRE

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The theoretical electronic structure and transport properties of Au and 8a,9,10,10a-tetrahydro-2,6-Bis-(2-phenylethynyl) anthracene have been calculated from high level Density functional theory (DFT) using B3LYP method with LANL2DZ basis set. The molecular geometric parameters predicted by DFT method are in agreement with the reported results. The 8a,9,10,10a-tetrahydro-2,6-bis-(2-phenylethynyl) anthracene molecule reveals the, energy level shifting, bond topological features and the electrostatic properties for Au substituted molecule. Further, the decrease of HOMO-LUMO gap from 2.12 eV to 0.94 eV determined from density of states spectrum for the applied field (0 – 0.21 VÅ-1) shows that thiol linked 8a,9,10,10a-tetrahydro-2,6-Bis-(2-phenylethynyl) anthracene molecule can act as efficient molecular nanowire for Au electrodes.

AB 23 BOND TOPOLOGICAL AND HOMO-LUMO ANALYSIS OF ANTHRAQUINONE MOLECULE BY DFT AND AIM METHOD

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The Structural and bond topological and electrostatic properties of Anthraquinone molecule have been studied using the DFT and AIM analysis. The optimized (B3LYP/6-311G** and B3LYP/aug-cc-PVDZ) geometric parameters are in excellent agreement with the experimental data.The molecule exhibits C2v/C1 chemical symmetry; it is confirms that this molecule is planner in nature. Interestingly, the bond topological analysis based on the AIM theory shows the difference of charge distribution in all bonds. The calculated total molecular orbital energy gape ranges from 3.75 to 3.63 eV. The value of HLG measured from these calculations is almost matching with the value calculated experimental methods The HLG gives the very good information of conductivity.These observations give an insight on this kind of super conducting material, which are useful to design navel electronic devices.

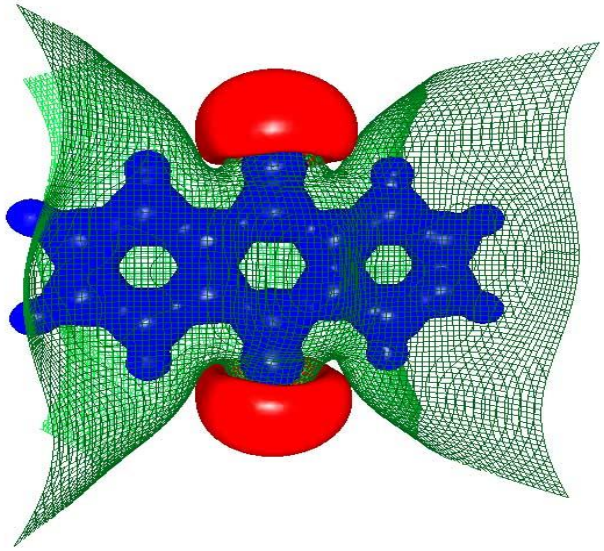

Figure shows Isosurface representation of electrostatic potential of anthraquinone molecule. Blue regions indicate the electropositive; red indicates electronegative regions and green regions indicate neutral. Isosurface values are ±0.5 eÅ^{-1}

AB 24 EXPLORING THE STRUCTURAL AND EXPLOSIVE PROPERTIES OF HIGHLY ENERGETIC 1,1-DIAMINO-2,2-DINITROETHANE (FOX-7) MOLECULE VIA *AB INITIO* AND DFT THEORY

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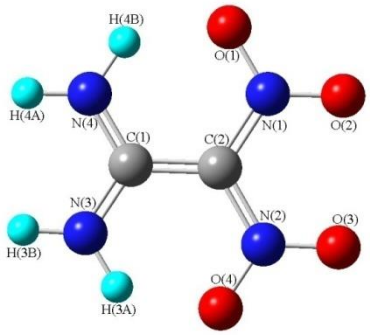
In the present study, the structural, electrostatic and explosive properties of FOX-7 molecule have been calculated from *ab initio* and DFT method with 6-311G** and aug-cc-PVDZ basis sets. The observed geometrical parameters are found very close to the experimentally reported structure. The bond sensitivity calculated from the nitro group charges and oxygen balance, shows, the nitro group attached C–N bonds are more sensitive than all other bonds in the FOX-7 molecule. Further, the bond sensitivity of molecules also calculated using ESP (V_{mid}), predicts the C–N bonds are the sensitive bonds in the molecules. On the basis of this investigation it is concluded that, the NO_2 group attached C–N bonds are the weak bonds in the molecule. Large electronegative regions are found near the nitrogen rich area, at the vicinity of NO_2 group; these are the expected nucleophilic sites of the molecule. The theoretically calculated structural and the explosive properties of insensitive FOX-7 energetic molecules at electronic level may be useful further studies.



Optimized structure of 1,1-diamino-2,2-dinitroethane (FOX-7).

AB 25 EXPLORING THE MOLECULAR STRUCTURE AND ELECTROSTATICPROPERTIES OF HIGH ENERGETIC 2,4,6-TRINITROPYRIDINEN-OXIDE MOLECULE VIA DFT CALCULATIONS

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The TNPyO molecule has been optimized using quantum chemical methods (B3LYP/Aug-cc-PVDZ) in order to find the potential HEDMs. The predicted optimized structural parameters are in good agreement with experimental value. This quantum chemical calculation reveals that, the TNPyO molecule C–NO_2 and N–O (N-oxide) bonds are weak, which confirms that these bonds are the weakest bonds in the molecule. The simulated TNPyO molecule reveals negative oxygen balance (-0.86%) and its energy gap is 3.45 eV. The calculated impact sensitivity and imbalance parameters show very good agreement with already known

explosives. These computational studies are the viable pathway and helpful for the experimental characterization and production of some of high energetic nitrogen rich molecules.

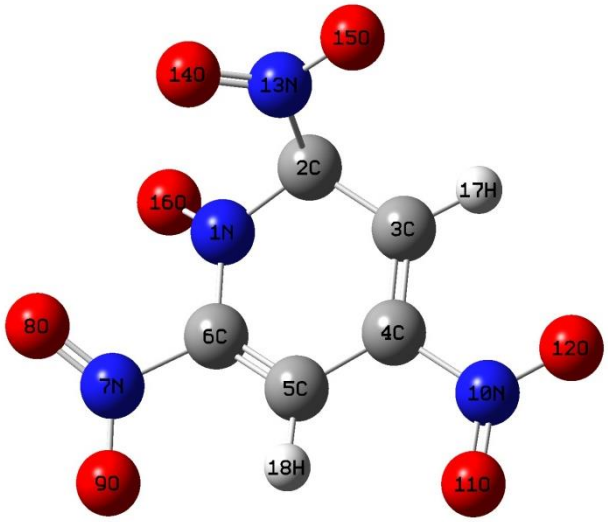

Figure shoes the optimized structure of 2,4,6-trinitropyridine-1-oxide (TNPyO) molecule.

AB 26 CRYSTAL GROWTH OF BENZPHOENONE BY BRIDGMANN TECHNIQUE USING A SOLAR CONCENTRATOR

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Benzophenone finds immense applications in products, such as sunglasses, food packaging, laundry and cleaning products to protect from UV light. It can contaminate drinking water and migrate from food packaging into food. Benzophenone is used in many food packaging inks too and may seep through foods. Benzophenone also occurs naturally in some foods (such as wine grapes and muscat grapes) and is added to other foods as a flavoring. In personal care products, benzophenone is used as a fragrance enhancer or to prevent products such as soaps from losing scents and colors in the presence of UV light. Derivatives of benzophenone such as BP2 and oxybenzone (BP3) are used in sunscreens. Oxybenzone is used as an ultraviolet light absorber and stabilizer especially in plastics and sunscreen agents. Benzophenone and oxybenzone are also used in nail polishes, and lip balms.

Benzophenone can be used as a photo initiator in UV-curing applications such as inks, imaging, and clear coatings in the printing industry. Benzophenone prevents ultraviolet (UV) light from damaging scents and colors in products such as perfumes and soaps. Benzophenone can also be added to plastic packaging as a UV blocker cum filter to prevent photo-degradation of the packaging polymers or its contents. Its use allows manufacturers to package the product in clear

glass or plastic PETE water bottles. Without it, opaque or dark packaging would be required. In biological applications, benzophenone has been used extensively as photo physical probes to identify and map peptide–protein interactions.

Crystal Growth of Benzophenone is achieved in both pure and doped forms using Bridgmann Technique using a solar concentrator aided fluid furnace which is optimally arranged. Bridgmann Technique coupled with solar concentrators and a fluid furnace which is a versatile technique for growing low melting materials (from 40 to 100˚C). The furnace used in this method is a very novel form where heat energy gets focused from a solar concentrator and a suitable fluid is utilized in the temperature capture which further leads to the melting process of the Benzophenone charge at 49-50˚C. Good quality crystals of Benzophenone were grown in pure form and doped forms using Sodium, Magnesium, Cobalt and Zinc as dopants. The grown crystals will be structurally confirmed by x-ray diffraction and characterized by spectroscopic investigations.

AB 27 CRYSTAL GROWTH OF BENZIL BY BRIDGMANN TECHNIQUE USING SOLAR HEATING PROCESS

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Benzil (otherwise known as 1, 2-diphenylethane-1, 2-dione) is the organic compound with the formula $(C_6H_5CO)_2$, generally abbreviated $(PhCO)_2$. This yellow solid is one of the most common diketones. Its main use is as a photo initiator in polymer chemistry. Most Benzil is used in the free-radical curing of polymer networks. Ultraviolet radiation decomposes Benzil, generating free-radical species within the material, promoting the formation of cross-links. Recently, Benzil has been demonstrated to be a potent inhibitor of human carboxyl esterase, enzymes involved in the hydrolysis of carboxyl esters and many clinically used drugs.

Crystal growth of good quality Benzil is achieved by Bridgmann Technique with the aid of a solar concentrator aided fluid fired furnace. The Bridgmann technique serves as a very good initiative mechanism where the crystals of Benzil can be grown both in good quality as well as in required specifications of size. The furnace used for this process is a very novel form of a fluid furnace which was fired using an induction heater placed at an optimal position. Good quality crystals of Benzil both in pure and doped forms were grown and harvested. The grown crystals will be characterized using structural and spectroscopic investigative methods to confirm the properties and investigate some new properties if any.

AB 28 CRYSTAL GROWTH OF BENZOPHENONE AND BENZIL BY BRIDGMANN TECHNIQUE USING A FLUID FURNACE

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Benzophenone is widely used as a protector from UV light. Benzophenone occurs naturally in some eatables and foods such as wine grapes and grapes and is added synthetically to other foods as a flavoring. Benzophenone is also used in personal care area as a fragrance enhancer or to prevent products such as soaps from losing scents and colors in the presence of UV light. Derivatives of benzophenone such as BP2 and oxybenzone (BP3) are used in sunscreens. Oxybenzone is used as an ultraviolet light absorber and stabilizer especially in plastics and sunscreen agents. Benzophenone and oxybenzone are also used in nail polishes, and lip balms.

Benzil (also known as 1, 2-diphenylethane-1, 2-dione) is the organic compound with the formula $(C_6H_5CO)_2$. This yellow solid is one of the most common diketones. It's prominently used as a photo initiator in polymer chemistry. Mostly Benzil is used in the free-radical curing of polymer networks. Ultraviolet radiation decomposes Benzil, generating free-radical species within the material, promoting the formation of cross-links. Ultraviolet radiation decomposes Benzil, generating free-radical species within the material, promoting the formation of cross-links. Recently, Benzil has been demonstrated to be a potent inhibitor of human carboxyl esterase, enzymes involved in the hydrolysis of carboxyl esters and many clinically used drugs.

Crystal Growth of Benzophenone and Benzil are achieved by adopting the Bridgmann process with the aid of a fluid furnace. The firing mechanism by which the fluid furnace gets heated is done by a host of heating mechanisms namely resistance heating and induction heating. Both pure and doped forms of Benzophenone and Benzil are grown and the prominent dopants used are Sodium, Magnesium, Zinc and Cobalt. Grown crystals of pure and doped forms will be characterized using structural, compositional and spectroscopic investigative methods and their results will be discussed in detail.

AB 29 ANNEALING EFFECT ON OPTICAL AND THERMAL PROPERTIES OF CdO NANOPARTICLES

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In the present study CdO nanostructured materials were synthesized using chemical co-precipitation method. CdO nanoparticles were prepared by using NaOH as a precipitating agent in water medium. The precursor was annealed at different temperatures at 300˚C, 400˚C, and 500˚C for 3 hours to produce nanocrystalline materials with different grain sizes. Fairly good nano particles of CdO were realized. The structural, optical and thermal properties were studied and analyzed for the effects of annealing by means of X-Ray diffraction, UV-VIS spectroscopy and Thermo Gravimetric analysis,

AB 30 CONCEPTUAL ARCHITECTURAL DESIGNING OF CRYSTAL GROWTH AND THIN FILM INSTRUMENTATION

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Crystal Growth and Thin Film Growth is nowadays becoming a more promising and prominent field which has very good scope in the areas of Scientific, Strategic, Solar Power Generation and Research and Development. Growing Crystals were an art earlier but now it is Technology. Growing Thin films were an expensive affair earlier. But nowadays scientific scenario especially in most Educational Institutions is such that we have to explore and design suitable alternatives for these two processes so that crystals and thin films are easily grown and harvested with a reasonable and economic expense. There are interesting alternatives to the expensive and complex instrumentation in both fields of Crystal Growth and Thin Films but if in case they are architecturally conceptualized, designed and developed in-house, indigenously in the laboratory, it costs a fraction of the procurement cost. The main hiccup of today's research and development is the costly instrumentation which is almost imported in large numbers.

So an earnest effort is taken in making some of the Crystal Growth and Thin film apparatus and equipments indigenously by our own expertise available in and around. The first apparatus made was the Solar Bridgmann Equipment (SBE) which involves the designing of a solar concentrator into an IR-furnace and thereby enabling it to grow crystals. Crystals can be grown upto 80 degrees C and when the concentrator array and focusing array is multiplied, then the temperatures can go fair higher. The second apparatus is the fluid furnace addendum which is installed inside the Solar Bridgmann Equipment. This fluid furnace perfected the annealing period of the crystals grown. The third apparatus is the Dip Coating apparatus which was used to grow

Zinc Oxide coatings and nano-rods on specific metal and metal-oxide substrates. The fourth apparatus is the primary electro deposition apparatus which used to grow thin films using the voltammetry idea. The fifth apparatus is the induction coupled Liquid Phase Epitaxy (IC-LPE) apparatus which can work with a simple induction hot plate. The sixth apparatus is the Microwave coupled Bridgmann Equipment. (MCBE) which can be used to grow crystals with the household microwave oven. The list continues. In this section we will see how we can build simple but architecturally superior instrumentation to inculcate complex growth methods in an effective manner.

AB 31 BASIC INSTRUMENTATION FOR PRIMARY CRYSTAL GROWTH RESEARCH

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Crystals both strategic and mystic are of use in both science and technology and in gemology alike. There are many techniques of growing these crystals of which some are functionally easy to handle with. The first versatile technique is solution growth which requires a small amount of space and little instrumentation like glassware. The constant temperature bath can be manufactured using locally available substances. The second technique is the Bridgmann Stockbarger which requires the fabrication of a temperature profiled furnace and an ascending puller which withdraws the ampoule with the melt. The third technique is the dip coating process which requires only some little glassware and some worthy salt which can be made into a thin film crystal coating. The fourth technique is the chemical bath deposition which employs the pickling process of coating crystalline surfaces onto the substrate. The fifth technique is crystal growth using induction heater where some solid crystals can be grown. The induction heating setup can be modified to be used as a LPE apparatus. The sixth technique is employing a microwave heater for both oxide growth and zone melting where good quality crystals are grown.

All the above techniques are tried presently many Arts and Science colleges can be possibly put to good use in other such similar colleges with interested students come together and congregate towards indigenous development of instruments.

AB 32 ESSENTIAL RESEARCH METHODOLOGY FOR SCIENCE AND HUMANITIES

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Research Methodology is a systematic, theoretical analysis of the methods applied to a specific field of study. It comprises the exhaustive and extended theoretical analysis of the body of methods and principles associated with that branch of knowledge. Typically, it encompasses concepts such as paradigms, theoretical models, phases and quantitative or qualitative techniques which will result in a specific useful scientific or socially beneficial finding. Research methodology does not set out to provide solutions in complete, but not the same as a method. Instead, research methodology offers the theoretical underpinning for understanding which method, set of methods, or best practices can be applied to specific case, for example, to calculate a specific result. There are several important aspects to research methodology. This is a summary of the key concepts in scientific research and an attempt to erase some common misconceptions in science.

Steps of the scientific method are shaped like an hourglass - starting from general questions, narrowing down to focus on one specific aspect, and designing research where we can observe and analyze this aspect. At last, we conclude and generalize to the real world. Researchers organize their research by formulating and defining a research problem. This helps them focus the research process so that they can draw conclusions reflecting the real world in the best possible way. There are several important aspects to research methodology. This is a summary of the key concepts in scientific research and an attempt to erase some common misconceptions in science. Steps of the scientific method are shaped like an hourglass - starting from general questions, narrowing down to focus on one specific aspect, and designing research where we can observe and analyze this aspect.

At last, we conclude and generalize to the real world. Researchers organize their research by formulating and defining a research problem. This helps them focus the research process so that they can draw conclusions reflecting the real world in the best possible way. After arriving at a Hypothesis, the researcher sets the variables and focuses his area of operation around the research problem chosen where measured evaluations are generalized for a clear conclusive and decisive result. The validity and reliability check is done in an exhaustive manner to make the research calibrated and ideal. Nowadays mandatory plagiarism checks are finally done to verify the originality of the research.

AB 33 ESSENTIAL AND EFFICIENT SCIENTIFIC INTERPRETATIONAL SKILLS

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Interpretation is an essential mode of able communication where the conversion and clarity of the subject is not lost after the literary conversion of the complete process. There are many interesting forms of interpretation skills which are finding appropriate uses in their respective areas. Nowadays there is an essential compelling need in the general mastery and vocabulary banking in English language with respect to Science since there is good scope of content development if there is a complete understanding of the underlying processes involved. An able interpreter would use some or all the listed types of interpretation skills given below in order to attain a precise description giving exactness and lucidity in each and every sphere. Science has grown in leaps and bounds by good interpretation where the processes, functions, theories and experiments reach a larger audience and gives vivid details invoking interest making the reader addictive and educating him in the easiest way ever possible. Thus, interpretation in total becomes an integral part of every scientific deliberation making it a functional part which explains even passive features most active including multidimensional skill sets in all possible dimensions.

There are many types of interpretation whereby the particular situation chooses the best form. Simultaneous Interpretation happens instantaneously and reflexively, Consecutive interpretation is carried out after taking abreast the full paragraph, absorbing it and then interpreting it. It normally happens in diplomatic circles and also in scientific circles where word by word interpretation becomes very much disjoint and unclear in totality. Whispered interpretation happens along with the speaker where the original and the interpretation goes hand in hand. Negotiation Interpretation happens in business circles where there it takes a very crucial and important form. Scientific Interpretation is an amalgamation of all the forms described above. An experiment should have simultaneous interpretation where the nature of the experimental process is explained. Consecutive Interpretation happens after each and every experimental routine. Whispered interpretation happens in very crucial experiments like launching of rockets in peace time or missiles during war. Negotiation interpretation happens when the same scientific experiment goes on industrial mode. Thus Interpretation is fully absorbed in all its forms totally in Scientific Interpretation. Thus these are the necessary and required skills which are essential for effective Interpretation.

AB 34 ESSENTIAL SIMULATION TECHNIQUES AND MODELS AIDING EFFICIENT SCIENTIFIC RESEARCH

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Computer simulation is the use of a computer with the aid of software or a package to represent the dynamic responses of one system by the behavior of another system modeled after it. A simulation uses a mathematical description, or model, of a real system in the form of a computer program. A computer simulation or a computer model is a computer program that attempts to simulate an abstract model of a particular system. Computer simulations build on, and are a useful adjunct to purely mathematical models in science, technology and entertainment. Simulation is the imitation of the operation of a real-world process or system over time. The act of simulating something first requires that a model be developed; this model represents the key characteristics, behaviors and functions of the selected physical or abstract system or process. Simulation modeling is the process of creating and analyzing a digital prototype of a physical model to predict its performance in the real world. Simulation modeling is used to help designers and engineers understand whether, under what conditions, and in which ways a part could fail and what loads it can withstand. Simulation is also known to be a set of techniques that use computers to imitate the operations of various real-world tasks or processes through simulation.

Computers are used to generate numeric models for the purpose of describing or displaying complex interaction among multiple variables within a system. Computer models are used to predict and investigate how a device or process might behave given a certain set of conditions. The rules of a model describe an object or process and the variables that can be changed to affect the way it behaves. A computer-based model is a computer program that is designed to simulate what might or what did happen in a situation. They are used in many ways including in astronomy, economics and sciences such as physics and biology. A computer-based model is a computer program that is designed to simulate what might or what did happen in a situation. They are used in many ways including in astronomy, economics and sciences such as physics and biology. Computer simulation, the use of a computer to represent the dynamic responses of one system by the behavior of another system modeled after it. A simulation uses a mathematical description, or model, of a real system in the form of a computer program.

Modeling and simulation (M&S) refers to using models – physical, mathematical, or otherwise logical representation of a system, entity, phenomenon, or process – as a basis for simulations – methods for implementing a model (either statically or) over time – to develop data as a basis for managerial or technical. Simulationis a way to model random events, such that simulated outcomes closely matcome situations do not lend themselves to precise mathematical treatment. Others may be difficult, time-consuming, or expensive to analyze. In these situations, simulation may approximate real-world results; yet, require less time, effort, and/or money than

other approaches and real-world outcomes. By observing simulated outcomes, researchers gain insight on the real world. The Monte Carlo method is a simulation technique using random numbers. Monte Carlo simulation techniques are used in business and industry to solve problems that are extremely difficult or involve a large number of variables.

Simulation is used when conducting experiments on a real system would be impossible or impractical: for example, because of the high cost of prototyping and testing, or because the fragility of the system will not support extensive tests, or because of the duration of the experiment in real time is impractical. Modeling and simulation (M&S) refers to using models – physical, mathematical, or otherwise logical representation of a system, entity, phenomenon, or process – as a basis for simulations – methods for implementing a model (either statically or) over time – to develop data as a basis for managerial or technical. An instructional simulation, also called an educational simulation, is a simulation of some type of reality (system or environment) but which also includes instructional elements that help a learner explore, navigate or obtain more information about that system or environment that cannot generally be acquired from mere instruction sets. They represent a reality within which students interact. Students experience the reality of the scenario and gather meaning from it. A simulation is a form of experiential learning. It is a strategy that fits well with the principles of Student-Centered and constructivist learning and teaching.

AB 35 SOLUTION CRYSTAL GROWTH OF PURE AND DOPED ZINC OXIDE CRYSTALS USING ACCELERATED EVAPORIZATION TECHNIQUES

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An indigenous solution growth workstation capable of room temperature crystallization and also working at various elevated temperatures is fabricated using locally available components. The starting materials in each case are taken in adequate quantities and then dissolved in double distilled de-ionised water in order to attain super saturation. The supersaturated solution is left to crystallize by slow evaporation process. Another supersaturated solution is prepared and filtered and loaded into 1000ml beakers and kept in a constant temperature water bath. Each of the crystals will appear spontaneously nucleated after a prescribed amount of time which is unique and proportional to the growth rate of the said crystal. While accelerated evaporation technique is

used, a gust of air is made to be constantly available on the vaporisation surface so as to speed up the process of crystallization. This happens when the particles of the solvent which is water in most cases is made to evaporate at a steady rate so as to form crystals. The rate of crystallization is at its optimally fastest pace. Care is taken so that excessive evaporation does not happen so that there is spurious nucleation and clustered nucleation where the formation of quality crystals is not seen. There may be some cases of poly- crystallization since the evaporation becomes intense and strong making more water molecules to leave the solution. The solution is made to evaporate using the solar concentrator in the next case. The beaker with the water bath is arranged inside a solar concentrator and made to crystallize at elevated temperatures. The increase in the speed of vaporization makes the crystals to grow at a faster pace. The grown thin films and crystals of pure and metal doped Zinc Oxide will be analyzed for their physical, scientific and spectroscopic properties.

AB 36 CRYSTAL GROWTH OF PURE AND MIXED CRYSTALS OF SODIUM CHORIDE AND SUCROSE USING FOXTAIL MILLET EXTRACT WITH ACCELERATED VAPORIZATION

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Growth of crystals from aqueous solution is one of the ancient methods of crystal growth. The method of crystal growth from low temperature aqueous solutions is extremely popular in the production of many technologically important crystals. It is the most widely used method for the growth of single crystals, when the starting materials are unstable at high temperatures and also which undergo phase transformations below melting point. The growth of crystals by low temperature solution growth involves days, weeks, months and sometimes years. Though the technology of growth of crystals from solution has been well perfected, it involves meticulous work, much patience and even a little amount of luck. A power failure or a contaminated batch of raw material can destroy months of work. The main disadvantage of the low temperature solution growth is the slow growth rate (but can be made faster) in many cases and the ease of solvent inclusion into the growing crystal. Under the controlled conditions of growth the solvent inclusion can be minimized and the high quality of the grown crystal can compensate the disadvantage of much longer growth periods. After many modifications and refinements, the process of solution growth now yields good quality crystals for a variety of useful and scientific applications. Growth of crystals from solution at room temperature has many advantages over other growth methods though the rate of crystallization is slow. Since growth is carried out at room temperature, the

structural imperfections in solution grown crystals are relatively low. Room Temperature Solution Growth of Sodium Chloride and Sucrose and mixed crystals of Foxtail Millet Extract is carried out in our department to produce good food quality crystals of scientific and technological importance.

AB 37 SPECTROSCOPIC ANALYSIS OF CERTAIN HERBAL MEDICINAL COMPOSITIONS AND THEIR CRYSTALLIZATION

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Extracts of Indian Medicinal plants namely Phyllanthous amarus, (Bhumi Amla) used for Aenimic, jaundice, Dropsy and Emblica officinalis (Amla) used for Vitamin - C, Cough , Diabetes, cold, Laxativ, hyper acidity and Lawsennia Lermis (Henna, Mehindi) used as Burning, Steam, Anti Inflammatory will be analyzed by spectroscopic investigations.

Spectroscopy is a method to find the functional groups and other important sub-groups in any given compound. It identifies the internal principles and its functional at a molecular scale. FTIR is used to obtain an infrared spectrum of absorption, emission, photoconductivity or Raman scattering of a solid, liquid or gas. An FTIR spectrometer simultaneously collects spectral data over a wide spectral range possible. This confers a significant advantage over a dispersive spectrometer which measures intensity over a narrow range of wavelengths at a time. FTIR has made dispersive infrared spectrometers opening up new applications of infrared spectroscopy. The term *Fourier transform infrared spectroscopy* originates from the fact that a Fourier transform being a mathematical process, is required to convert the raw data into the actual spectrum. The goal of any absorption spectroscopy namely FTIR, ultraviolet-visible "UV-Vis" spectroscopy, etc., is to measure how well a sample absorbs light at each wavelength. Using the "dispersive spectroscopy" technique, a monochromatic light beam is shined at a sample, measure how much of the light is absorbed, and repeat for each different wavelength.

A spectrum can be used to obtain information about atomic and molecular energy levels, molecular geometries, chemical bonds, interactions of molecules, and related processes. Often, spectra are used to identify the components of a sample (qualitative analysis). Spectra may also be used to measure the amount of material in a sample (quantitative analysis). There are several instruments that are used to perform a spectroscopic analysis. In simplest terms, spectroscopy requires an energy source (commonly a laser, but this could be an ion source or radiation source) and a device for measuring the change in the energy source after it has interacted with the sample (often a spectrophotometer or interferometer).

Herbal extracts are obtained in their pure form either by independent extraction or by fluid assisted extraction. The extracts are filtered and preserved simultaneously. A crystallization precursor like Sucrose, Fructose, Lactose or Sodium Chloride will be essential since they can be crystallized by solution growth method. Adding the precursor in a desired form and optimal strength until super saturation will be required to be left in a crystallization environment under room temperature. The crystallization will be carried out by evaporation process or by activated evaporation process.

AB 38 CONCEPTUAL DESIGN AND FABRICATION OF A LOW COST INDIGENOUS SOLAR WATER HEATER

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Solar Energy is an abundant form of energy which has good amount of heating by IR radiation in all conductive, convective and radiative forms. The energy which is available in enormous quantities rather freely is made to converge, convect and radiate so that energy capture occurs and heat-exchange is done whereby a suitable fluid is passed into hollow conductive metal tubes which is made to heat-up when arranged optimally in a black body like orientation. Hollow pipes of any conductive metal were soldered on another conductive metal sheet which is blackened on all visible surfaces. The top portion of the convective chamber is fixed with a transparent glass lid so that there would be little loss due to convection and radiation since there would be internal reflections of infra-red radiations. When there is abundant supply of sunlight, the infra-red radiations are trapped inside the heat chamber and the converged IR radiations transfer heat onto the liquids which circulate inside the hollow pipes. Now there is a specific amount of heat exchanged into the circulating fluid which collects heat and which upon recirculation maximises the quantum efficiency of the heat collected. Now water seems to flow out in its hottest phase which can be used to domestic and industrial applications. When the number of the hollow pipes are maximised there is a possibility that water can be converted into steam and can activate a steam engine or serve as a hot source. Simulation of the heat energy absorbed by conduction, convection and radiation using physical principles and the total quantum yield of solar energy, and its conversion into heat energy will be done. Theoretically simulated readings are compared with experimentally and practically available results.

AB 39 ELECTRODEPOSITION OF ZNO THIN FILM SOLAR CELLS

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Zinc Oxide is a good material both in crystalline and amorphous form is used for photoconductive and photovoltaic applications widely used as Solar Cells. Solar cells can be fabricated by many methods. Physical Vapour Deposition, Chemical Vapour Deposition, Electrodeposition are some of the methods available in which coatings for solar cells can be easily made. Electrodeposition is a versatile method which has an edge over all the methods in terms of coatings and the methodology of application. The main advantage in this process of thin film making is where the basic precursor of all solar cells which is Indium Tin Oxide (ITO), is judiciously replaced by conducting metal substrates or insulating polymers since it can cut costs and the substrate itself can be used as the electrode.

Pure and doped thin films of Zinc Oxide are initially grown on aluminium, Zinc and other metal substrates with thickness varying so as to reach the optimal solar cell quality. When inert polymer substrates are employed they require a mandatory primary layer of coating by dip-coating process where a supersaturated solution of the precursor is taken. Zinc Oxide is doped with metal dopants in order to increase the density of electrons making these solar cells more irradiation efficient. These pure and doped substrates of ZnO thin films are investigated for their structural, photoconductive and optical properties.

AB 40 CRYSTAL GROWTH OF NAPTHALENE & CAMPHOR BY BRIDGMANN-STOCKBARGER TECHNIQUE

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Bridgmann-Stockbarger Technique is a technically superior method of Crystal Growth using a congruent melt. The Vertical Bridgmann-Stockbarger workstation has a choice of interchangeable resistive heating or optical heating facility which can go up to 350˚C but having a uniform vertical temperature gradient. It is provided with an optimal sintering, melting and annealing profile vertically along the z-axis axially. A hollow cylindrical resistive/ optical heater capable of reaching 350°C is arranged vertically centred and co-incident with the geometric centre of the insulation blanket which is axially symmetrical. Refractory heat shields and tiles are

arranged on the top and bottom part and all possible parts of the apparatus so that there is good heat insulation and a good thermal gradient. A translation assembly is appended in order to pull the ampoule with the charge in the sintering, melting, crystallization and annealing zones. A rotor with an optimal translation speed is arranged so that the ampoule is hooked with the rotor and engaged for experimentation. A transparent ampoule is charged with the essential starting materials necessarily sintered and hooked to the translation assembly. An optimal translation is set and the growth run is commenced to produce crystals of the desired orientation and quality. The grown crystals of pure and doped Napthalene and Camphor will be characterised for their structural, morphological and optical properties.

AB 41 CRYSTAL GROWTH OF PURE AND DOPED CRYSTALS OF LEAD OXIDE BY BRIDGMANN-STOCKBARGER TECHNIQUE

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The Bridgman technique is a method of growing single crystalingots or boules. It is a popular method of producing certain semiconductor crystals, such as gallium arsenide, II-V Crystals (ZnSe, CdS, CdTe) and BGO, where the Czochralski process is more difficult. The method involves heating polycrystalline material in a container above its melting point and slowly cooling it from one end where a seed crystal is located. Single crystal material is progressively formed along the length of the container. The process can be carried out in a horizontal or vertical geometry. The Bridgman technique is a directional solidification process. The ampoule contains the charge which is made into a melt and moves through a vertical axial temperature gradient of a resistive heated furnace. Single crystals can be grown using either seeded or unseeded ampoules. Many novel organic single crystals can be grown by this unseeded method. The solid-liquid interface should be investigated during growth to improve crystal quality. A vertical bridgemann with a resistive heating single zone furnace is designed and fabricated in our Department for the growth of crystals. Crystals of pure and doped Lead Oxide is grown and characterized for their structural, optical and technical properties.

AB 42 GROWTH OF THIN FILM SOLAR CELLS BY SPIN COATING PROCESS

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Spin coating is an effective technique for the growth of both crystalline and amorphous thin films especially solar cells. The conceptualization, design and fabrication of an optimal spin coating apparatus was done indigenously. The spin coater is capable of reaching optimal speeds resulting in the growth of thin films. A substrate holder-clasper or clamp is fabricated on the top of the rotor stub firmly fixed so that not to spin off while reaching such high speeds. A transparent lid with a gaping hole is fixed with a provision for applying the liquefied charge periodically as regularly formed droplets onto the top substrate. A spill container is also arranged around the spinning platform in order to reduce the splashing thereby wasting the liquid charge.

The charge is taken as a supersaturated solution with an optimal texture and so that crystallization evolves easily else there is a possibility of accumulation and multiple nucleation which will prevent the film formation. Homogeneous and Heterogeneous combinations of single layered and multiple layered thin films are grown after arranging for a thin film coating with an optimal spin speed. Zinc Oxide thin films in pure and doped forms using metal dopants like Cobalt, Magnesium, Lead, Ferrous, Copper are formed on suitable metal and glass substrates. The thin films grown by this process will be subjected to structural, functional and optical characterizations.

AB 43 SOLUTION CRYSTAL GROWTH OF PURE AND DOPED ZINC OXIDE CRYSTALS USING ACCELERATED VAPORIZATION TECHNIQUES

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An indigenous solution growth workstation capable of room temperature crystallization and also working at various elevated temperatures is fabricated using locally available components. The starting materials in each case are taken in adequate quantities and then dissolved in double distilled de-ionised water in order to attain super saturation. The supersaturated solution is left to crystallize by slow evaporation process. Another supersaturated solution is prepared and filtered and loaded into 1000ml beakers and kept in a constant temperature water bath. Each of the crystals will appear spontaneously nucleated after a prescribed amount of time which is unique and proportional to the growth rate of the said crystal. While accelerated evaporation technique is used, a gust of air is made to be constantly available on the vaporisation surface so as to speed up the process of crystallization. This happens when the particles of the solvent which is water in most cases is made to evaporate at a steady rate so as to form crystals. The rate of crystallization is at its optimally fastest pace. Care is taken so that excessive evaporation does not happen so that there is spurious nucleation and clustered nucleation where the formation of quality crystals are not seen. There may be some cases of poly- crystallization since the evaporation becomes intense

and strong making more water molecules to leave the solution. The solution is made to evaporate using the solar concentrator in the next case. The beaker with the water bath is arranged inside a solar concentrator and made to crystallize at elevated temperatures. The increase in the speed of vaporization makes the crystals to grow at a faster pace. The grown thin films and crystals of pure and metal doped Zinc Oxide will be analysed for their physical, scientific and spectroscopic properties.

AB 44 FABRICATION OF THIN FILM SOLAR CELLS BY EPITAXIAL GROWTH

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With the present day energy demand, the ratio over production and consumption seems to be imbalanced. Search of greener and non-conventional energy resources is under full swing. Solar Cells are one of the promising contenders expected to play a very important part in the near future. Till now solar cells were predominantly Photovoltaic cells which were made of special materials called semiconductors such as Silicon, Germanium etc,. There are two types of solar cells: Crystalline and Amorphous. In both cases the key ingredient is silicon. Amorphous panels are typically cheaper to manufacture, less susceptible to breakage, and use less silicon, however their power output is typically lower than crystalline panels meaning that an amorphous solar installation would take up more space than a similarly power-rated crystalline installation. Amorphous solar panels deteriorate faster than crystalline solar panels and so their power output will fall more quickly during the years of use. A new emerging conceptualization in solar cell design and technology are Nanocrystalline solar cells which are advantageous than Crystalline or Amorphous solar cells. Most of these nanocrystalline cells require a very small amount of starting substances which makes it very attractive and efficient since the coated layer is obviously a nanometer thick. A detailed review of nano crystalline solar cells with a special emphasis on dye synthesized organic solar cell and its fabrication is discussed in this paper.

AB 45 FABRICATION OF SOLAR THIN FILM SOLAR CELLS USING DIP COATING

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In the dip-coating process, the substrate is slowly dipped into and withdrawn from a tank containing the sol, with a uniform velocity, in order to obtain a uniform coating. The deposition

operations were completely automated by computerised control system. The whole experimental set-up, entirely made in our laboratory, is isolated on a vibration damping table to ensure that the liquid surface remains completely undisturbed, thus granting the homogeneity of thickness at each deposition.

Physical manual withdrawal or Mechanised automated withdrawal can be organized based on the need and the requirement. Coating thickness generally increases with faster withdrawal speeds and decreases with slower speeds. The thickness is determined by the balance of forces at the stagnation point at the solidus-liquidus interface on the liquid surface. Faster withdrawal speed pulls more fluid up onto the surface of the substrate before it has time to flow back down into the solution. The thickness is primarily affected by fluid viscosity, fluid density, and surface tension.

Dip-coating, while excellent for producing high-quality, uniform coatings, requires precise control and a clean environment. The applied coating may remain wet for several minutes until the solvent evaporates. This process can be accelerated by heated drying. In addition, the coating may be cured by a variety of means including conventional thermal, UV, or IR techniques depending on the coating solution formulation. Once a layer is cured, another layer may be applied on top of it with another dip-coating / curing process. In this way, a multi-layer AR stack is constructed.

Very uniform and transparent Zinc oxide thin films doped with metal derivatives will be fabricated by the dip-coating technique. As starting material zinc acetate was prepared into a suitable supersaturated solution. The prepared solutions were very stable and suitable for dip-coating. The film formation of Zinc Oxide and its effect in film formation with the addition of the metals will be investigated in full. Structural, Optical, PV characterizations will be carried out on the said films.

AB 46 ZnO Thin Film growth using Chemical Bath Deposition

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The Chemical bath deposition (CBD) method is one of the effective methods to deposit thin films and nanomaterials, as it does not depend on expensive equipment and is a scalable technique that can be employed for large area batch processing or continuous deposition. The major advantage of CBD is that it requires only solution containers and substrate mounting devices. The one drawback of this method is the wastage of solution after every deposition. A large amount of the solution is so needed which has to be made a new and fresh. Chemical solution deposition (CSD) or Chemical bath deposition (CBD) uses a liquid precursor, usually a solution

of organometallic powders dissolved in an organic solvent. This is a relatively inexpensive, simple thin film process that is able to produce stoichiometrically accurate crystalline phases. This technique is also known as the sol-gel method because the 'sol' (or solution) gradually evolves towards the formation of a gel-like diphasic system. The chemical bath deposition involves two steps, nucleation and particle growth, and is based on the formation of a solid phase from a solution. In the chemical bath deposition procedure, the substrate is immersed in an aqueous solution containing the precursors.

Zinc Nitrate or Zinc Acetate was taken as precursors and made into a suitable supersaturated solution. A suitable electrode is taken and arranged for chemical bath deposition in the bath containing a suitable silica ge.. The temperature of the bath can be varied or deposition can be arranged at room temperature. The samples which were coated using this Chemical Bath Deposition method will be analysed for their structural, optical and technological properties.

AB 47 INSTRUMENTATION FOR THIN CRYSTALLINE AND AMORPHOUS NANOFILMS FOR IMPORTANT APPLICATIONS IN SCIENCE AND TECHNOLOGY

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A thin film is a layer of material ranging from fractions of a nanometer (monolayer) to several micrometers in thickness. Electronicsemiconductor devices and optical coatings are the main applications benefiting from thin film construction. The performance of optical coatings (e.g. antireflective, or AR, coatings) are typically enhanced when the thin film coating consists of multiple layers having varying thicknesses and refractive indices. Similarly, a periodic structure of alternating thin films of different materials may collectively form a so-called superlattice which exploits the phenomenon of quantum confinement by restricting electronic phenomena to two-dimensions. Work is being done with ferromagnetic and ferroelectric thin films for use as computer memory. It is also being applied to pharmaceuticals, via thin film drug delivery. Thin-films are used to produce thin-film batteries too.

Thin film applications can also be adopted on dye-sensitized solar cells. Ceramic thin films are presently in wider use owing to their cost effectiveness. The relatively high hardness and inertness of ceramic materials make this type of thin coating of interest for protection of substrate materials against corrosion, oxidation and wear. In particular, the use of such coatings on cutting tools can extend the life of these items by several orders of magnitude. Now research is being done on a new class of thin film inorganic oxide materials, called amorphousheavy-metalcation

multicomponent oxides, which could be used to make transparent transistors that are inexpensive, stable, and environmentally benign.

The act of applying a thin film to a surface is *thin-film deposition* – any technique for depositing a thin film of material onto a substrate or onto previously deposited layers. "Thin" is a relative term, but most deposition techniques control layer thickness within a few tens of nanometres. Deposition techniques fall into two broad categories, depending on whether the process is primarily chemical or physical. Plating relies on liquid precursors, often a solution of water with a salt of the metal to be deposited. Some plating processes are driven entirely by reagents in the solution (usually for noble metals), but by far the most commercially important process is electroplating. Chemical solution deposition (CSD) or Chemical bath deposition (CBD) uses a liquid precursor, usually a solution of organometallic powders dissolved in an organic solvent. This is a relatively inexpensive, simple thin film process that is able to produce stoichiometrically accurate crystalline phases. A thermal evaporator uses an electric resistance heater to melt the material and raise its vapor pressure to a useful range. This is done in a high vacuum, both to allow the vapor to reach the substrate without reacting with or scattering against other gas-phase atoms in the chamber, and reduce the incorporation of impurities from the residual gas in the vacuum chamber. The design and development of an improvised Electro-deposition equipment, Chemical Bath Deposition equipment, Physical Thermal Evaporator is being done for deposition of thin nano-films for various important applications in science and technology.

AB48 CRYSTAL GROWTH AND CHARACTERIZATION OF KDP DYE DOPED CRYSTALS

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Crystal Growth from solution is a very important process used in many applications from the laboratory to the industry. Potassium di-hydrogen phosphate (KDP) having important applications in electro-optics and harmonic generation was grown by rapid evaporation technique at room temperature.

Nonlinear optical single crystals of potassium dihydrogen phosphate KDP doped with Congo red dye were grown by slow evaporation method using a suitable solvent. Good quality single crystals have been harvested in the period of 23 days. The lattice parameters of the crystal and structural confirmation were obtained by single crystal X-Ray diffraction analysis.

The optical transmission observed from the specimen, FTIR confirms the presence of functional groups in the grown crystal. The nature of solidity of the crystal has been studied by Vicker's micro hardness values. The relative second harmonic generation ability has been tested by Kurtz and Perry powder technique. The thermal studies of the crystal has been carried out by TGA/DTA analysis.

AB 49 STRUCTURAL AND ELECTROCHEMICAL PROPERTIES OF SYNTHESIZED BUNKER C FUEL OIL WITH COLLECTED SiO_2 NANOPARTICLES

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Electrochemical (Energy storage) works are familiar to the technology world, wherein, in this work we prepare petroleum homogeneously mixed with metal oxide (collected SiO_2 from the beach sand) nano particles for efficiency enhancement studies on morphology, structure and associated electrochemical properties. Naturally petroleum is a complex liquid mixture of hydrocarbons of various molecular weights and other liquid organic compounds that are the found in geologic formations beneath the earth's surface. It's used mostly by volume for producing fuel oil and petrol that are both important "primary energy" sources. 84 vol.% of hydrocarbons present in petroleum is converted into energy-rich fuels.

Basically petroleum is branched out as crude oil and refined oil. Crude oil is characterized according to its geographical source and vary from light volatile fluid to a semi-solid [Class-A(Light, volatile), Class-B(Graden sticky), Class-C(Heavy Sticky) and Class-D(Graden fluid))], refined petroleum is derived from crude oils through processes such as catalytic crocking and fractional distillation [Gasoline, kerosene, Grade-2,4,5(Bunker B) & 6(Bunker C) and lubricant Oil].

Bunker C fuel oil and Collected SiO_2 are used to synthesized SiO_2 nanoparticles introduced to study structural and electrochemical properties. crystal size and structure are calculated used XRD, Functional groups and chemical compositions are studied FT-IR & NMR. Surface morphological and electrochemical studies are characterized used for SEM & CV. From the CV analysis of Bunker C fuel oil with SiO_2 prepared NPs are have electrochemical property.

AB 50 PETROLEUM (BUNKER C FUEL OIL) WITH COPPER OXIDE PWCO GEL: SYNTHESIS AND CHARACTERIZATION FOR ELECTROCHEMICAL APPLICATION

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One important derivative derived from Pertoleum of the fuel Oil is bunker C fuel Oil (heavy fuel oil or residency fuel oil), it has a big role in the transport sector where most of the vehicles and means of transport for every bit of the entire world. It is a chemical admixture of paraffins (alkanes), naphthenes (cycloakanes), aromatic and olefins (alkenes). The ratios vary based on a variety of derivatives. In petroleum compound the C chain in very important since it chooses its property and various factors mostly depend upon the molecular reactions.

By sol-gel method the synthesized gel is used to characterize the structure, morphology and electrochemical property which is studied because petroleum is one of the wide used organic fuel and has a good concoction of chemical properties whereby more than two hundred products are fractured from petroleum except its inherent but versatile electrochemical property. In this work we have verified the electrochemical property of Petroleum (Bunker C fuel oil) with transition copper oxide by cyclic voltammetry, Crystal structure & particle size by XRD, complex mixture by ^{1}H &^{13}C-NMR, functional groups study by FT-IR, morphological factors by SEM.

AB 51 TRACE ELEMENTAL ANALYSIS IN RANDOM SELECTIVE SOIL SAMPLES FROM RAINWATER HARVESTED FORMATIONS BY SEM AND EDAX ANALYSIS

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Environmental pollution is becoming the most challenging threat of human beings as a result of rapid sewage disposal and growth of population throughout the world. The problem of water and soil pollution due to industrial effluents as well as sewage waste have attained greater dimensions day-by-day in India (Bhosale, 1985). Conventional methods of liquid waste disposal for homes in un-sewered areas consisting of cesspool treatment followed by subsurface soil disposal (Simons and Magdoff, 1979. Bouma et.al., 1973).

While such systems can provide effective and economical treatment, they are not always reliable. Malfunctioning of systems are a risk to public health by contaminating ground and near by surface waters with pathogens (Scandria and Sobey, 1997). Recent studies indicate that significant amounts of organic and inorganic contaminants have been introduced into ground water through septic tank system (U.S. Envrionmental protection Agency, May 1980).

The distribution of trace and toxic elements in the environment is constantly altered by human activities as well as by natural biogeochemical process. Changes in metals, chemical binding, environment and solubility can potentially alter their mobility, availability and toxicity (Martinez et.al., 2001). The present paper deals with the SEM-EDAX analysis of soil samples collected from four different location at various depths in the environment of rainwater harvests

from Muthiah nagar, Chidambaram, Tamil Nadu and the identification of the elements were carried out.

An attempt has been made to study the extent of trace element content in the morphological structure of soil. Trace elements like Na, Mg, Al, Si, P, S, Cl, K, Ca, Mn, Fe, Cu, Zn, Cd and Pb were qualitatively and quantitatively analysed by Energy Dispersive X-ray spectrometer (EDAX) attached to the SEM (Scanning Electron Microscope) from soil samples in rainy season at different depth from the rainwater harvested drainfield leachate and the Spectroscopic results are analysed in detail.

The surfactant-mediated method is adopted to achieve tin dioxide nanoparticles with a high surface area which are generated within the template of the cationic surfactant (cetyltrimethylammonium bromide) micelle assembly. X-ray diffraction (XRD), field emission scanning electron microscopy, and transmission electron microscopy (TEM) were employed to characterize the annealed product, and optical property of the sample was studied by UV-visible diffuse reflectance spectroscopy (DRS). The XRD pattern of the sample is indexed to the tetragonal structure of SnO_2, and the calculated particle size is 22.4 nm, which is further confirmed by TEM. The selected area electron diffraction patterns showed continuous ring patterns without any additional diffraction spots and rings of secondary phases which is revealing their crystalline structure. Analysis of the DRS spectrum showed the bandgap of the synthesized SnO_2 to be 3.6 eV. The anionic surfactant CTAB plays a key role in the formation of the SnO_2 nanostructures.

AB 52 EFFECT OF PICRIC ACID ON THE CRYSTAL GROWTH OF SOME NLO MATERIALS

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The crystal growth of nonlinear optical (NLO) materials is essential since they have imminent potential applications in the field of telecommunications, optical signal processing, and switching. Nonlinear optics (NLO) is the branch of optics that describes the behavior of light in nonlinear media, in which the dielectric polarization P responds nonlinearly to the electric field E of the light. The nonlinearity is typically observed only at very high light intensities (values of the electric field comparable to interatomic electric fields, typically 108 V/m) such as those provided by lasers. Above this limit known as Schwinger limit, the vacuum itself is expected to become nonlinear. In nonlinear optics, the superposition principle no longer holds. Nonlinear optics remained unexplored until the discovery in 1961 of second-harmonic generation by Peter Franken et al. at University of Michigan, shortly after the construction of the first laser by Theodore Harold Maiman. However, some nonlinear effects were discovered before the development of the laser.

The theoretical basis for many nonlinear processes were first described in Bloembergen's monograph "Nonlinear Optics".

Some of the NLO properties are Second-harmonic generation (SHG), or frequency doubling, generation of light with a doubled frequency (half the wavelength), two photons are destroyed, creating a single photon at two times the frequency. Third-harmonic generation (THG), generation of light with a tripled frequency (one-third the wavelength), three photons are destroyed, creating a single photon at three times the frequency. High-harmonic generation (HHG), generation of light with frequencies much greater than the original (typically 100 to 1000 times greater). Sum-frequency generation (SFG), generation of light with a frequency that is the sum of two other frequencies (SHG is a special case of this). Difference-frequency generation (DFG), generation of light with a frequency that is the difference between two other frequencies. Optical parametric amplification (OPA), amplification of a signal input in the presence of a higher-frequency pump wave, at the same time generating an idler wave (can be considered as DFG).Optical parametric oscillation (OPO), generation of a signal and idler wave using a parametric amplifier in a resonator (with no signal input). Optical parametric generation (OPG), like parametric oscillation but without a resonator, using a very high gain instead. Spontaneous parametric down-conversion (SPDC), the amplification of the vacuum fluctuations in the low-gain regime. Optical rectification (OR), generation of quasi-static electric fields. The effect of Picric acid in the crystal growth of L-valine, glycine, L-asparagine, and L-proline is studied in detail. The grown crystals will be subjected to structural, optical, and spectroscopic investigations and NLO investigative characterizations.

AB 53 MICROWAVE SYNTHESIS OF TUNGSTEN OXIDE (WO_3) NANOPARTICLES

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Tungsten oxide nanoparticles (WO_3) were synthesized using microwave assisted method. Then as prepared nanoparticles was characterized to know their structural, optical and morphological properties. The monoclinic and orthorhombic (WO_3)crystal structure was obtained from the prepared nanoparticles by using X-ray diffraction (XRD). The functional groups were analyzed by using Fourier transform infra-red spectroscopy (FTIR) and the W-O chemical bonding

nature was confirmed. The surface morphology of the samples was observed by using scanning electron microscopy (SEM) and high resolution transmission electron microscope (HRTEM). From SEM studies, the surface morphology was unclear and careful observation in HRTEM studies shows that it contains rod shape structure. The optical properties were investigated by using ultra-violet visible spectroscopy (UV-VIS) and a blue-shifted optical absorption spectrum was observed when compared with bulk spectrum of WO_3. The PL emission behaviors were investigated by using spectrofluorometer and an enhanced defects reduced emission was obtained.

AB 54 THEORETICAL ANALYSIS OF QUANTUM MODELING & DFT: A REVIEW

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This study demonstrates the computation of structures and properties of the molecule using density functional theory (DFT). Computational methods dealing with the prediction and analysis of spectroscopic measurements and of their interpretation in terms of stereo-electronic, environmental, and dynamical effects. This topical introduction focuses on the most important conceptual aspects.

The basis of cluster model and quantum chemical methods of different level is critically discussed. This work illustrated by a great deal of theoretical *ab initio* and semi-empirical calculations and basis-set choices. It deals with Gaussian, which optimizes geometries; calculate vibrational frequencies, thermodynamic properties of the molecule etc. It can be used further to study their stability and potential interactions with other species.

AB 55 THERMAL, OPTICAL AND MECHANICAL PROPERTIES OF $B_2O_3 – Na_2O$ - CdO TERNARY GLASS SYSTEMS

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The borate glass composition of 70 B_2O_3 – (30-x) Na_2o - XCdO (where x= 0, 5, 10, 15, and 20%) was prepared for a melt quenching technique, All the glass had excellent thermal stability against crystallization; the structural analysis of glasses is carried out by XRD, The FTIR spectra studies have pointed out the conversation with structural units of BO_3+BO_4, The absorption spectra of the examined alkali borate glass containing transition metal ions, Thesis visible spectra are the result of d-d electron transfers of the transition metal ions, when linked with oxygen, The glass stability and weight loss measured for thermal properties TG-DTA. The optical absorption

measurements carried out for well-polished samples, calculated the band gap and ultrasonic velocity. TGA-is used to measure the weight loss as s function of temperature. DTA-is used to identify the glass transition temperature, crystallization temperature and melting temperature.

AB 56 QUANTUM CHEMICAL STUDY OF INDOLO [3, 2, 1-JK] CARBAZOLE FOR DYESENSITIZED SOLAR CELLS: EFFECTS OF ACCEPTOR GROUPS ONOPTOELECTRONIC PROPERTIES

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In this work, we designed and screened a series of indolo [3, 2, 1-jk] carbazole based dye sensitizer for Dye-Sensitized Solar Cells (DSSCs). The electron-donor containing indole-carbazole, thiophene as spacer and cyanoacrylic acid an electron acceptor based on donor-spacer-acceptor (D-π-A) as reference dye IC-2 are discussed. In order to enhance the effect in rhodamine acetic acid was investigated at IC-2 dye. The effect elector acceptor of the substituent on the absorption spectra and photovoltaic properties has been investigated by the combination of density functional theory (DFT) and time-dependent DFT (TD-DFT) approaches. Different exchange-correlation functional was initially evaluated in order to establish a proper methodology for calculating the excited-state absorption spectra of the IC-2. Consequently, TD-WB97XD method and 6-31G (d, p) of the basis set have used with the comparison of experimental value. From the calculated results, concluded that the rhodamine acetic acid dye was strongly grouped for more red-shift and electrons injected into semiconductors effectively and also reduced aggregation of dyes in TiO_2. 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.

AB 57 SPR BASED BIOSENSOR FOR DETECTING BIOMOLECULES USING MAGNETIC MATERIAL WITH GRAPHENE LAYERS

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In the present work we have investigated the angular response of Surface Plasmon resonance biosensors with magnetic material (Ni) and Graphene. The numerical calculation of presented work shows the high sensitivity and other parameters such as FWHM, Detection accuracy, Quality factor. The thicknesses of these materials are optimized. In this field the gold

material are have the good sensitivity compared with other materials but in the case of cost wise it possesses drawback, also gold is not good absorber of bio molecules, when replacing gold with nickel it gives good sensitivity and the Graphene layers helps to adsorb biomolecules well.

AB 58 SENSITIVITY ENHANCEMENT OF A SURFACE PLASMON RESONANCE BASEDBIOSENSOR USING SILVER - (MOS_2)-PLATINUM-GRAPHENE

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In the present theoretical work, the performance of surface plasmon resonance (SPR) based biosensor consisting of BK7 prism-silver (Ag)-Molybdenum Disulfide (MoS_2)-platinum (Pt)-graphene structure is analysed numerically, based on angular interrogation method. The performance of the sensor has been quantified in terms of sensitivity and it is found that can be tuned by selecting number of MoS_2 and graphene layer. The proposed biosensor with Ag,Pt, three layers of MoS_2 and a single layer of graphene demonstrates the highest sensitivity of 246°/RIU.

AB 59 QUANTUM CHEMICAL STUDIES, SPECTROSCOPIC ANALYSIS AND MOLECULARSTRUCTURE INVESTIGATION OF 4-CHLORO-2-[(FURAN-2-YLMETHYL)AMINO]-5-SULFAMOYLBENZOIC ACID

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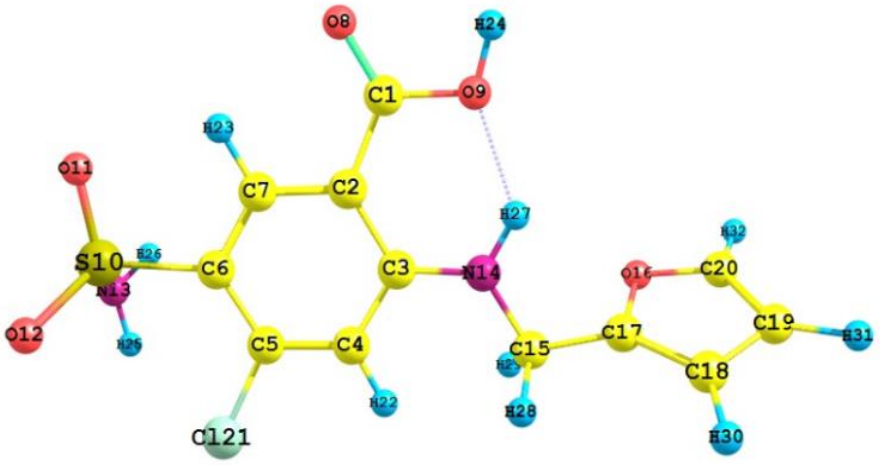

In this study, the FTIR, FT-Raman and UV-visible Spectra of furosemide molecule,C_{12}H11ClN2O5S, (with synonym,4-Chloro-2-[(furan-2-ylmethyl)amino]-5-sulfamoylbenzoic acid were recorded experimentally and theoretically. Optimized geometrical structure, harmonic vibration frequencies and chemical shifts were computed using hybrid-DFT (B3LYP)method and 6-31G (d,p) as the basis set. The complete assignments of fundamental vibrations were performed on the basis of the experimental results and Total Energy Distribution (TED) of the vibrational modes. The molecule orbital contributions were studied by density of energy states (DOSs). UV-visible spectrum of the compound was recorded in the range 200-400nm and the electronic properties such as HOMO and LUMO energies were determined by Time-Dependent DFT approach. Furthermore thermodynamic properties were performed using B3LYP-6-31G (d,p) level for the furosemide compound.

AB 60 EXPERIMENTAL ASSESSMENT OF THERMAL PERFORMANCES OF SOLAR COLLECTORS WITH NANO-CARBON AND METAL OXIDE COATED FINS

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This applied research is devoted not only to develop the nano-carbon and metal oxide coated solar fins but also to experimentally analyze the solar collector integrated with the nano-carbon and metal oxide coated fins. In this connection, the present research work was carried out with the objectives such as (i) preparation and deposition of absorptive coatings with nano sized carbon and metal oxides (ii) characterization of absorptive coatings effected on aluminium

substrates and (iii) experimental evaluation of thermal performances of solar collectors with the nano carbon and metal oxide coated fins. In the present research work, the absorptive coatings with optimized composition of carbon and metal oxides were prepared and they were spray coated on aluminium substrates. The prepared solar absorbers were characterized and it was found that the crystallite sizes of carbon and metal oxides were in nano sizes. Subsequently, the thermal performance and losses of solar collectors integrated with the optimized fins were experimentally estimated. The experimental results showed that the thermal performance of solar collectors with fins of different nano-carbon and metal oxide coatings was higher than 65.0 %. The experimental results also showed that the thermal loss of solar collectors with fins of different nano-carbon and metal oxide coatings was lower than 4.0 $Wm^{-2}°C$. On the basis of generated database, it could be concluded that solar collectors with nano-structured fins would be used due to their enhanced thermal performances and reduced thermal losses Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were performed to examine geometry, electronic structure, polarizability and hyperpolarizability of sensitizer in dye-sensitized solar cell. The calculations were carried out using hybrid functional B3LYP. A ZnO cluster was used as a model semiconductor towards determining conversion efficiency of the dye. The efficiency of the designed dye molecule is analyzed using various parameters such as the HOMO–LUMO energy gap, absorption spectra. The simulated absorption spectra of the selected dye molecule are good candidates for DSSC applications. Furthermore, the study on the polarizability and hyperpolarizability of the designed molecule is good candidates for NLO applications. The Photovoltaic measurements were carried out to determine the V_{oc}, J_{sc}, V_{max}, J_{max}, FF and overall energy conversion efficiency (η) of the samples by using J-V studies under 100 mW/cm^2 of stimulated sunlight.

AB 61 QUANTUM CHEMICAL INVESTIGATIONS OF 4-HYDROXY- 3-METHOXYPHENYL FOR DYE-SENSITIZED SOLAR CELL APPLICATIONS

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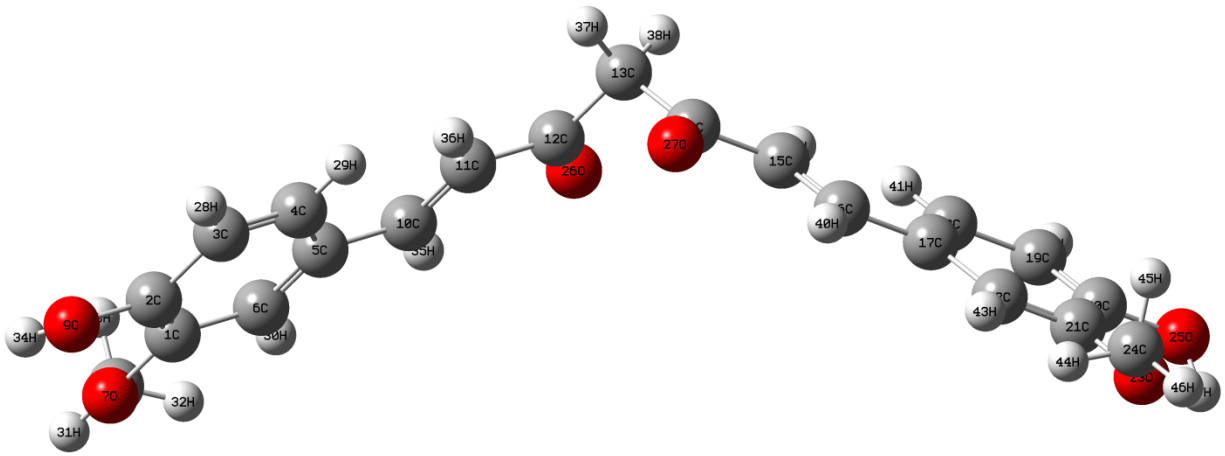

Optimized geometrical structure of 4-hydroxy- 3-methoxyphenyl

AB 62 PHARMACOLOGICAL INVESTIGATION OF 2-AMINOBENZOTHIAZOLIUMETHYLBENZENESULFONATE : SYNTHESIS, SPECTRAL CHARACTERIZATION AND STRUCTURAL ELUCIDATION

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The novel organic compound synthesized and structure was confirmed by various spectral studies. Single crystal X-ray diffraction analysis to confirms the strong hydrogen bonding interactions. Furthermore, biologically activity of the compound is examined by in *vitro* antimicrobial, DNA binding/cleavage and antioxidant studies. The microbial activities of synthesized compound were examined against various fungi and bacteria species possesses a good inhibition activity. DNA interaction with compound shows that the compound could interact with CT-DNA *via* intercalation binding mode. Investigation of antioxidant properties showed that the compound have strong radical scavenging potencies.

AB 63 STUDY OF GEOMETRICAL AND NLO PROPERTIES OF ALIZARIN FOR DSSC APPLICATIONS

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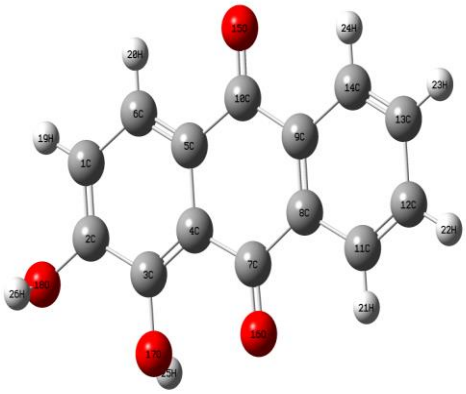
The geometries, electronic structures, polarizabilities, and hyperpolarizabilities of organic dye sensitizer Alizarin was studied based on ab initio Hartee Fock (HF) and Density Functional Theory (DFT) using the hybrid functional B3LYP. UV-Visible (UV-Vis) spectrum was investigated by Time Dependent- DFT (TD-DFT). Features of the electronic absorption spectrum in the visible and near-UV regions were assigned based on TD-DFT calculations. The absorption bands are assigned to $\pi \rightarrow \pi^*$ transitions. Calculated results suggest that the three excited states with the lowest excited energies in *Alizarin* dye are due to photo induced electron transfer processes. The interfacial electron transfer between semiconductor TiO_2 electrode and dye sensitizer *Alizarin* dye is due to an electron injection process from excited dye to the semiconductor's conduction band. The role of cyanine and methyl group in *Alizarin* dye in geometries, electronic structures, and spectral properties were analyzed.



AB 64 INFLUENCE OF IRON OXIDE NANOPARTICLES ON THE GROWTH OF *TRIGONELLAFOENUM-GRAECUM* IN THE RED SOIL ENVIRONMENT

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In the present study Iron oxide (Fe_3O_4) nanoparticles was synthesized using Ferric nitrate as the precursor and sodium hydroxide as the precipitating agent. Synthesized nanoparticles were characterized using X-ray diffraction, SEM, FTIR, and UV-visible spectrometer. The results showed that synthesized iron oxide nanoparticle exhibited UV-visible absorption peaks at 278nm,

which indicates that the particles were photosensitive and the XRD study confirmed that nanoparticles were crystalline in nature. The various functional groups present in the synthesized nanoparticleswere analyzed and the peak at 515 nm was assigned to Fe-O stretching and bending mode. The SEM results revealed thatiron oxide nanoparticles were cubic spinal in shape and having the particle size in the range of 20nm to 25nm.As to test agricultural impact of the synthesized iron nanoparticles about 5gm of iron oxide was incorporated to the red soil and moisturized for 7days and the seeds of *Trigonellafoenum-graecum* were sowed in to the soil , its germination and agronomical traits were measured using POT studies and found that iron oxide nanoparticle really enhanced the germination and the growth factor. The samples were harvested after 70 days of complete observation, dried in shadow and grinded well for the Flame emission spectroscopic study. From the results the elemental composition of the nutrients found to be increased and it was proposed that due to the action of micronutrient in the form of nanoscale promotes the growth along with the increased concentration of sodium and potassium

AB 65 EFFECTS OF ELECTRON TRAPPING ON DEGRADATION OF ORGANIC POLLUTANTS BY REDUCED GRAPHENE BASED HYBRID NANOCOMPOSITE

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A visible light driven novelreduced grapheme (rGO) based hybrid photocatalyticnanocomposite was synthesized via hydrothermal assisted homogeneous precipitation method. The phase, crystal structure, surface morphology and elemental composition of synthesized nanocomposite was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FE-SEM) and energy dispersive X-ray spectroscopy (EDX) . Absorption range and band gap energy were investigated by UV−Vis diffuse reflectance spectroscopy (UV-Vis DRS). The photocatalytic examination was carried outby degrading a target organic pollutant (Reactive Blue 160). The ternary hybrid nanocomposite shows enhanced degradation efficiency than pure and binary nanocomposites. The effect of electron trapping on the degradation of organic pollutants were studied by using $AgNO_3$as an electrontrapping material. From the results we observed the reduction of degradation efficiency due to the lack of superoxide radical generation. Thus it can be concluded that, in combination of rGO with binary nanocompositessuperoxide radical plays key role in organic pollutant degradation.

AB 66 THERMAL INFLUENCE ON ZINC OXIDE NANO PARTICLES BY CO-PRECIPITATION METHOD

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` In the recent era Zinc oxide (ZnO) which belongs to II-VI compound semiconductor materials attracted the researcher due to their promising properties like direct band gap for optoelectronics, transparent electronics, spintronic devices and sensor applications. ZnO has numerous attractive characteristics for the preparation of certain devices. Zinc is also the best nutrient and it is used in pharmaceuticals field. Therefore zinc is added with oxide and the nature of the zinc oxide is investigated and it is analyzed in the nano particle size. In the percent investigation, Zinc Oxide nano particles were synthesized using simple precipitation method with zinc acetate and sodium hydroxide as starting precursors and de-ionized (DI) water as solvent. The samples were synthesized for different concentration and calcined at different temperatures for 2 hrs. The average crystallite size of the samples were revealed by X-ray diffraction(XRD) spectroscopy. The large excitation binding energy which is obtained at room temperature and found that nanoparticles were environmental friendly due to non-toxic and its transparency over the entire range of visible spectrum were confirmed by UV-Visible analysis. The optical properties were comfirmed by photoluminescence analysis. The enhancement of optical properties may be utilized for the composition of drugs based on Hausner's ratio and also for biosensors. zinc oxide nanoparticles attracted the researchers due to their unique properties and applications in optoelectronic devices. The synthesis method has potential for application in manufacturing units due to ease processing and more economical reagent. Semiconductor nanoparticles have recently attracted significant attention for their role in fundamental studies and technical application [1], mainly due to their unusual photonic characteristics.

AB 67 INFLUENCE OF AMMONIA CONCENTRATION ON THE STRUCTURAL BEHAVIOUR OF PYRITE FILMS

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Chemical bath Deposition method (CBD) is employed to prepare the pyrite thin films at different ammonia concentration as a complexing agent, XRD and Raman methods were used to study the structural characterization of the iron pyrite films. XRD (110), (200), (211) and (023)

planes were observed corresponding to both marcasite and pyrite phases of FeS_2 as the AC of the bath was increased. Also, the intensity of the peaks corresponding to marcasite decreased without any phase conversion. The presence of appropriate ammonia concentration in the reaction bath that results in the release of necessary Fe^{2+} ions in order to formate the pyrite films. XRD pattern was estimated at the highest crystallite size of 8.07 nm at AC precursor 14 mole. Raman bands for both marcasite at 217 $cm^{-1}$and triolite at 250 cm^{-1} are observed along with pyrite phase at low concentration and all the secondary phases were absent except the pyrite phase while at high concentration. The surface properties of the films were revealed by the literature provided by XRD and Raman measurements. This paper explains the complete structural behaviour of pyrite films used in optoelectronics devices.

AB 68 A REVIEW ON MAGNETIC NANOFLUID

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Nanofluids, the engineered colloidal suspensions of nanoparticles in a base fluid have shown many interesting properties, and the distinctive features offer unprecedented potential for many applications. Magnetic nanofluids (ferrofluids) have received special attention due to their unique feature of both the liquid and magnetic properties, and find several applications such as magneto- optical wavelength filter, optical modulators, nonlinear optical materials, tunable optical fiber filter, optical grating, optical switches, drug targeting, drug delivery, MRI contrast, and hyperthermia stability. This review summarizes the preparation of nanofluids, synthesis of ferrofluids and characterization techniques used for evaluation. Among the diverse applications of ferrofluid, this review emphasis on SEAL, Heat transporting applications, NDT sensors, Nanofluid based optical filters. This paper also identifies the opportunities for future research.

AB 69 SYNTHESIS AND CHARACTERIZATION OF ZNO NANOPARTICLES THROUGH A CHEMICAL PRECIPITATION METHOD

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In this paper, highly dispersed Zinc Oxide (ZnO) nanoparticles have been successfully synthesized in Deionised water mixed solvent by a chemical precipitation method. The prepared ZnO nanoparticles were characterized by high-resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD). Several kinds of ZnO particles with different shapes were

obtained including particle-like, spherical-like, spindle-like and rod-like ZnO particles. The effects of processing parameters on the size and shape of ZnO particles such as the volume ratio of water, the increasing temperature of NaOH. It is found that higher volume ratio and water, higher adding temperature of NaOH and higher molar ratio of Zinc and O result in smaller size of ZnO particles. The nucleation and growth kinetic of the resulting ZnO particles were also discussed.

AB 70 MOLECULAR STRUCTURE, VIBRATIONAL SPECTRAL ASSIGNMENTS (FT-IR AND FT-RAMAN), NMR, NBO, HOMO-LUMO AND NLO PROPERTIES IN THE BINARY MIXTURES OF BENZYL ALCOHOL WITH ALKYL AMINES BY HF AND DFT CALCULATIONS

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We have performed quantum mechanical calculations on both pure and equimolar binary systems of benzyl alcohols with alkyl amines by HF and DFT method (B3LYP) with 6-311^{++}G basic sets using Gaussian 3W software. The theoretical vibrational frequencies (FT-IR, FT-Raman), NMR and optimized geometric parameters had been found in good agreement with the corresponding experimental data. Chemical shifts of the molecule were recorded using ^{1}H and ^{13}C NMR spectra and compared to TMS by using the Gauge-Independent Atomic Orbital (GIAO) method. Natural bond orbital (NBO) analysis helped to calculate different intramolecular interactions which were responsible for the stabilization of this Mannich base. The result confirmed the occurrence of intramolecular charge-transfer (ICT) within the molecule. The dipole moment (μ), polarizability (α) and hyperpolarizability (β) of pure and binary mixtures have been computed using HF/B3LYP basic set 6-311++G (d,p) method. HOMO and LUMO energies were also calculated.

AB 71 GROWTH AND CHARACTERISATION PURE AND $ZnSO_4$DOPED SULPHAMIC ACID SINGLE CRYSTAL: AN INORGANIC MATERIAL

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Sulphamic acid is a well known nonlinear optical inorganic material has significantly attracted in recent years because various field of applications such as harmonic generators, nonlinear optical devices and optical communication. The nonlinear optical potassium chloride doped sulphamic acid single crystals are grown by solution growth especially solvent evaporation technique at room temperature. The grown crystal structure was confirmed by single crystal X-ray diffraction study. The UV visible spectrum shows that UV cutoff wavelength of the grown crystals have less than 300 nm and crystal has wide transparency range through entire visible region. Second order nonlinear optical property of the grown crystal was tested by Kurtz powder technique. The grown pure and $ZnSO_4$ doped sulphamic acid single crystals shown in figure 1& 2.

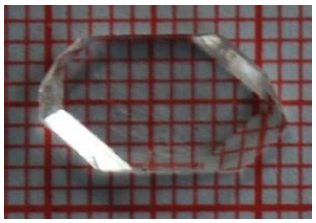

Fig: 1 Pure Sulphamic Acid crystal

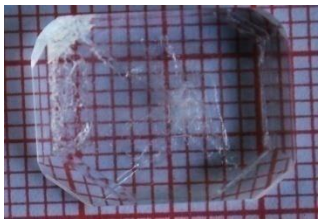

Fig: 2 $ZnSO_4$ doped sulphamic crystal

AB72 ELECTRICAL BEHAVIOUR OF METAL DOPED COPPER SELENIDE THIN FILMS

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In this work, the pure and Na doped Cu_2Se thin films were deposited on a glass substrate using chemical bath deposition method and the films were annealed at 200 ˚C. The effects of Na doping on the structural, morphological, optical and electrical properties of the Cu_2Se thin films were studied using X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Diffuse Reflectance Spectra (DRS) and Hall effect techniques. The XRD analysis confirms that all the films were crystallized with cubic structure. The broadening in the primary crystalline peak of Na doped film corroborates the incorporation of Nain to the Cu_2Se lattice. The average crystallite size was decreased for doped film.FESEM images of pure and doped film shows uniformly distributed particles over the surface. The strong optical absorption is observed for pure and Na doped Cu_2Se film in the visible region. The values of band gap energy for pure and Na doped Cu_2Se thin films are respectively 1.75 and 2.5 eV. The electrical property of the deposited

films show that the films were found to be p type with high electrical conductivity than undoped Cu_2Se films due to the introduction of large charge carriers by the dopant ions.

AB 73 BULK MELT GROWTH AND MICROSTRUCTURAL INVESTIGATIONS OF LAYERED TIN SELENIDE SEMICONDUCTING CRYSTALS

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Tin based layered chalcogenide materials are extremely useful for the fabrication of photovoltaic devices. Since tin selenide is an economical and environmental friendly material for energy conversion applications, the present research work emphasizes the bulk growth of good quality single crystals of this compound from melt, adopting Bridgman-Stockbarger method with an indigenously developed translation mechanism. High pure (99.999%) tin and selenium of stoichiometric proportions were filled in a pre-cleaned and dried quartz ampoule and sealed under a vacuum ~ 10^{-6} mbar. The ampoule was then kept in a muffle furnace and rocked at regular intervals to maintain homogeneity. The prepared ingot was ground and then filled in a specially designed 10 cm long quartz ampoule for growth process. The molten ingot was translated down slowly to the cold zone at the rate of 5 mm/h with a precise control on the movement of liquid-solid interface. The crystals were carefully cleaved at liquid nitrogen temperature to minimize deformation and the micro structural investigations were carried out with the aid of an inverted metallurgical and scanning electron microscopes. The structure and composition of the powder sample was probed by X-ray diffraction (XRD) and energy dispersive analysis by X-rays (EDAX) techniques. It crystallized in layered form with orthorhombic structure and the lattice parameters were found to be a = 11.497 Å, b = 4.150 Å and c = 4.445 Å. The density of grown crystals estimated based on the Archimedes principle is equal to 6.178 g/cm^3. Crystals with cleaved, shining and homogeneous surface were selected for microindentation analysis and grain growth engineering. The grown SnSe samples exhibited high value of microhardness due to the development of mono-phase and chemical homogeneity.

AB 74 PHOTOLUMINESCENCE PROPERTIES OF DY^{3+} IONS DOPED TELLURO PHOSPHIDE GLASSES

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Phosphate glasses are technologically important materials because they generally have higher thermal expansion co-efficient, high electrical conductivities etc..than other glasses. Photoluminescence properties of rear earth ion, Dy^{3+} doped telluro phosphate based glasses were prepared by Differential Thermal Analyzing (DTA) method for fundamental studies of the glass transition and devitrification effects. These were characterized through absorption spectra, emission spectra and decay rate analysis. The energy level structure of Dy^{3+} ion observed in absorption and emission spectra have been analyzed by the method of free-ion Hamiltonian model. All these co-efficient exponential behavior obeys the urbach empirical relation. Jadd-Ofsett theory was also employed for the absorption intensities of an f-f transition. A good correlation was found between f_{exp} and f_{cal} and J-O intensity parameters were obtained from the experimental oscillator strengths. J-O parameters indicate that present glasses are fairly rigid and parameters Ω_4 and Ω_6 reflect the rigidity of the glass. This work observes the higher value of stimulated emission cross-section peak in order to produce higher lasing action. The glass transition (T_g), crystallization (T_c) and melting temperature (T_m) of the Dy^{3+} have been evaluated by DTA thermogram. The direct and indirect optical band gaps were estimated using UV absorption spectra due to their practical importance in laser applications.

AB75 CRYSTAL GROWTH AND CHARACTERIZATION OF PURE AND PICRIC ACID DOPED LITHIUM SULPHATE NON LINEAR SINGLE CRYSTALS

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Now a days, numerous research activities have been in progress on non linear optical crystals owing to their key functions in different application like optical modulation, optical switching, frequency doubling and optical memory. Picric doped lithium sulphateis a having wide application in various field. Picric acid is added with Lithium Sulphate in 1:2 molar ratio and the crystal were grown by slow evaporation method in normal room temperature and it will compare with pure crystal of Lithium sulphate. The grown crystal was subjected to XRD, UV, FTIR, Micro hardness. The crystal structure, lattice parameter and the group were determined by XRD. The band gap, absorption and emission wave length are determined by UV spectrum. The different functional groups were found by FTIR instrumentation. The Hardness of the crystal was analyzed by vikers micro hardness.

AB 76 High-Density All-Optical Magnetic Recording Using a High-Na Lens Illuminated By Circularly Polarized Multi-Gaussian Beam

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Based on the vector diffraction theory and inverse Faraday Effect,circularly polarized multi Gaussian beam superimposed with a helical phase and modulated by an optimized multi belt complex phase filter (MBOPF) is analyzed numerically. It is found that a super long (24.8λ) magnetization chain, composed of eight ,six and four subwavelength (0.45λ) spherical spots with longitudinal magnetization field, can beachieved in the focal volume of the objective. These unique focal field distributions may find potential applications in confocalmicroscopy, atom control, and magneto-optical data storage.These characteristics are useful to next-generation high-density all-optical magnetic storage.

AB 77 THERMOPHYSICAL PROPERTIES OF FEW NLO CRYSTALS USING PHOTOACOUSTIC SPECTROSCOPY

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Photoacoustic spectrometer (PAS) is a non-destructive tool to measure the thermophysical properties of the solids, liquid and gas phase materials. Since heat transfer processes are involved in high-power laser devices, suppressing the excess temperature is of paramount importance in order to save the device from thermal damage due to sudden heat exchange to ensure durability. Hence, to design high-power laser systems, it is mandatory to know the information regarding the thermal conductivity, thermal diffusivity and thermal effusivity of the materials. Since L-Tartaric Acid (LTA), Ammonium Dihydrogen Phosphate (ADP) and Nickel Sulphate Hexahydrate (NSH) crystals were grown from an aqueous solution by Sankaranarayanan-Ramasamy(SR) method. The grown LTA, ADP and NSH crystal has been subjected to thermal characterization using Photoacoustic spectrometer (PAS) which was indigenously constructed in our laboratory. Thermal characterization involves measurement of the thermal parameters such as thermal diffusivity, thermal effusivity, thermal conductivity. The experimental results of Photoacoustic spectrometer show that the thermal diffusivity of LTA, ADP and NSH is compared of few other well known NLO materials.

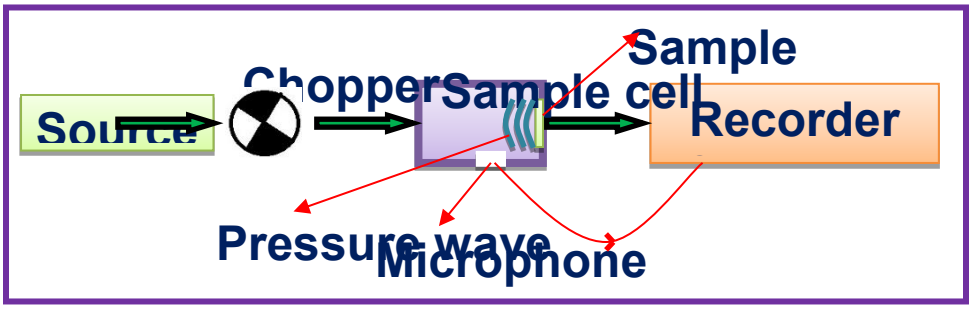

Fig.1 Block diagram of photoacoustic spectrometer

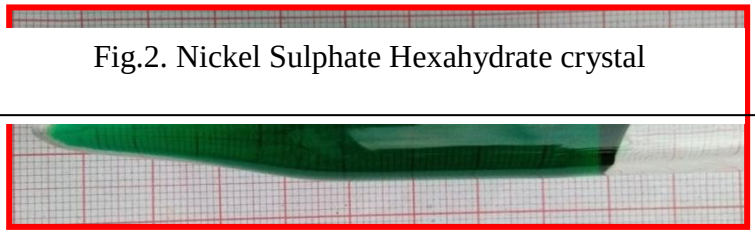

Fig.2. Nickel Sulphate Hexahydrate crystal

AB 78 **LOW**

TEMPERATURE EPITAXIAL ELECTROCHEMICAL DEPOSITION OF N-TYPE CDSE THIN FILMS AND THEIR CHARACTERISATION

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Cadmium selenide (CdSe) epitaxial thin films on ITO coated glass substrate have been grown by an electrochemical deposition technique at different bath temperatures (ambient temperature, 40°C, 50°C, 60°C and 70°C). The as-deposited epitaxial thin films from different bath temperatures were reddish and smooth, well adherent and specularly reflective. The as-deposited epitaxial thin films were characterized by glancing angle X-ray diffraction (GAXRD), high resolution scanning electron microscopy (HRSEM), energy dispersive X-ray analysis, optical absorption, photoluminescence (PL) spectra and electrical measurements. GAXRD studies reveals that cubic CdSe with a preferred orientation along (200) plane and the micro-structural parameters such as crystallite size, microstrain, dislocation density and number of crystallites per unit area were estimated. The HRSEM micrographs showed that the films surface was composed of spherically shaped grains and the elemental analyses confirmed that the atomic percentage of Cd:Se is very close to one, indicating that the as-deposited epitaxial thin films were stoichiometric.

AB 79 **FOCUSING PROPERTIES OF SPIRALLY POLARIZED SINH GAUSSIAN BEAM**

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The tight focusing properties of spirally polarizedsinh-Gaussian beam areinvestigated by vector diffraction theory.Results show that theoptical intensity in focal region of spirally polarized sinh Gaussian beam can be altered considerably by thebeam order, relative waist width and spiral parameter that indicatesthe polarization spiral degree of the spirally polarized sinhGaussian beam.Many novel focal patterns including flattop profile, focal hole and focal spots of long focal depth and axially separated focal spots are evolved. We expect such a tunable focal patterns are useful for optical manipulation of micro particles.

AB 80 SYNTHESIS AND CHARACTERISATION OF Mg DOPED HYDROXYAPATITE POWDER BY SOL-GEL METHOD

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Hydroxyapatite (HAp) is generally a unique material with high adsorption capacity, high biological compatibility, low water solubility and it is a good biomaterial as it closely resembles bone apatite and it is used as a bioimplant material. This paper describes the synthesis technique of Mg doped HAp powder by sol gel method using Calcium Hydroxide [$Ca(OH)_2$], Diammonium hydrogen phosphate [$(NH_4)HPO_4$] and Magnesium nitrate tetrahydrate [$Mg(NO_3)_2$]. Calcium Hydroxide and Diammonium hydrogen phosphate were added by dissolving it in deionised water and allowed to constant stirring for half an hour and aged for 24 hours and then it was washed repeatedly and filtered, then dried at 150^0C and calcinated at 450^0C for 5 hrs. The obtained powder was separated into three equal parts, of the three, two parts were doped with 25% and 50% of magnesium nitrate and dried. The final nanopowder was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier Transform Infrared Spectroscopy to reveal its crystallite size, morphology and types of bond present within it.

AB 81 HIGH SENSITIVITY FIBER OPTIC SENSOR BASED Fe DOPED ZnO NANOPARTICLES

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Fiber optic sensors based on semiconducting oxides have certain advantages when compared to other types of fiber optic sensors, such as low cost, simple construction, small size and ease of placing the sensor in the operating environment. The present work deals with Fe doped ZnO nanoparticles by hydrothermal method. The structural, morphological, and optical properties of the nanopowders were analyzed by using powder X-ray diffraction (XRD), Transmission electron microscope (TEM), UV-Vis transmission spectra, Fourier transform infra-red spectra and photoluminescence spectra analysis. The Fe doped sample showed high sensitivity fast response and recovery time as compared to other samples. The fiber optic sensing result showed that Fe ZnO can be used as active nanostructures for fiber optic sensors.

AB 82 SYNTHESIS OF PVP BASED TIN DIOXIDE NANOPARTICLES FOR PHOTOCATALYIC APPLICATION

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Poor metal oxides are an important classes of semi conductors which find application is almost all the fields. **SnO_2** has attracted much attention due to its wide spread application in the fileds of electronics, catalysis, gas sensing and etc. In the paper **SnO_2** nanoparticles was prepared by hydrothermal method. samples were prepared at three different time reactions 3h, 8h,12h at 380^0c. The **PVP** is used as the surfactant for preparing SnO_2 nanoparticles. The **SnO_2** nano particles were characterized with several techniques PXRD, TEM, FT-IR, UV-VIS absorbance spectra. Photocatalyic activities of the **SnO_2** nanoparticles are evaluated in the photo degradation reaction of **(MB)** methyelene blue under visible light irradiation. This type of **SnO_2** nanoparticles can be used as a good photocatalyst.

AB 83 SYNTHESIS, NMR STUDY AND CRYSTAL ETERMINATION OF 7-BENZOYLOXYCOUMARIN

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The title compound, 7-benzoyloxycoumarin, C16H10O4, crystallizes into monoclinic space group $P2_{(1)}$ with unit-cell parameter: a = 3.8479(7), b = 27.693(5), c = 5.7259(10) Ao. Z =

2. The crystal structure was solved by direct methods and refined to a final R-value of 0.0535 for 3295 observed reflection. The benzoyloxy ring present on 7- position was found to be almost coplanar with coumarin. The structure is stabilized by vander Waal's interactions. The structure of this compound was also established by 1H NMR spectrum of its solution in CDCl3. IR and Raman spectra were obtained directly in the synthesis process of coumarin with computational study of geometry such as bond lengths, bond angels and different molecular properties like Molecular Electrostatic Potential (MESP), Mulliken Charge Distribution, Global and Local Reactivity Descriptors (chemical hardness, softness, chemical potential, electronegativity, electrophilicity index). Hartee–Fock (HF) and B3LYP level of theory with 6-31G++(d,p) basis set are employed for all sorts of calculation. IR and Raman information made up training set and a quantitative analysis model of the Benzoyloxycoumarin mixed system was established by applying partial least squares (PLS). The molecular geometry was compared with the experimental data and a good agreement with the experimental data was found.

AB 84 GROWTH AND CHARACTERIZATION OF L-LYSINEDOPED MANGANESE (II) SULPHATE SINGLE CRYSTAL

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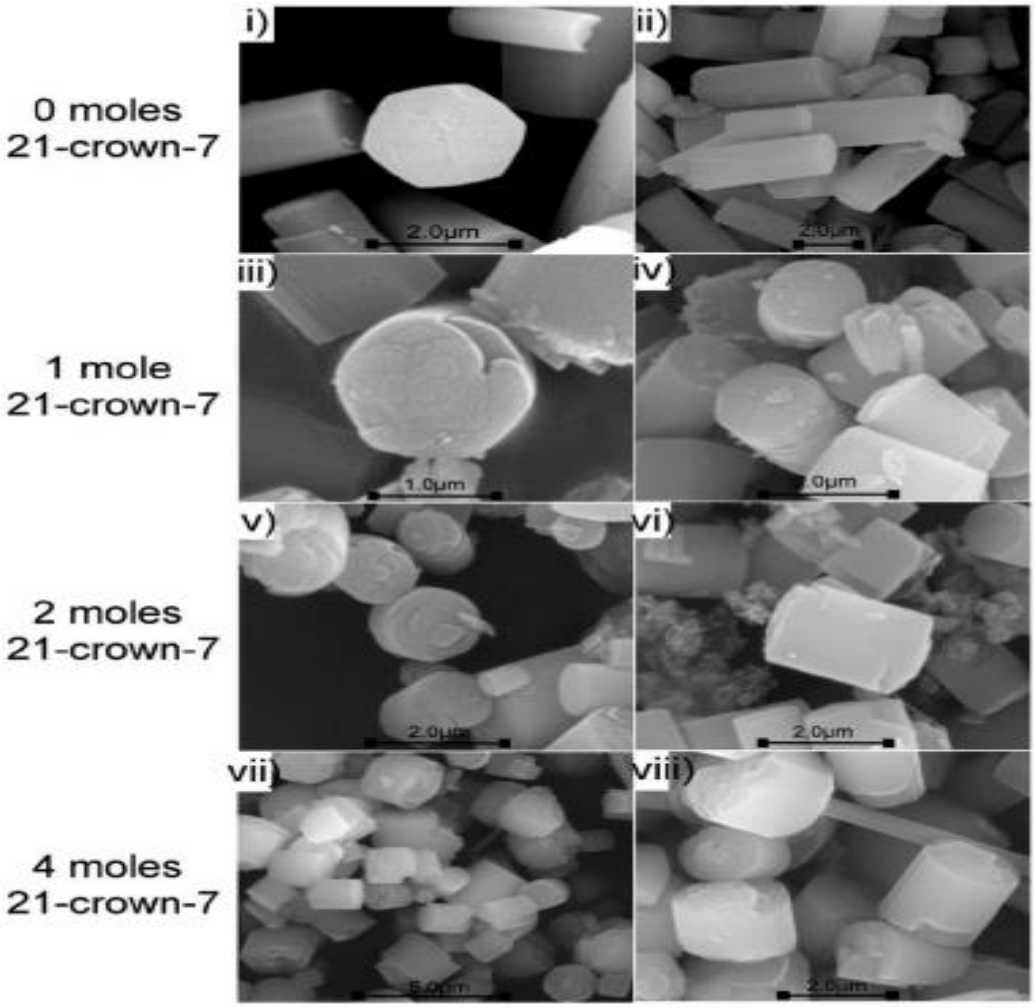
The crystal of l-Lysine and Manganese (II) sulphate was synthesized and grown by adopting slow evaporation technique at room temperature. The FITR spectrum illustrated that presence of characteristic absorption band due to the presence of various functional group in the L-Lysine and $MnSo_4$ crystal are highly transparent. The dielectric constant and dielectric loss at higher frequency is a desirable property to enhance the SHG efficiency.



TEM image of Benzoyloxycoumarin for different crown

AB 85 ABERRATION OF THE CHARACTERISTICS OF GROWN CRYSTAL DUE TO DYE IMPURITIES

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Single crystals of non-linear optical have been grown by slow evaporation and grown crystal were characterized by powder x-ray diffraction analysis and the vibration frequencies of various functional groups in the crystals have been derived from FTIR spectrum. And the percentage of optical transmission is determined by recording UV spectrum. Thermal behavior of the crystal has been investigated by DSC and TGA analyses. The NLO property of the grown crystal has been confirmed by Kurtz-powder SHG test.

AB 86 INFLUENCE OF ALKALI METAL [Li(I)] DOPING ON THE PROPERTIES OF POTASSIUM HYDROGEN PHTHALATE CRYSTALS

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The effect of dopant Li(I) (over a concentration range from 5mol% to 1:1) on the growth process and properties of KHP single crystals by slow evaporation solution technique (SEST) has been investigated. Incorporation of dopant in to the crystalline matrix even in the presence of low dopant concentration in aqueous growth medium is well confirmed by energy dispersive X-ray spectroscopy (EDS) and ICP analysis. Doping with light metal facilities nonlinearity. Power XRD and FT-IR spectral analysis confirmed the slight distortion of the structure of the crystals by dopant incorporation. TG/DTA studies reveal the purity of the material and no decomposition is observed up to the melting point. Considerable influence of doping the alkali metal on the structure, optical properties and morphology of KHP crystals are observed. The crystal structure has been determined by X-ray crystallography studies.

AB 87 SYNTHESIS AND CHARACTERIZATION OF GLYCINIUM MALEATE: A NOVEL OPTICAL CRYSTAL

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Single crystals of an organic glycinium maleate were successfully grown from the supersaturated aqueous solution of glycine and maleic acid in 1:1 molar ratio for the first time by the slow solvent evaporation method at ambient temperature (30° C) with the ph value of 2. The grown crystals were subjected to single crystal X-ray diffraction and the resultant cell parameter values were compared with the reported values to confirm the coordination. In order to identify the functional groups present in the grown crystal, FTIR studies were carried out from 4000 to 450 cm -1. They were further characterized by UV-Vis-NIR studies to determine its optical properties. Powder X-ray diffraction of the grown crystal was recorded and indexed on the corresponding major peaks. Thermal studies such as thermo gravimetric (TGA) and differential thermal analysis (DTA) were carried out to find the thermal stability of the crystal. Dielectric behavior was measured at different temperatures and frequencies. To reveal the surface hardness micro hardness testing was made on the as grown crystal, from which yield strength also was calculated.

AB88 DESIGN AND THERMAL PERFORMANCE OF A PASSIVE TYPE SOLAR STILL

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Solar still is a very simple device for supplying potable water to small communities where the sun shine is abundant. The simplest and easily accessible type of solar distillation is passive type. This paper presents the design, fabrication and thermal analysis of a passive type single basin double slope solar still. Hourly and daily measurements of the still productivity, temperature of water, glass cover and ambient air were recorded during both on cloudy and sunny days. The internal heat transfer was analysed for all the days experiment. The main performance parameters such as hourly yield, daily productivity and efficiency were calculated and it was found that the theoretical and experimental values are in good agreement. The hourly efficiency ranges from 19 % to 46% and the maximum yield obtained was 1.875 litres /m^2. The physical and chemical analyses were done on the water samples before and after distillation and the solar distilled water are found to be in good in quality and it is superior to the water sample before distillation.

AB 89 EXPERIMENTAL INVESTIGATION OF A PYRAMIDAL SOLAR STILL

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Solar distillation is the promising method which uses the solar energy for supplying potable water where the natural supply of fresh water is inadequate or of poor quality. This work describes about the thermal performance analysis of a pyramidal solar still. A heat transfer model is developed to study the thermal performance of the still. The internal and external heat loss coefficients were calculated for every hour time interval during the period of experiment. The climatic parameters such as ambient temperature, solar insolation and the system temperatures are clearly measured with the help of K – type thermocouple wires. Experimental results showed that the average distillate output is 1150ml/sq. metre and the maximum efficiency achieved is 31%. The total dissolved solids (TDS) of the distilled water are 9.1 ppm.

AB90 GROWTH AND CHARACTERIZATION OF NON LINEAR OPTICAL INORGANIC MAGNESIUM CHLORIDE DOPED AMMONIUM SULPHATE (MCAS) SINGLE CRYSTAL

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A crystalline material of magnesium chloride doped ammonium sulphate (MCAS) was grown using slow evaporation solution growth technique. The solubility measurement shows that the temperature increases the concentration of solute is also increases which indicates the positive solubility of the material. An average of crystal size up 11 × 11 × 3 mm^3were harvested and characterized by FTIR analysis, NLO studies, single crystal XRD analysis, Vicker's microhardness test, dielectric and thermal studies. The Non-linear optical property of the grown crystal was confirmed by the Kurtz- powder SHG test. Lattice parameter of the grown crystal has been studied by single crystal X-ray diffraction analysis. The mechanical property of the title compound has been assessed by Vicker's microhardness measurements. Dielectric constant and dielectric loss for various frequencies at different temperatures were performed on MCAS single crystal. The results were discussed in detail.

AB 91 CELL PHONE CONTROLLED DOOR LOCK SYSTEM

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The cell phone controlled door latch system was successfully designed and soldered on the PCB using the toner and decoder IC with resistors, relay driver and diodes in our lab. It explains how add-on power door locking systems actually work and also the basics of installing them. Most of them are built up using only three different types of component. There are,

- Master lock actuators for the doors which enables to lock and unlock with a conventional key
- Slave lock actuators for the remaining doors
- A lock control relay unit to make it all work.

MT8870DE acted as the receiver for the digital signal along with NOKIA 1616-2.The relay driver acts as switch for ON/OFF of the entire system so that it latches the door as soon the electrical signal is received.

AB 92 GROWTH AND CHARACTERIZATION STUDIES OF VAM AND VGM CRYSTALS

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Crystal of l-Valine acta master and VGM is characterized using following technique. FTIR spectral analysis (4000-400 cm^{-1}) was used to confirm the functional group present in the grown samples. The FTIR analysis was performed with PERKIN – ELMER- FTIR spectrometer. It provides information about structure of a compound and molecule absorbs at definite frequency and it is reason for various bands to bend or stretch the molecule. Peaks were observed in the region **542.02 cm^{-1} to 1448.59 cm^{-1}**corresponding to **SO_4** vibrational**2712.01 to 3905.98** corresponding to **HOH** vibrational frequencies. Hence assignment is in conformity with characteristic transmission bands of VAM and VGM crystals. The UV- visible transmittance spectra were recorded in the wavelength region 190-1100nm by using LAMBDA 35 UV- Visible spectrometer. The material must be transparent in the wavelength region for studying the optical property. The optical transmission spectrum of l-valine crystal with acta master, l-valine with potassium sulphate and dopants was recorded in the wavelength region 190-1100nm. A strong absorption was observed at 372.32nm, 287.97nm, 262.5nm and 382.12nm. This illustrates the optical quality of the grown VAM and VGM crystals. The transparent nature of crystals in UV-Vis region can be used for NLO applications.

AB 93 GROWTH AND CHARACTERIZATION STUDIES OF GTC AND GS CRYSTALS

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Crystal of pure glycine and doped glycine with thio carbamide and saline obtained are characterized by the following technique. The FT-IR spectral analysis (4000-400 cm^{-1}) was used to confirm the functional group present in the grown samples. The FTIR analysis was performed with PERKIN – ELMER- FTIR spectrometer. It provides information about structure of a compound and molecule absorbs at definite frequency and it is reason for various bands to bend or stretch the molecule. Peaks were observed in the region **683.94cm^{-1} to 3107.28cm^{-1}**corresponding **NH stretching** frequencies and **2228.52 cm-1** corresponding **R-N=C=S thiourea** stretching frequency. Hence assignment is in conformity with characteristic transmission bands of glycine thio carbamide and glycine saline crystal. The UV- visible transmittance spectra were recorded in the wavelength region 190-1100nm by using LAMBDA 35 UV- Visible spectrometer. The material must be transparent in the wavelength region for studying the optical property. The optical transmission spectrum of glycine thio carbamide crystal and glycine saline was recorded in the wavelength region 190-1100nm. A strong absorption was observed at 236.45nm and 280nm. This illustrates the optical quality of the grown GTC and GS crystals. The transparent nature of crystals in UV- Vis region can be used for NLO applications.

AB 94 A STUDY OF COUPLED HIGGS EQUATION USING LIE SYMMETRY AND G'/G –EXPANSION METHOD- A REVIEW

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Evolution depends on the nature of force and the initial state which is the basis for nonlinear dynamics. Dynamics of nonlinear system depends heavily on initial condition while it is not for linear system.Coupled Higgs field which is a second order nonlinear partial differential equation is analyzed using lie symmetry analysis and G''/G expansion method. Lie's method is a theoretic technique involving the invariance of point transformation and transforms solutions of the system to other new solutions from known ones depending on monomials (using one parameter). For understanding the complex analysis in science we must find exact solution for the travelling wave solutions (soliton) and so G''/G – expansion method is one explicit method from unknown ones with soliton expressed by a polynomial in G''/G.

AB 95 THIN FILM DEPOSITION PROCESSES AND CHARACTERIZATION TECHNIQUES

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[2]**V.Vinodhini,** *Pachamuthu College of Arts & Science for women, Dharmapuri*

The field of material science and engineering community's ability to conceive the novel materials with extraordinary combination of chemical, physical and mechanical, properties has changed the modern society. Thin film technology is the basic of astounding development in solid state electronics. The usefulness of the optical properties of metal films, and scientific curiosity about the behaviour of two-dimensional solids has been responsible for the immense interest in the study science and technology of the thin films. Thin film studies have directly or indirectly advanced many new areas of research in solid state physics and chemistry which are based on phenomena uniquely characteristic of the thickness, geometry, and structure of the film. For a thin film the limit of thickness is considered between tenths of nanometers and several micrometers. The vast varieties of thin film materials, their deposition processing and fabrication techniques, spectroscopic characterization and optical characterization probes that are used to produce the devices. It is possible to classify these techniques in two ways.

- Physical Process
- Chemical Process

AB 96 CRYSTAL GROWTH AND CHARACTERISATION OF ANILINIUM PICRATE SINGLE CRYSTALS

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Single crystal of Anilinium Picrate (AP) was successfully grown by slow evaporation method with the dimensions 12×6×3 mm^3**.** Thesolubility of AP was determined at various temperatures.The structure ofAnilinium Picrate was elucidated using single crystal X-ray diffraction study. The compound crystallized in monoclinic space group $P2_1/c$, lattice parameters a=13.03Å, b=7.09Å, c=14.85Å, Fourier transform infra red (FTIR) spectral analysis are performed for the identification of functional groups present in the compound. Absorption of the grown crystal are examined using UV-visible spectral studies and it was found that the crystal has a cut off wavelength around 476.3nm.Mechanical stability of the grown crystal was tested with Vicker`s micro hardness tester and the work hardening coefficient (n) of the grown material was estimated.

AB 97 QUANTUM CHEMICAL AND CHARGE DENSITY STUDIES ON GOLD SUBSTITUTED 8A,9,10,10A-TETRAHYDRO-2,6-BIS-(2-PHENYLETHYNYL) ANTHRACENE BASED NANO-MOLECULARWIRE

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The theoretical electronic structure and transport properties of Au and 8a,9,10,10a-tetrahydro-2,6-Bis-(2-phenylethynyl) anthracene have been calculated from high level Density functional theory (DFT) using B3LYP method with LANL2DZ basis set. The molecular geometric parameters predicted by DFT method are in agreement with the reported results. The 8a,9,10,10a-tetrahydro-2,6-bis-(2-phenylethynyl) anthracene molecule reveals the, energy level shifting, bond topological features and the electrostatic properties for Au substituted molecule. Further, the decrease of HOMO-LUMO gap from 2.12 eV to 0.94 eV determined from density of states spectrum for the applied field (0 – 0.21 VÅ-1) shows that thiol linked 8a,9,10,10a-tetrahydro-2,6-Bis-(2-phenylethynyl) anthracene molecule can act as efficient molecular nanowire for Au electrodes.

AB98 C NMR CHEMICAL SHIFT OF NAPHTHALENE AND SOME N-SUBSTITUTEDNAPHTHALENE USING QUANTUM CHEMICAL CALCULATION

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The organic molecule chosen in this study are naphthalene, Quinoline, Isoquinoline, Quinazoline, Naphthyridine. The 13C isotropic shielding constants(σ) of the molecules under study were calculated employing Gauge Invariant Atomic Orbital method (GIAO).From the 13C isotropic shielding constant values the isotropic chemical shifts (δ) were obtained with reference to tetramethylsillane.The geometries of naphthalene and N-substituted naphthalene's are optimized by density functional method namely B3LYP using two different basis sets 6-31G+(d) and 6-311G++(d, p) and also at a higher level of theory employing MP2 method using a smaller basis set 6-31G+(d).All the calculations were performed using Gaussian 03W suite of package. Shielding constants for various optimized structures were calculated at the Hartree-Fock(HF) level with an accurate basis set namely 6-311G++(2d,p).As experimental chemical shift values are in general evaluated with reference to TMS, we have also used TMS as the reference. The calculated isotropic shielding constants have been compared with the available experimental values.

AB 99 GROWTH AND CHARACTERISATION ZTCl CRYSTALS

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Crystal growth has been a subject of absorbing interest for many years and the recent development of technology has stimulated the commercial importance of the subject. A crystal is an array of atoms arranged in a three dimensional structure which of a crystalline solid and the perfect ordering in the crystal gives rise to many of the physical properties of crystals such as ferromagnetism, birefringences, piezo-electricity etc., A poly crystal is an aggregate of crystals which might or might not be of different kinds, generally irregular shaped and interlocked together at the boundaries of contact. ZTCl is among the organic NLO materials, they have been grown by solution growth method at room temperature. From X-RD we confined that the ZTCl structure is orthorhombic space group. The cell parameters of ZTCl have been obtained by powder X-ray diffraction. The FTIR spectra have been studied for identification of functional groups. We observed that N-H present at higher energy. C.H present at lower energy. In the characteristics of aromatic ring protons are present and there is no other peaks in the spectrum, the crystal is free from any impurities.

Variation of Hardness with Load for BTC Crystals.

AB 100 GROWTH, XRD AND HARDNESS STUDIES ON SUCCINIC ACID CRYSTALS

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The growth of Succinic Acid crystals is carried out in the Sodium Metasilicate Gel medium under optimum conditions. The desired value of gel density was 1.04 gm/cc and pH of the above gel solution is to be above 5. The neutral gel medium in the U – Tube also suggested for the well-developed crystals. Since this crystal is organic in nature, the Gel method has gained considerable importance due to its simplicity and effectiveness of growing crystals. For Biological applications this crystal was suitable and their growth rate was also analysed. The X – Ray Diffraction studies using Richie- Siefert Diffractometer was also carried out and the theoretical values are in good agreement with the Experimental values. The hkl values and the Interfacial angles and other diffraction angles are calculated and their I/I_0 values are calculated. The FTIR studies are carried out on the grown samples and the vibrational assignments are made. The wagging out of phase stretching and scissoring are the factors available in the FTIR spectrum . This will be useful in analyzing the structure and confirmation of compounds.

AB 101 ENHANCED STRUCTURAL, BIOLOGICALAND CORROSION PROPERTIES OF HYDROXYAPATITE/CNT FILMS COATED ON 316L SS SUBSTRATE USING SPRAY PYROLYSIS TECHNIQUE

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We report on the synthesis of hydroxyapatite (HA)/carbon nanotube (CNT) thin films on 316L SS substrates by spray pyrolysis method for a new generation of implants.The deposited films were characterized by scanning electron microscopy, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and energy dispersive X-ray spectroscopy (EDX). On incorporation of CNT in HA lattice, the phase of the HA was not changed, but it reduced the crystallite size and increased the specific surface area of HA. Surface morphology of CNT-HA (CHA) coated implant was found to show uniform particle size without any defects. FTIR analysis confirmed the presence of CNT and HA. CHA composites indicated enhanced antibacterial activity against gram-negative bacterial strains. The corrosion resistance of the resultant coating was investigated by the electrochemical analysis, which revealed the higher corrosion resistance performance in stimulated body fluid (SBF).

AB 102 PHOTOCATALYTIC ACTIVITY OF CR DOPED ZNO NANOCOMPOSITE PREPARED VIA HYDROTHERMAL METHOD

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In this present work, we focused on improving the zinc oxide nanoparticles properties by doping chromium (Cr), synthesized by hydrothermal method. The structural, morphological and optical properties of the samples were investigated. The crystallite sizes ZnO were reduced after Cr incorporation in to the ZnO lattice. The XRD analysis also confirms that ZnO has a hexagonal (wurtzite) crystal structure with c-axis orientation.SEM micrographs displayed the formation of hexagonal-spheroid shaped of Cr doped ZnO nanoparticles with high porosity.The optical band gap of ZnO nanoparticles decreases from 3.18 to 3.07 eV when Cr added into Zn lattice. The photocatalytic properties of Cr doped ZnO nanocomposite were evaluated by degradation of Rhodamine B under visible light irradiation. It has been found that photocatalytic efficiency was significantly improved when ZnO doped by Cr.

AB 103 COMPARITIVE STUDY OF ZNO NANOPARTICLES BY CHEMICAL AND GREEN METHOD AND ITS ANTI-BACTERIAL ACTIVITIES

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In this present study. ZnO nanoparticles were synthesized using eco-friendly green method and environmental chemical method. The effect of green and chemical synthesized ZnO nanoparticles on structural and optical property were analysed. This study reports the exploit of phyllanthus emblica stem extract as an eco-friendly agent for the pattern of Zinc Oxide nanoparticles using Zinc Acetate and KOH as a surrogate for chemical method. Structural, morphological and optical properties of the synthesized nanoparticles were characterized. The EDS analysis shows that the elemental composition of ZnO nanoparticles chemical and 50ml P.Emblica stem extract shows best anti bacterial activity for Klebsiella Pneumoniae(gram –ve) bacteria more than Staphylococcus Aureus(gram +ve) bacteria. Though chemical and green method are trendier for nanoparticle synthesis, the biogenic green fabrication is a better choice due to eco-friendliness. Green synthesized nanomaterial finds extensive applications in photovoltaic and photocatalytic fields.

AB 104 MOLECULAR EXCITATIONS IN TERMS OF SPLAY MODE IN NEMATIC LIQUID CRYSTALS

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In this project work, we try to investigate the nature of molecular excitations in terms of splay- mode for an hometropically aligned nematic under pure elastic field. We solved the steady state of governing equation of motion numerically. For this we consider the pulse type of solution of the governing equation of motion governed by vector field which act as their potential for the splay mode governing scalar field equation. Here we equation represent the steady state equation in terms of splay mode. We made an attempt to solve Equation numerically both for the case of elastic isotropy (where the elastic constants are equal) and anisotropy (where the elastic constants are equal). The data's are plotted both for the cases of elastic isotropy and elastic anisotropy. Figures represent the molecular excitations in terms of splay mode corresponding to the case of elastic isotropy and elastic anisotropy respectively. From the figures it is evident that the envelope pattern exhibits the molecular excitations in terms of splay mode which is in the form of solitan – type pattern or the cases of elastic isotropy. However, for the case of elastic anisotropy the envelope pattern does not perfectly matches with the solitan , where the localized envelope wave does not approaches to zero both at the positive are negative are infinity. Thus it has been concluded that the molecular excitation in terms of splay mode only.

AB 105 NOVEL SYNTHESIS ROUTE FOR ZNS:FE HYBRID QUANTUM DOTS

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In the present work, a novel simple chemical synthesis route is used to prepare the ZnS:Fe hybrid quantum dots which is efficient and environmental friendly method. Then, the obtained hybrid QDs structural, optical, magnetic properties were thoroughly measured using various characterization techniques, and the multifunctional applications performances were investigated in detail. Moreover, the investigation on bi-functional behavior of photoluminescence as well as magnetism from this hybrid QDs is interesting one. Hence, it is highly suitable for magnetic resonance imaging and cancer cell target applications.

AB 106 GREEN SYNTHESIS APPROACH AND BACTERIAL ACTIVITY OF STARCH CAPPED ZNO NANO-DOTS

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In the present work,ZnO and starch capped ZnONDs are synthesized through precipitate green synthesis technique. Because of the "green" synthesis of metallic nanoparticles it has received increasing attention due to the development of eco-friendly technologies in materials science. Also the synthetic methodologies should be designed to use and generate substances that possess little or non-toxicity to human health and the environment. Therefore, starch was used as capping agent and the encapsulation of ZnO NDs plays an important role. Importantly, the starch encapsulation controls the agglomeration as well as toxicity of the nanoparticles.The bacterial study of *E.coli bacteria* is helpful to confirm the starch capped ZnONDs are less toxic for living organisms. Therefore, this can be bio-compatible and also suitable for drug delivery systems.

AB 107 SYNTHESIS AND CHARACTERIZATION OF NANO-SIZE HYDROXYAPATITE CAPPED WITH CHEMICAL(L-ARGININE MONOHYDROCHLORIDE) AND BIOLOGICAL PLANT-MEDIATED LEAF EXTRACT(AZADIRACHTA INDICA)

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Nanomaterials are cornerstones of nanoscience and nanotechnology. Hydroxyapatite(HAP) is an inorganic biomaterial, it is effectively used as a bioimplant material because it closely resembles bone apatite and exhibits good biocompatiability. In the present work, in order to improve itsbiological behavior, HAP was capped with both biological and chemical capping agents. L-Arginine monohydrochloride [$C_6H_{15}CIN_4O_2$] was used as a chemical capping agent andAzadirachta indica leaf extract was used as abiological capping agent. The synthesized sample was dried at 100˚c.The prepared samples were characterized by XRD, SEM, EDAX, and FTIR.The biological behavior was investigated by Antimicrobial activity and Cytotoxicity test.

AB 108 SYNTHESIS AND CHARACTERIZATION OF PURE AND CHEMICAL [SILICA GEL] CAPPED NANO HYDROXYAPATITE

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HAP a main inorganic phase of human hard tissue have be extensively investigated for medical application. Although HAP is bioactive and biocompatible, the brittleness and low fracture toughness limit its application as bulk material and under load-bearing conditions. A way to improve its biological and medical application is by adding capping agent in HAP. In the present work HAP was synthesis in pure form and also Silica gel (white) was used as a capping agent. The above prepared samples were characterized by XRD, FTIR, UV-Vis, SEM and EDAX. The synthesized sample was dried at 100^0 C. The biological behavior was investigated by Antimicrobial activity and Cytotoxicity test.

AB 109 DOCKING AND THEORETICAL CHARGE DENSITY ANALYSIS OF ACE ENZYME WITH CAPTOPRIL MOLECULE

Dr. G. Rajalakshmi*, A. Logeswari, J. Chitra, M. Nandhini

Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri

Angiotensin-converting enzyme "ACE" indirectly increases blood pressure by causing blood vessels to constrict by producing angiotensin (II) from angiotension (I). A substance which acts as vasoconstrictor and thereby narrowing the blood vessel which inturn raise the blood pressure and make the heart to work harder. It also degrades bradykinin, a potent vasodilator. This makes ACE inhibition is necessary in the treatment of high blood pressure, heart failure, diabetic nephropathy and type 2 diabetes mellitus. Inhibiting the formation of angiotensin II leading to dilation of arteries and veins and hence decrease in arterial blood pressure. So many medications are available captopril drug is one of the best ACE inhibitors. Hence docking analysis of captopril with ACE was carried out to know the docked energy, conformational variation of ligand when it present in the active site. Docking also provide intermolecular interactions between the ACE and ligand.

AB 110 DOCKING AND TOPOLOGICAL ANALYSIS OF DISULFIRAM DRUG MOLECULE VIA THEORETICAL CHARGE DENSITYANALYSIS

A. Logeswari, M. Nandhini, J. Chitra,l G. Rajalakshmi*

Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri- 636 701, Tamil Nadu, India

A charge density analysis of Disulfiram drug molecule in gas phase (form I) and in the active site of cytochrome P450 (form II) were performed using DFT method with 6-311G** basis set. The charge density analysis reveals the difference in conformational modification, charge distribution and the electrostatic properties between the isolated molecule (I) and the molecule present in the active site (II). The bond charges of C–S bond and S–S bonds are highly depleted after it entering the active site. The dipole moment of the molecule (I) is ~0.98D

whereas for molecule to (II) it is increased to 5.36D. The difference in dipole moment is ~4.4D. This large dipole moment enhancement is due to the intermolecular interaction that exist between the disulfiram molecule and the aminoacid residues present in the active site of cytochrome P450. A reactivity hole is seen on the surface of the electronegative region of (I) but it disappears in the form (II). Positive region represents the electrophilic sites of the molecule. Sulphur acts as the nucleophilic region.

AB 111 INSIGHTS OF DRUG DEISGN

A. Logeswari, M. Nandhini, J. Chitra,l G. Rajalakshmi*

Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri- 636 701, Tamil Nadu, India

The field of SBDD is a rapidly growing area in which many drugs are discovered so far. In this presentation let us have the glimpses of Drug design, types of drug design, and some of its applications

AB 112 COMPUTATION STUDY ON SOME MOLECULAR PROPERTIES OF 4-NITROANILINE 4-AMINOBENZOIC ACID

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Recent days, search for organic single crystal in the application of telecommunication, frequency doubling and optoelectronics has been increased considerably. The organic molecules exhibiting nonlinear optical (NLO) properties have been motivated by their potential for applications in optical communications, optical computing, data storage, dynamic holography, harmonic generators, frequency mixing, and optical switching. The advantages of using organic molecules as NLO materials are that they can be designed to optimize the desired NLO property by having different donor and acceptor groups in the molecules. This is because of their efficient physicochemical properties such as molecular nonlinearity over a broad frequency range, low cost, low dielectric constant, inherent synthetic flexibility, high optical damage threshold(>10 GW/cm2), ultrafast response with better process ability, ease of fabrication and possible integration into devices.

4-Aminobenzoic acid (4-ABA) is one of the well known carboxylic acids to promoting molecular self assembly by means of strong hydrogen bonding through its carboxylic acid group and the ring substituted amino group of 4-nitroanilne (4-NA). Strong hydrogen bonds occur due to the polarizable hydrogen atom covalently bonded to an electron-withdrawing donor nitrogen atom and interact with a partially negatively charged and comparatively less polarizable acceptor

oxygen atom, which will also increase the molecular hyper polarizability. Smith et al reported the structure of 4-nitroaniline 4-aminobenzoic acid(4NAABA). In this study, the first order hyperpolarizability, FT-Raman, FT-IR, NMR and UV spectroscopic studies along with HOMO (highest occupied molecular orbital)–LUMO (lowest unoccupied molecular orbital) of 4NAABA have been investigated by applying density functional theory(DFT) calculations based on Becke3-Lee–Yang–Parr (B3LYP) with 6-311++G(d, p) as basis set.The theoretically calculated values have been compared with the experimentally measured data and also the results have been discussed.

AB 113 STRUCTURAL, MORPHOLOGICAL, OPTICAL AND THERMOELECTRIC PROPERTIES OF NANOSTRUCTURED CDTE

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Thermoelectric systems have recently received an increasing amount of attention because they facilitate direct and reversible conversion between heat and electrical energy, thus enabling environmentally friendly refrigeration and electric power generation. The performance of TE material is assessed using a dimensionless figure of merit (ZT) = $\alpha^2\sigma T/\kappa$, where α, σ, T, $\alpha^2\sigma$, and κ are the Seebeck coefficient, electrical conductivity, absolute temperature, power factor, and total thermal conductivity, respectively. In the present work, Chalcogenides based CdTe materials were prepared by wet chemical method. The synthesized materials were characterized by XRD, SEM and UV analysis for structural, morphological and optical analysis. The XRD analysis confirms the crystal structure of the prepared material. The SEM images show that the synthesized CdTe particles are highly mono dispersed with less agglomerations. The particles have spherical morphology with sizes in the range of 30 to 40 nm. Thermoelectric properties of the CdTe were studied by measuring the Seebeck coefficient as a function of temperature. The Seebeck coefficient increases with temperature in the temperature range from 30ºC to 650ºC.

AB 114 SYNTHESIS AND CHARACTERIZATION OF ZINC TITANATE NANOCRYSTALS FOR THERMOELECTRIC APPLICATIONS

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[d]Centre for Nanoscience and Technology, Anna University, Chennai-600025, India

[e]*Department of Mechanical Engineering, A.R.S College of Engineering, Maraimalai Nagar, Chennai*

$ZnTiO_3$ nanocrystals were synthesized by sol-gel method with different Zn and Ti ratios. The synthesized nanocrystals were annealed at different temperatures to study the impact of annealing temperature on the structural and optical properties of the titanates. The structural, morphological and optical properties of sol-gel synthesized $ZnTiO_3$ nanocrystals were studied. The structural properties and phase transition from one phase to another phase as a function of annealing temperature were studied by X-ray diffraction analysis. The surface morphology of the as synthesized and annealed samples was analysed by FE-SEM. The thermoelectric properties of the samples were systematically investigated as a function of Zn to Ti ratio and annealing temperature.

AB 115 NANOSTRUCTURED SEMICONDUCTOR MATERIALS FOR THERMOELECTRIC APPLICATIONS

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Thermoelectric nanomaterials have received much attention because of its high performance compared to bulk material due to increased phonon scattering at grain boundaries. Bismuth telluride (Bi_2Te_3) is a well-known low temperature TE material, and is commercially available for practical applications. Despite of huge efforts made by the researchers for the preparation of Bi_2Te_3 material, the large scale synthesis using conventional processes such as directional crystallization, is quite complicated as it requires sophisticated systems, due to the volatile nature and high vapour pressure of tellurium. Cobalt antimony ($CoSb_3$) is one of the skutterudite material for moderate temperature thermoelectric applications. In the present work, Bi_2Te_3 and $CoSb_3$ nanocrystals were synthesized by sol-gel method and pellets of nanocrystals were made by high pressure and high temperature sintering (HPHTS) process. The pellets were sinterred at different temperatures. The impact of sinterring temperature on phase transformation and morphological evolutions of pelletized nanocrystals were studied. Thermoelectric properties of as-prepared and sintered pellets were measured. Seebeck coefficient of Bi_2Te_3 and $CoSb_3$ nanocrystals has increased and the electrical resistivity decreased with sintering temperature. The variations of Seebeck coefficient and power factor are explained by a proposed model.

AB 116 COMPUTATION STUDY ON SOME MOLECULAR PROPERTIES OF 4-NITROANILINE 4-AMINOBENZOIC ACID

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Recentdays, search for organic single crystal in the application of telecommunication, frequency doubling and optoelectronics has been increased considerably. The organic molecules exhibiting nonlinear optical (NLO) properties have been motivated by their potential for applications in optical communications, optical computing, data storage, dynamic holography, harmonic generators, frequency mixing, and optical switching. The advantages of using organic molecules as NLO materials are that they can be designed to optimize the desired NLO property by having different donor and acceptor groups in the molecules. This is because of their efficient physicochemical properties such as molecular nonlinearity over a broad frequency range, low cost, low dielectric constant, inherent synthetic flexibility, high optical damage threshold(>10 GW/cm2), ultrafast response with better process ability, ease of fabrication and possible integration into devices.

4-Aminobenzoic acid (4-ABA) is one of the well known carboxylic acids to promoting molecular self assembly by means of strong hydrogen bonding through its carboxylic acid group and the ring substituted amino group of 4-nitroanilne (4-NA). Strong hydrogen bonds occur due to the polarizable hydrogen atom covalently bonded to an electron-withdrawing donor nitrogen atom and interact with a partially negatively charged and comparatively less polarizable acceptor oxygen atom, which will also increase the molecular hyper polarizability. Smith et al reported the structure of 4-nitroaniline 4-aminobenzoic acid(4NAABA). In this study, the first order hyperpolarizability, FT-Raman, FT-IR, NMR and UV spectroscopic studies along with HOMO (highest occupied molecular orbital)–LUMO (lowest unoccupied molecular orbital) of 4NAABA have been investigated by applying density functional theory(DFT) calculations based on Becke3-Lee–Yang–Parr (B3LYP) with 6-311++G(d, p) as basis set.The theoretically calculated values have been compared with the experimentally measured data and also the results have been discussed.

AB 117 INCREASE IN EFFICIENCY OF THE SOLAR STILL DUE TO THE EFFECT OF DIFFERENT ABSORBING MATERIALS

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The most important factor that helps for the production of distilled water in solar still as the amount of solar radiation which is received on the glass cover. It is not assured that all the solar energy that falls on the surface of glass cover will be transmitted inside the solar still. It may get reflected and absorbed by when it passes through. Part of the sunlight is reflected and observed by

the glass, the water, and the basin surface. If the still is not perfectly sealed and insulated there will be heat losses to the surroundings. The different absorbing materials like charcoal, few selective coating materials, iron fillings etc., The performance of the still is studied by using these materials. The improvements in efficiency due to these absorbing materials are predicted.

AB 118 THERMO - ACOUSTICAL STUDIES ON INTER IONIC INTERACTIONS OF SOME A-AMINO ACIDS IN AQUEOUS SOLUTION AT .01 MASS PERCENTAGES.

P.Inbam,Ragavendiran and Rajadurai*,Don Bosco College, Dharmapuri

The present study deals with the structure-making and breaking behaviour of some alpha-amino acids in aqueous sodium acetate solution at 301.15K. Experimental values of density, viscosity and speed of sound were carried out on the binary mixtures of sodium acetate + amino acids namely (L-histidine) at 301.15K. The binary solvent mixtures was prepared by taking amino acids at the mass percentages, say at .01% was added with water. The given amino acids under study were added with aqueous solvent under different molarities at normal atmospheric pressure. Besides, our investigation also explores about the presence of possible inter ionic interactions such as solute-solvent, solute-solute, ion-solvent and ion-ion in the solution.

AB 119 THERMODYNAMIC AND TRANSPORT STUDIES ON SOME BASIC AMINO ACIDS IN AQUEOUS SODIUM ACETATE SOLUTION AT DIFFERENT TEMPERATURES

P.Inbam, Mullaivendan and priya*, Don Bosco College, Dharmapuri

The present study deals with the structure-making and breaking behaviour of some alpha-amino acids in aqueous sodium acetate solution at 301.15K. Experimental values of density, viscosity and speed of sound were carried out on the binary mixtures of sodium carbonate + amino acids at 301.15K. The binary solvent mixtures was prepared by taking amino acids at the mass percentages, say at .01% was added with water. The given amino acids under study were added with aqueous solvent under different molarities at normal atmospheric pressure. Besides, our investigation also explores about the presence of possible inter ionic interactions such as solute-solvent, solute-solute, ion-solvent and ion-ion in the solution.

AB 120 ULTRASONIC STUDY OF INTERMOLECULAR ASSOCIATION THROUGH HYDROGEN BONDING IN BINARY LIQUID MIXTURES

P.Inbam, and Vennila*, Don Bosco College, Dharmapuri

The present study deals with the structure-making and breaking behaviour of some alpha-amino acids in aqueous sodium acetate solution at 301.15K. Experimental values of density, viscosity and speed of sound were carried out on the binary mixtures of sodium nitrate + amino acids. The binary solvent mixtures was prepared by taking amino acids at the mass percentages, say at .01% was added with water. The given amino acids under study were added with aqueous solvent under different molarities at normal atmospheric pressure. Besides, our investigation also explores about the presence of possible inter ionic interactions such as solute-solvent, solute-solute, ion-solvent and ion-ion in the solution.

AB 121 SYNTHESIS OF PURE TIO_2 BY SOL-GEL METHOD FOR PHOTO CATALYTIC AND ANTIMICROBIAL ACTIVITY APPLICATIONS

M.Sangeetha, T.S. Senthil*

Nanotechnology Laboratory, Department of Physics, Erode Sengunthar Engineering College, Erode 638057, Tamil Nadu, India.

Pure Tio2 nanoparticles are synthesized by sol-gel technique. The prepared materials are characterized by x-ray diffraction analysis (XRD), UV-Visible, Field emission scanning electron microscopy (FESEM). The obtained results illustrate an aggregative structure at high calcined temperatures with the formation of spherical particles. The effects of chemical compositions and calcined temperature on surface topography and crystallization and crystallization of phase are studied. The photocatalytic activity was examined in details. In vitro antibacterial activities of the synthesized Tio2 nanoparticles were investigated against gram positive and gram negative bacteria's by using Agar diffusion method.An Antibacterial activity study carried out the strong inhibitory and antibacterial effects also a broad spectrum of antimicrobial activities against human pathogens.

AB 122 EFFECT OF EPSOMITE DOPED ON ASCORBIC ACID CRYSTAL CHARCTERIZATION STUDIES

[1]**A.Murugan** *M.Sc Physics, Don Bosco College, Dharmapuri.*

[2]**Prof.V.Vinodhini**,*M.Sc., M.Phil., Assistant Professor, Pachamuthu College of Arts & Science for women, Dharmapuri*

NLO materials are getting a greater attention in the every field of optical telecommunication, second harmonic generation and optical signal processing replacing inorganic compounds. The chemical on doping change their dielectric properties and are used in NLO application. The materials for non-linear optical are formed from a system of delocalized π electrons. A single crystal of Epsomite doped with ascorbic acid was grown successfully by slow evaporation solution growth technique at room temperature. The various group functional groups

were confirmed by FT-IR spectrum analysis. The optical transparency of grown crystal was studied by the UV-Visible spectrum based on absorption and emission rates, the band gap of 4.6771 ev.

AB 123 GROWTH AND CHARCECTERIZATION STUDIES OF ANEURIN CRYSTALS BY SLOW EVAPORATION

[1]**A.Shamala** *M.Sc Physics, Don Bosco College, Dharmapuri.*
[2]**Prof.V.Vinodhini**,*M.Sc., M.Phil., Assistant Professor, Pachamuthu College of Arts & Science for women, Dharmapuri*

For the growth of the above crystal, the Saturated solution of pure aneurin using distilled water was prepared in a magnetic stirrer with rotation speed of 460-700 for 10 minutes for uniform stirring. The saturated solution of aneurin using distilled water was prepared using a 250ml cleaned beaker as growth vessel. For the growth by slow evaporation, the vessel was covered with a performed polythene cover. The temperature of the solution is maintained constant keeping the growth vessel in the laboratory near the window. At constant temperature constant took place with resulted in super saturation of the solution. After 21 days few seeds of a single aneurin were obtained. This is the quickest and most useful way of growing crystal. The crystals were harvested after a typical growth of 41 days. The single crystal of aneurin was obtained.

AB 124 SLOW EVAPORATION GROWTH OF PYRIDOXIN HYDROCHLORIDE CRYSTALS

M.USHA, *M.Sc Physics, Don Bosco College, Dharmapuri.*
[2]**Prof.V.Vinodhini**,*M.Sc., M.Phil., Assistant Professor, Pachamuthu College of Arts & Science for women, Dharmapuri*

For the growth of the single crystal of Pyridoxin, the saturated solution was prepared using distilled water was prepared in a magnetic stirrer with rotation speed of 680-740 for 30 minutes in a 250ml cleaned beaker as growth vessel. For the growth of solution by slow evaporation, the vessel was covered with a performed polythene cover. The temperature of the solution is varied at different temperature by keeping the growth vessel in the laboratory near the window. The constant evaporation took place which resulted in super saturation of the solution. After 15 days few seeds of a single crystal of pyridoxine were obtained. The solution should be supersaturated and the beaker should be sealed to avoid evaporation. The seed grows as excess salt in the solution and slowly crystallization occurs on it. The crystals were harvested after a typical growth of seed crystal after 20 days.

AB 125 LOW TEMPERATURE SOLUTION GROWTH OF ASCORBIC ACID ON WHITE VITRIOL CRYSTALS

C.PRIYANKA, *M.Sc Physics, Don Bosco College, Dharmapuri.*
[2]**Prof.V.Vinodhini**,*M.Sc., M.Phil., Assistant Professor, Pachamuthu College of Arts & Science for women, Dharmapuri*

NLO materials are getting a greater attention in the every field of optical telecommunication, second harmonic generation and optical signal processing replacing inorganic compounds. By doping a chemical to another the dielectric properties of the crystal change with applies to NLO. The materials for non-linear optical are formed from a system of delocalized π electrons. A single crystal of white vitriol doped with vitamin C was grown successfully by slow evaporation solution growth technique at room temperature. The various functional groups were confirmed by FT-IR spectrum analysis. The optical transparency of the grown crystal was studied by the UV visible spectrum.

AB 126 THERMODYNAMIC AND TRANSPORT STUDIES ON SOME BASIC AMINO ACIDS IN AQUEOUS SODIUM ACETATE SOLUTION AT DIFFERENT TEMPERATURES

(P Inbam * *Don Bosco College,Dharmapuri)*

Ultrasonic velocity (U), density (ρ) and viscosity (η) of three amino acids namely L-arginine, L-lysine and L-histidine in aqueous sodium acetate solution (0.4 mol. kg-1) as a function of composition at 298.15, 308.15 and 318.15 K, have been measured. Using these experimental values, the acoustical parameters such as adiabatic compressibility(β), molal hydration number (nH), apparent molal compressibility (φK), apparent molal volume (φV), limiting apparent molal compressibility (φK0), limiting apparent molal volume (φV0), the constants (SK, SV) and viscosity B-coefficient of Jones-Dole equations were calculated for all the three systems. These parameters have been thoroughly analysed and eventually emphasizing the possible molecular interactions in terms of structure-making and structure-breaking effects of the above amino acids in the solvent mixture.

AB 127 EFFECT OF KCL DOPING ON THE GROWT H OF GLYCINE CRYSTAL AND ITS PROPERTIES

C.George Arokia Raj ,Arokia Mary.M*,*Don Bosco College*

Glycine usually crystallizes as the metastable alpha-polymorph from pure aqueous solution. The polymorph, gamma-form of glycine can be crystallized only in presence of additive. In the present work, gamma-glycine has been crystallized by using potassium chloride (KCl) as additive at ambient temperature by solvent evaporation method. The form of crystallization is confirmed by FTIR ,UV method. Spectroscopic and thermal studies have been carried out for analyzing the presence of functional groups, thermal stability and decomposition of the sample. The results indicate that the KCl is doped into the gamma-glycine.

AB 128 SYNTHESIS AND CHARACTERIZATION OF ZINC SULPHIDE NANOPARTICLES PREPARED BY COPRECIPITATION METHOD

C.George Arokia raj,Mageswari.P*Don Bosco College,Dharmapuri*

Zinc sulphide (ZnS) nanoparticles have been synthesized by the mechanochemical route. The prepared nanoparticles have been analyzed by Coprecipitation method, Fourier transform infrared spectrophotometer. The crystallite size of as prepared nanoparticles are found to be in the 9 nm range. XRD spectrum confirmed the composition of ZnS sample.

AB 129 SYNTHESIS AND CHARACTERIZATION OF ZINC TITANATE NANOCRYSTALS FOR THERMOELECTRIC APPLICATIONS

P. Chandrasekaran[a], T.M.V.Murugu Thiruvalluvan[b], P.Anandhan[c], M.Arivanandhan[d], K. Pazhanivel[e]

[a]Department of Physics, Annamalai University, Annamalai Nagar, Chidambaram, India
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[c]Department of Physics, Thiru Kolanjiappar Government Arts College, Virudhachalam
[d]Centre for Nanoscience and Technology, Anna University, Chennai-600025, India
[e]Department of Mechanical Engineering, A.R.S College of Engineering, Maraimalai Nagar, Chennai

$ZnTiO_3$ nanocrystals were synthesized by sol-gel method with different Zn and Ti ratios. The synthesized nanocrystals were annealed at different temperatures to study the impact of annealing temperature on the structural and optical properties of the titanates. The structural, morphological and optical properties of sol-gel synthesized $ZnTiO_3$ nanocrystals were studied. The structural properties and phase transition from one phase to another phase as a function of annealing temperature were studied by X-ray diffraction analysis. The surface morphology of the as synthesized and annealed samples was analysed by FE-SEM. The thermoelectric properties of the samples were systematically investigated as a function of Zn to Ti ratio and annealing temperature.

AB 130 FUNCTIONS AND THERAPEUTIC APPLICATIONS OF VENOM PROTEINS

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Venomous animals are a serious threat to the life of victims both animal and human and 1.45 million people around the world are affected by snake bite. As per the report of Kasturiratne et al. 2008, annually 20,000-94,000 deaths are recorded globally and the main reason is untreated (especially in poor countries) due to expensive of antivenoms and the limitation and complication of the drugs. Targeting the toxins which cause the serious or immediate death can be neutralized by new effective drugs thus can save the victims and large scale production can lead to the easy available to all people. On the other hand, understanding the biochemical property of venom will help us to treat the envenomation, as well as some specific functional toxin molecule with protein engineering, can be developed as a lifesaving drug. This article gives a glimpse of the venom proteins and their functional properties and the list of drugs approved from animal toxins. The overall study focused on the functional specificity of the venom proteins, molecular evolution with their biological importance which can be targeted for treatment and developing drugs from the proteins.

AB 131 GROWTH AND CHARACTERIZATION WITH MOLECULAR MODELING STUDIES OF BENZOTRIAZOLE SALICYLIC ACID (BSA) SINGLE CRYSTAL

P.Sathya, N.Karthikeyan

Department of physics, Anna University, Chennai – 25

Benzotriazole salicylic acid (BSA) single crystal was grown by slow evaporation solution growth method. The grown crystal was confirmed by single crystal X-ray diffraction analysis. The BSA compound crystallises in monoclinic system with space group P21/n which is recognized as centro-symmetric nature. The lattice parameters were obtained as a = 13.80(7) Å, b = 5.41 (1) Å, c = 16.66 (2) Å, α = 90°, β = 102.27 (3) °, γ = 90°, V = 1216 (4) Å3. The vibrational spectroscopy (FT-IR and Raman spectra) of BSA compound has been studied under both theoretically and experimentally. The optimized geometrical parameters of BSA obtained by B3LYP/6-31g(d,p) density functional calculations. The HOMO and LUMO energy values were calculated along with their plot has been presented to understand the charge transfer occurring within the compound. Molecular electrostatic potential (MEP) surface map, hyperpolarisability and dipolemoment were calculated. Number of protons was identifying by 1H NMR spectrum. The material is thermally stable up to 134°C and the compound starts to decompose at 216°C. The biological activities of BSA molecule have also been explored as a best potential inhibitor of Bacillus cereus bacteria. These findings may guide to design new triazole compounds with interesting biological activity.

AB 132 INVESTIGATIONS ON THE SUPRAMOLECULAR ASSEMBLIES OF PYRIDINE BASED ORGANIC CRYSTALS FOR NONLINEAR OPTICAL APPLICATIONS

RO. MU. Jauhar, P. Murugakoothan*

MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai – 600 030.

Present work aims at the crystal growth and characterization of 2-amino 4, 6 dimethoxy pyrimidine p-toluenesulfonic acid monohydrate (2ADPTS), 2, 6 diaminopyridinium tosylate (2,6DPT), isonicotinamidium picrate (ISPA) and 2-aminopyridinium diphenylacetate diphenylacetic acid (2APD) by slow evaporation solution technique (SEST). The essential properties, such as structural, linear and nonlinear optical, thermal and laser damage threshold of the grown crystals have been investigated.

AB 133 SYNTHESIS, CHARACTERIZATION AND DFT CALCULATIONS OF 1-(QUINOLIN-3-YL) PYRROLIDIN-2-OL (P7)

M. Suresh

Department of Chemistry,
Anna University(CEG), Chennai-25

The experimental and theoretical vibrational frequencies of a newly synthesized compound, namely 1-(quinolin-3-yl)pyrrolidin-2-ol are analyzed. The experimental FT-IR (4000-400 cm−1) and FT-Raman (4000-100 cm−1) of the molecule in solid phase have been recorded. The optimized molecular structure, vibrational assignments of P7 have been investigated experimentally and theoretically using Gaussian03W software package. The stability of the molecule arising from hyper-conjugative interaction and charge delocalization has been analyzed using NBO analysis. The first order hyperpolarizability (β0) is calculated to find its character in Non-linear optics. Gauge including atomic orbital (GIAO) method is used to calculate1H-NMR chemical shift calculations were carried out and compared with experimental data. The electronic properties like UV-Visible spectral analysis and HOMOLUMO energies were reported. The energy gap shows that the charge transfer occurs within the molecule. Thermodynamic parameters of the title compound were calculated at various temperatures.

AB 134 STRUCTURAL, MORPHOLOGICAL, OPTICAL AND THERMOELECTRIC PROPERTIES OF NANOSTRUCTURED CDTE

R.Rajkumar[a], J.Senthil Selvan[a*], G.Anbalagan[a], M.Arivanandhan[b]

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Thermoelectric systems have recently received an increasing amount of attention because they facilitate direct and reversible conversion between heat and electrical energy, thus enabling environmentally friendly refrigeration and electric power generation. The performance of TE

material is assessed using a dimensionless figure of merit (ZT) = $\alpha^2\sigma T/\kappa$, where α, σ, T, $\alpha^2\sigma$, and κ are the Seebeck coefficient, electrical conductivity, absolute temperature, power factor, and total thermal conductivity, respectively. In the present work, Chalcogenides based CdTe materialswere prepared by wet chemical method. The synthesized materials were characterized by XRD, SEM and UV analysis for structural, morphological and optical analysis. The XRD analysis confirms the crystal structure of the prepared material. The SEM images show that the synthesized CdTe particles are highly mono dispersed with less agglomerations. The particles have spherical morphology with sizes in the range of 30 to 40 nm. Thermoelectric properties of the CdTe were studied by measuring the Seebeck coefficient as a function of temperature. The Seebeck coefficient increases with temperature in the temperature range from 30ºC to 650ºC.

AB 135 SYNTHESIS, NMR STUDY AND CRYSTAL DETERMINATION OF 7-BENZOYLOXYCOUMARIN

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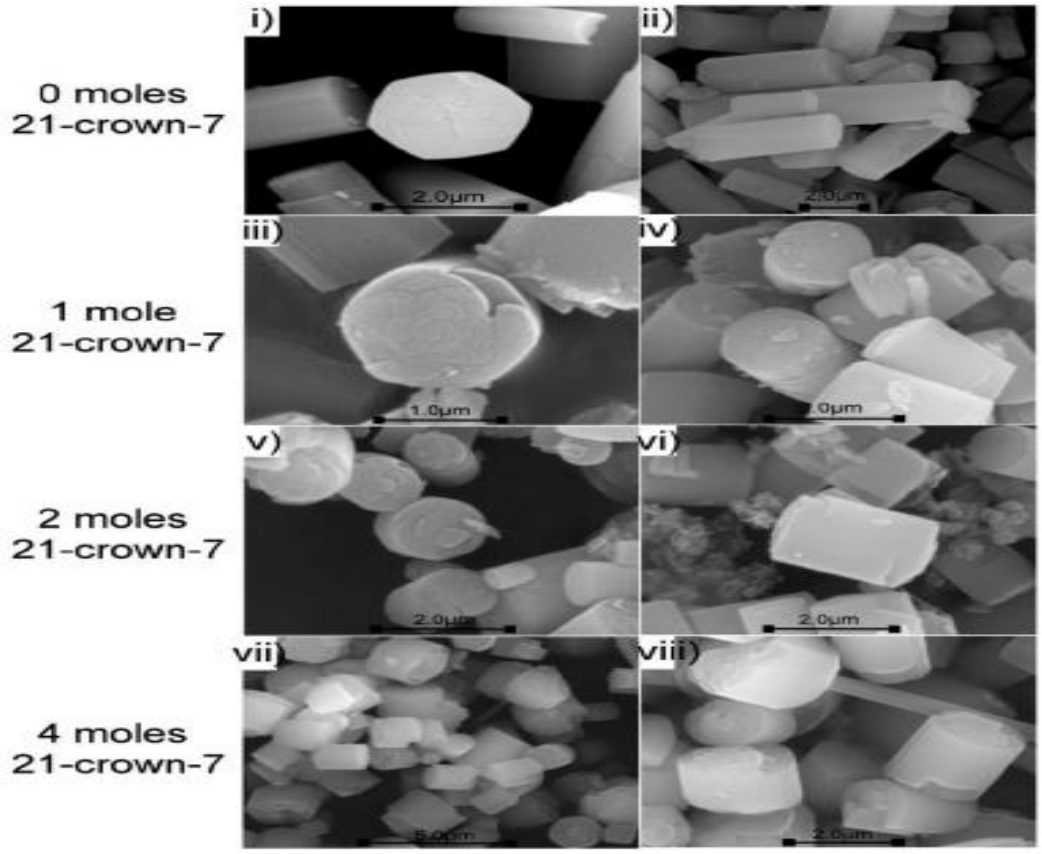
The title compound, 7-benzoyloxycoumarin, C16H10O4, crystallizes into monoclinic space group $P2_{(1)}$ with unit-cell parameter: a = 3.8479(7), b = 27.693(5), c = 5.7259(10) Ao. Z = 2. The crystal structure was solved by direct methods and refined to a final R-value of 0.0535 for 3295 observed reflection. The benzoyloxy ring present on 7- position was found to be almost coplanar with coumarin. The structure is stabilized by vander Waal's interactions. The structure of this compound was also established by 1H NMR spectrum of its solution in CDCl3. IR and Raman spectra were obtained directly in the synthesis process of coumarin with computational study of geometry such as bond lengths, bond angels and different molecular properties like Molecular Electrostatic Potential (MESP), Mulliken Charge Distribution, Global and Local Reactivity Descriptors (chemical hardness, softness, chemical potential, electronegativity, electrophilicity index). Hartee–Fock (HF) and B3LYP level of theory with 6-31G++(d,p) basis set are employed for all sorts of calculation. IR and Raman information made up training set and a quantitative analysis model of the Benzoyloxycoumarin mixed system was established by applying partial least squares (PLS). The molecular geometry was compared with the experimental data and a good agreement with the experimental data was found.



TEM image of Benzoyloxycoumarin for different crown

AB 136 CORROSION ANALYSIS OF MILD STEEL IN HYDROCHLORIC ACID USING PYRIDINE N-OXIDE AS INHIBITORS

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Inhibition of corrosion of mild steel material in hydrochloric acid medium has been tried with many synthetic and green inhibitors. Each inhibitor has its own merits and limitations. The present study aims at the synthesis of Pyridine N-Oxide (PyNO) and the study of their inhibition behaviour on the corrosion of mild steel in 2N hydrochloric acid. The inhibition behaviour of the synthesized compound was studied by subjecting to weight loss measurements, polarisation studies and electrochemical impedance spectra (EIS) for the assessment of its performance. The studies were made with 2N hydrochloric acid as the corroding medium, but with the inhibitor

concentration in the range of 50 -350 ppm. The results revealed that the inhibitor studied perform better in the medium and function by the mechanism of adsorption onto the metal surface.

AB 137 LUMINESCENCE STUDIES OF ERBIUM DOPEDBARIUM LITHIUM FLUOROBORATE GLASSES

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The present spectral investigations on erbium doped barium lithium fluoroborate glasses of the composition (H_3BO_3- Li_2CO_3 - $BaCO_3$ - CaF_2– ZnO - Er_2O_3) and different varying erbium oxide concentrations were prepared by conventional melt quenching technique. Dielectric constant, refractive index, electronic susceptibility, reflection loss and interionic distance were calculated for all the glass samples. The amorphous nature of the glass was confirmed by X-Ray diffraction analysis. Functional groups were determined from the FTIR measurements. The optical properties of the prepared glasses were investigated by UV-Vis-NIR absorption and emission spectra. Nephelauxetic ratio and bonding parameters were determined from the absorption spectra and were found to be ionic. Optical bandgap corresponding to the direct and indirect allowed transitions were calculated to understand the electronic band structure and Urbach energy values. Judd-Ofelt intensity parameters (Ω_λ=2, 4 and 6) were determined from the absorption spectra in order to study the site occupancy of the rare earth ion and its surrounding region. The JO parameters were used to analyse the transition probability (A), branching ratio (β_R), and stimulated emission cross section (σ_P^E) for the different emission intensities.The infrared emission at 1550 nm indicates that the glass material is a promising candidate to be employed as wave guide laser source and optical fiber amplifier.

Keywords: Absorption; Intensity parameter; branching ratio; optical amplifier; Solid state laser;

AB 138 GROWTH AND CHARACTERIZATION OF STRONTIUM BIS (HYDROGEN L-MALATE) HEXAHYDRATE SINGLE CRYSTALS FOR NLO APPLICATIONS

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Department of Physics, SRM University, Ramapuram, Chennai

**SSN College of Engineering, Kalavakkam, Chennai*

L-malic acid derivative, semi-organic single crystals are vital candidateas for NLO and electro optical applications. Recent studies on organic and semi-organic crystals have shown that

L-malic acid ($C_4H_6O_5$), one of the simplest chiral dicarboxylic acids, is a suitable building block in crystal engineering, being used to create two dimensional anionic networks held together by hydrogen bonds. Moreover, its chirality ensures the absence of a center of symmetry, essential for optical nonlinear second harmonic generation. Semi-organic, good quality single crystals of strontium bis (hydrogen L-malate) hexahydrate (SrLM) were successfully grown by unidirectional SR method. Optically transparent SrLM crystal was grown by conventional solution growth methods and a well faceted crystal was chosen as a seed for SR Method. Based on the morphology of the slow cooling method grown SrLM crystal, the (010) plane was selected in the present study to impose the orientation in the growing crystal.By this method, crystal with the diameters 10 mm and 20 mm and length maxium up to 70 mm were grown. The structural perfection and growth features of SrLM was analysed by chemical etching studies. The grown crystals were characterized by UV-Vis-NIR spectrum, birefringence, laser damage threshold and dielectric studies. The value of birefringence and quality were ascertained by birefringence interferometer. The birefringence interferogram shows good refractive index homogeneity of the SrLM crystal. Optical damage tolerance of SR grown SrLM crystal was investigated by laser damage threshold studies. The dielectric behaviour and perfection of the SrLM crystals are studied and reported.

AB 139 STABILITY CONSTANTS OF TRANSITION METAL COMPLEXES OF SOME ORGANIC ACIDS

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The present work deals with the study of proton-ligands and metal ligands of oxalic acids,malonic acid,maleic acid,glycine and alanine with Mn(II),Fe(III),Ni(II),La(III),Ce(III)and UO_2(II).The metal ligands stability constant of binary and ternary complexes were evaluated using Irving-Rossotti titration technique.

Keywords: Potentiometric,Determination,Binary,Ternary,Formation constants,Cu(II),Mn(II),Fe(III),Ni(II),La(III),Ce(III) and UO_2(II),complexes.

AB 140 GROUND WATER POLLUTION BY DISTILLERY WASTE

D.AGALYA[1] and C.SENTHILKUMAR[2]

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The objective of this study is to evelute contamination in ground water due to distillery effluent irrigation. A study was conducted from 2016 to 2017 at 2 different times in a year, that is in march and October for 10 per- identified location at pennagaram and its suburbs of dharmapuri district. The PMDE(post machinated distillery effluent)was applied twice at the rate of about 230-50m^3/ha as a pre-sown irrigation. The analysis showed that PH,EC,CT,SO_4^{2-} and Zn were all within acceptable limits. Elevated levels of TDS,NO^{3-},PO_4^{3-},BOD and Fe values proximity to pollution sources were exceeded the World Health Organization(WHO)for recommended threshoulds for potable water.

Ketwords-Contamination,Groundwater,Industrial pollution,Distillery,Effluent irrigation.

AB 141 EVALITION OF EXCESS FLUORIDE IN GROUND WATER AND ITS IMPACTS ON HUMANHEALTH IN PAPPIREDDIPATTI,DHARMAPURI DISTRICT

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[1]Department of chemistry,Pachamuthu college of arts and science for women,Dharmapuri Dt

[2] Department of chemistry,Pachamuthu college of arts and science for women,Dharmapuri Dt

Water is one of the most important nature gifts for all living things. The ground water is one of the major sources for drinking and other irrigation purposes in this region. Most of the villages mainly they depend ground water sources for all purposes. The present studies explain the excess amount of fluoride in ground water and also explain the variation of some physic-chemical parameters. This study also explains the fiuorosis problems among the peoples.

AB 142 STRUCTURAL PROPERTIES OF MGO NANO PARTICLES:SYNTHESIZED BY CO-PRECIPITATION METHOD.

A.Padmacini,R.Saritha,M.Bhuvaneshwari,M.nithya,S.Vidhya*

Pachamuthu college of Arts and Science for women,Dharmapuri.

Metal oxide nano materials are important and excellent materials, because of its special properties like chemical stability, high electric permittivity, non-toxic nature .so it is used in various applications like optical, electrical, environmental and semiconductor. Present work focused on to synthesis of MgO nano particles and, its applications in the field of environment. Thus nano particles are prepared by simple suitable chemical method like chemical Co-Precipitation using magnesium nitrate as Core precursor. The synthesized metal oxide nano particles have been characterized by XRD, UV, FTIR.

AB 143 SYNTHESIS AND CHARACTERIZATION OF CADMIUM SULFIDE NANOPARTICLES

A.Padmacini,A. Lilitha ,M.Dhivya ,P.Rajeshwari ,M. Vaitheswari,K.Aswini*

Pachamuthu college of Arts and Science for women,Dharmapuri.

Cadmium Sulfide is one of the most promising materials for solar cells and of great interest for their practical applications in up to electronics and photonics.the optical properties get modified due to the confinement of charge carrier within the nano particles. the physical and chemical properties of thus nano-particles are found to be size depended. In the present work describes synthesis and characterization of cadmium sulfide using chemical precipitation techniques. A pure nano structure cadmium sulfide is synthesized at room temperature. The Crystallite sizes of cadmium sulfide crystals were estimated from the peaks of XRD.The optical properties of the samples were estimated by UV visible Spectroscopy. The absorption spectrum were studied FTIR and Scanning Electron Microscopy is used to carry out the structural characterization of the nano particles.

AB 144 SYNTHESIZED AND STUDY OF MAGNESIUM OXIDE AND CADMIUM DOPED MAGNESIUM OXIDE NANO PARTICLES BY CO-PRECIPITATION METHOD.

A.Padmacini ,S.Vidhya,M.Bhuvaneshwari,R,Saritha,M.nithya*

Pachamuthu college of Arts and Science for women,Dharmapuri.

Metal oxide nano materials are important and excellent materials, because of its special properties like chemical stability, high electric permittivity, non-toxic nature .so it is used in various applications like optical, electrical, environmental and semiconductor. Present work focused on to synthesis of Cadmium doped MgO nano particles and, its applications in the field of environment. Thus nano particles are prepared by simple suitable chemical method like chemical

Co-Precipitation using magnesium nitrate as Core precursor. The synthesized metal oxide nano particles have been characterized by XRD, UV, and FTIR.

AB 145 SYNTHESIZED AND STUDY OF MAGNESIUM OXIDE AND CADMIUM DOPED MAGNESIUM OXIDE NANO PARTICLES BY CO-PRECIPITATION METHOD.

A.Padmacini ,S.Vidhya,M.Bhuvaneshwari,R,Saritha,M.nithya*

Pachamuthu college of Arts and Science for women,Dharmapuri.

Metal oxide nano materials are important and excellent materials,because of its special properties like chemical stebility ,high electric permittivity,non-toxic nature .so it is used in various applications like optical, electrical, environmental and semiconductor.Present work focused on to synthesis of Cadmium doped MgO nano particles and ,its applications in the field of environment.thus nano particles are prepared by simple suitable chemical method like chemical Co-Precipitation using magnesium nitrate as Core precursor.The synthesized metal oxide nano particles have been characterized by XRD,UV,FTIR.

Day-2 [29/08/2017]

9.15 a.m -9.55a.m	Chemical bonding and Electrostatic properties of Molecules from High resolution X-ray diffraction and AIM theory	**Prof.P. Kumaradhas** Head &Professor, Department of physics, Periyar University, Salem
9.55a.m -10.30 a.m	Recently Developed Unidirectional Organic Single Crystal Cylinders for Scintillator Application	**Prof. K. Shankaranarayanan** Professor & Director Department of Physics Alagappa University Karaikudi
10.30a.m-10.40a.m	Tea Break	
10.40a.m-11.15a.m	Modelling Molecules, Materials and Processes: Basics and Applications	**Prof P. Venuvanalingam** CSIR Emeritus Scientist School of Chemistry Bharthidasan University, Tiruchirappalli.
11.15 a.m to 11.50 p.m	Mechanism and Drug Inhibition of Influenza A (H1N1) virus	**Prof. P. Kolandhaivel** [Former Director, School of Physical Sciences] UGC BSR Faculty Fellow Department of Physics Bharathiyar University Coimbatore
11.50a.m to 12.25 p.m	Nanostructured Semiconductor Materials for Thermoelectric Applications	**Dr. M. Arivanandhan,** Centre for nanoscience and technology, Anna University, Chennai
12.25p.m to 01.00 p.m	Oral Presentations (OP-XX to OP-XX)	
01.00p.m to 02.00 p.m	Lunch Break & Poster Presentation(PP-XX to PP-XX)	
02.00p.m to 02.45 p.m	Single Crystal XRD for precise drug designing	**Dr. K. Gunasekaran** Centre of Advanced Study in Crystallography and Biophysics University of Madras Chennai.
02.45p.m to 03.20 p.m	Manganese based Cathode Materials for Rechargeable Li-ion Batteries	**Dr. Kumar Raju** Materials Science and Manufacturing, CSIR Pretoria 0001, South Africa.
3.20 p.m to 3.50 p.m	Improvement in crystallinity of unidirectional method grown nonlinear optical (NLO) and ferroelectric single crystals for Second Harmonic Generation and Infrared (IR) Detector Applications	**Dr. Muthu Senthil Pandian** Research Scientist Photovoltaic Devices Laboratory SSN Research Centre SSN Institutions Chennai
03.50 p.m to 04.25 p.m	Oral Presentations (OP-XX to OP-XX)	
04.25 p.m to 04. 35p.m	High tea	
04.40 p.m to 05.00p.m	Valedictory	

VALEDICTORY FUNCTION

Welcome Address : **Dr. Philomene**
Chair Person

Valedictory Address : **Prof P. Venuvanalingam**
CSIR Emeritus Scientist
School of Chemistry
Bharthidasan University,
Tiruchirappalli.

Feed Back : Participants

Vote of Thanks : **Prof. M. Anitha**
HOD, Convener- ICMAST 2017