INTERNATIONAL E-CONFERENCE ON FRONTIERS OF ENERGY EFFICIENT MATERIALS AND DEVICES (ICEEMD-2021)

13th MARCH 2021

ABSTRACTS

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Dr. P. JAYAMURUGAN

Organized by
Department of Physics
Sri Ramakrishna Mission Vidyalaya College of Arts and Science
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Swami Nirmaleshananda
Secretary
Sri Ramakrishna Mission Vidyalaya
College of Arts and Science
Coimbatore - 641020

Message

I am extremely happy and delighted to note that the Department of Physics our college is organizing an **International E-conference on Frontiers of energy efficient materials and devices (ICEEMD-2021) on 13.3.2021**.

I strongly believe that this conference will provide a platform for fresh concepts and young researchers to exhibit their talents in various fields of Physics. The thought provoking and resourceful lectures of our Alumni and other resource persons will definitely have a great impact.

Swami Nirmaleshananda
Patron

Dr. R. Thangavel
Principal
Sri Ramakrishna Mission Vidyalaya
College of Arts and Science
Coimbatore - 641020

Message

As the principal of SRMV college of Arts and Science, I am pleased to send this message on the occasion of the **International e-conference on Frontiers of energy efficient materials and devices (ICEEMD - 2021) organized** by the Departments of Physics on 13th March 2021.

I am certain the conference will be an excellent platform to deliberate on the issue relation to the selection of the materials for higher efficiency.
I congratulate all the Faculty Members and Research Scholars with heartful of wishes for the success of the conference.

Dr. R. Thangavel
Conference Chair

Dr. J. Chandrasekaran,
Head of Physics
Sri Ramakrishna Mission Vidyalaya
College of Arts and Science
Coimbatore - 641020

Message

It gives me immense pleasure and happiness that my dear colleagues have come forward in organizing the International E-conference on Frontiers of Energy Efficient Materials and Devices (ICEEMD-2021) in a grand way during 13th march 2021. Many eminent scientists around the globe are giving keynote address and delivering novel lectures during this conference. The conference will address critical issues of recent advances in materials research and is very much useful to develop our society.

I am confident that, this conference will definitely provide an interactive platform where scholars from various institutes, research laboratories and industries can meet, discuss and project a roadmap for materials science research towards novel applications in various fields.

It is important to develop an attitude towards research and evidence building in every scientific sphere and this conference would be a major step towards this goal in this field.

I wish the conference great success.

I am sure the conference is a grand scientific extravaganza.

Dr. J. CHANDRASEKARAN,
Convener

Sri Ramakrishna Mission Vidyalaya College of Arts and Science

Coimbatore - 641020

Ramakrishna Mission Vidyalaya was founded by 'Ayya' Sri.T.S Avinashilingam in the year 1930, to implement great education ideals placed before the country by Sri Ramakrishna, Swami Vivekananda and Mahatma Gandhi. It cherishes a life of purity, discipline, simplicity and inculcates the ideals of devotion to duty and sincerity in service.

Sri Ramakrishna Mission Vidyalaya College of Arts and Science, a constituent institution of Ramakrishna Vidyalaya was started in the year 1964 with Pre-University course. The Degree Programmes were started in 1966 and Post Graduate Programmes in 1971. The M.Phil programmes were begun in 1978 and affiliation for Ph.D programmes was granted in the year 1979. The college has completed 57 years of noble service in the field of higher education.

Recently the college has undergone the NAAC Re-Accreditation (3rd cycle) with the vision:

> "*Imparting moral ethical and socially relevant holistic education to devolope multidimensional personality of every youth to be an asset of our nation"*. and is awarded 'A' grade with CGPA 3.25.

Department of Physics

The Department of Physics was established in 1964 with a view to impart the scientific thoughts among the students. In addition to UG and PG Programmes, active M.Phil and Ph.D research in the fields of Solar Energy, Thin Film Technology, Crystal Growth, Non-Linear Optics, Conducting Polymers, Nano Technology, Solar Cells, Molecular Quantum Mechanics and Ultrasonics are being carried out. So far, more than 300 M.Phil and 35 Ph.D degrees were awarded. The department has published more than 500 research papers in SCI indexed international journals. During the last five years, the department has carried out five major research projects to the tune of 1.2 Cr. funded by UGC, DST and DRDO. It is a FIST sponsored department having advanced research instrumentation facilities.

SRI RAMAKRISHNA MISSION VIDYALAYACOLLEGE OF ARTS & SCIENCE
Coimbatore - 641 020
Department of Physics

PROGRAMME SCHEDULE

Time: 10.00 am – 4.45 pm **Date: 13th March 2021**

Inaugural Session

10.10 am	**Welcome Address**	**Dr. R. Thangavel** Principal Sri Ramakrishna Mission Vidyalaya College of Arts and Science Coimbatore - 641020
10.15 am	**Benedictory Address**	**Swami Nirmaleshananda** Secretary Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore - 641020
10.25 am	**Dynamics of the workshop**	**Dr. J. Chandrasekaran** Convener Sri Ramakrishna Mission Vidyalaya College of Arts and Science Coimbatore - 641020
10.30 am	**Vote of Thanks**	**Dr. P. Jayamurugan** Coordinator Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore – 641020

Technical Sessions

10.30 to 11.00 am	**Technical Session –I** Topic: Nonlinear Dynamics	
11.00 to 11.30 am	**Technical Session-II** Topic: Thin films for Super capacitor applications	
11.00 to 11.30 am	**Technical Session-III** Topic: Flame synthesis metal oxide nanoparticles for Gas sensor application	
11.30 to 12.00 pm	**Technical Session-IV** Topic: Non-thermal plasma on biomedical applications	
12.30 to 01.00 pm	**ORAL PRESENTATION**	
01.00 to 02.00 pm	**LUNCH BREAK**	
02.00 to 02.30 pm	**Technical Session-V** Topic: An overview of Lithium – ion storage devices	
02.30 to 03.00 pm	**Technical Session-VI** Topic: Resistive switch memory - materials and device fabrication	
03.00 to 03.30 pm	**Technical Session-VII** Topic: Mesocrystals: New materials design for different applications	
04.00 to 04.30 pm	**ORAL/POSTER PRESENTATION**	

Concluding Session

04.30 to 04.40 pm	**Feed Back**	**Dr. R. Suresh** Co-Coordinator Sri Ramakrishna Mission Vidyalaya College of Arts and Science Coimbatore - 641020
04.40 to 04.45 pm	**Vote of Thanks**	

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Dr. D. Sridher, *Assistant professor of Physics*

TABLE OF CONTENTS

INVITED TALKS

INV-01

Nonlinear Dynamics: An evolving Science

Dr. R.Gopal

Research Scientist Centre for Nonlinear Science and, School of Electrical and Electronics Engineering SASTRA DEEMED University,
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ABSTRACT

The lecture presents in a systematic manner the basic physical ideas in nonlinear dynamics of continuous dynamical systems considered from a common background. This approach allows one to reach goals in different aspects. In this lecture, we mainly focused on how the mathematical experiments based on numerical computation have led to the modern development of Nonlinear Science/ Nonlinear Physics, leading to the concepts of solitons, bifurcations, chaos, patterns, and various collective dynamical states.

In particular,the crucial role of the famous Fermi- Pasta- Ulam (FPU) recurrence phenomenon in nonlinear existence of various collective states and the existence of various collective states arrays and networks of coupled nonlinear oscillators will be explained.

References:

1. M. Lakshmanan & amp; S. Rajasekar Nonlinear Dynamics: Integrability and Chaos, Springer-Verlag, Berlin (2003).
2. R. Gopal, V. K. Chandrasekar, A. Venkatesan and M. Lakshmanan, Phys. Rev. E 89, 052914 (2014).
3. P. Chandran R. Gopal, V.K. Chandrasekar and N. Athavan Chaos 29, 053125 (2019).

INV-02

Highly saturated ferromagnetic cobalt doped cuprous oxide thin films for Super capacitor application

Dr.N.Anandhan

Advanced Materials and Thin film Laboratory, Department of Physics, Alagappa University, Karaikudi –630003, India.

*__Corresponding author email__: anandhan_kn@rediffmail.com

ABSTRACT

As prepared and different concentrations of cobalt (Co^{2+}) ions incorporated into cuprous oxide $Cu_{2-x}Co_xO$ (x=0-14 mM) thin films were successfully deposited in FTO glass substrate by employing electrode position technique. The X-ray diffraction (XRD) patterns confirm the cubic structure of pure and Co doped thin films that grow along the preferential (111) growth orientation. Scanning Electron Microscope (SEM) images display three side pyramid shape morphology of pure Cu_2O thin films that get significantly changed, as and when Co concentrations get increased. The band gap increased from 2.13 to 2.30 eV, as Co dopant concentrations get increased. Energy Dispersive X-ray (EDX) spectra confirm that the elemental composition of Co ion continuously increases with an increase in Co-doped concentrations.

Vibrating Sample Magnetometer (VSM) pictures the film that exhibits a better ferromagnetic property with saturation magnetism for 14 mM Co dopant. X-ray photoelectron spectroscopy (XPS) confirm the presence of cobalt (Co^{2+}) as a dopant in the host Cu_2O thin films.

The $Cu_{2-86}Co_{14}O$ (x=14 mM) thin film has a higher specific capacitance of 164.90 F/g at the current density of 2 A/g. It has good energy and power density in the higher concentration Co doped Cu_2O thin films.

Keywords: Cu_2O thin films; Electrode position; Co doping; Ferromagnetism; specific capacitance.

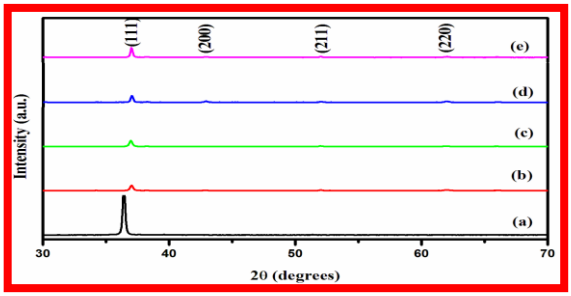

Fig. XRD patterns of pure and Co doped Cu_2O thin films deposited at different dopant concentrations (a) 0 mM (b) 8 mM (c) 10 mM (d) 12 mM, (e) 14 mM.

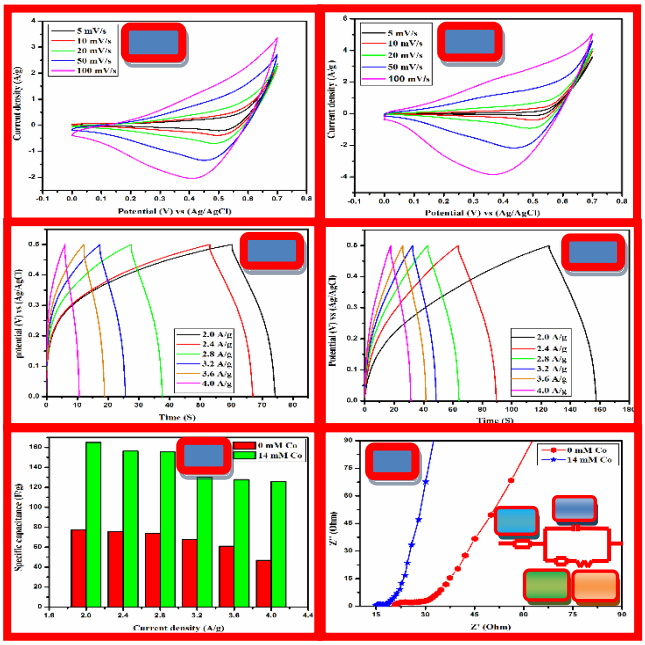

Fig. (a) and (b) CV curve, (c) and (d) GCD curve, (d) Bar chart of specific capacitance $v_{s.}$ current density, (e) EIS spectra of pure and Co doped Cu_2O thin films deposited at different concentrations of 0 mM and 14 mM.

INV-03

Nanomaterials for Gas Sensor cum Environmental Monitoring

Dr. P. Kathirvel

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ABSTRACT

Rapid increase in environmental risks due to the fast industrialization along with the modern technological comforts is becoming a growing threat to our everyday life. Similarly, improper usage of pesticides in the agricultural sector as well as accidental industrial/domestic leakages of various toxic chemicals and gases may also result in a number of health hazards. Moreover, if the hazard materials are in gas form, the need of a proper sensing devices for an early detection and proper precaution are even more crucial as many of the toxic gases are either not detectable by our human sense organs or detected only after a significant harm is already caused. Hence, gas sensors are becoming an integrated part of our daily life as preventive tools such as fire alarm/smoke detector, LPG/CNG leak detectors, H_2, etc.

Even there are several reports on various gas sensors based on metal oxide nanostructures, but many of them are either having limited selectivity (ethanol, NO2, H2S) or the sensitivity of them is not up to the accepted level for various safety issues. Hence, superior quality gas sensors with wider selectivity (LPG, CH4, CO) are still a global technological challenge. Moreover, the response and recovery time as well as sensitivity and reproducibility of a gas sensor need a rigorous optimization process to reach the accepted level.

Therefore, the proposed work will have a great opportunity for further improvement of the existing sensor materials for device applications.

It has been observed that Metal oxide based nanostructures are grown either (majority) using the chemical roots or (few) through the physical pathway. However, in both cases vacancy/impurities can play a very crucial role on defect induced band bending of the surface charge states of Metal oxide which further reflects the surface conductivity of the oxide materials. Therefore, chemical purity and crystal stoichiometry of Metal oxide can be the most deciding factors to tailor the surface electronic property and hence sensor performance. However, the chemical growth scheme is more prone to the unintentional contaminations as compared to vacuum assisted physical growth roots. In addition, precise control over the film thickness is somehow more challenging in the case of chemical growth approach as compared to the growth via physical roots.

On the other hand, controlled doping with wide varieties of dopants for oxide materials are more challenging in physical growth process and mostly limited within the chemical methods. Therefore a comparative study between the physical and the chemical growth mechanism of Metal oxide nanostructures and desired modification of electronic properties using controlled doping will be of real time technological demand. for a better understanding of the optimization process of the gas sensor performance.

INV-04

Role of non-thermal plasma in biomedical applications

Dr. K. Navaneetha Pandiyaraj*

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Abstract

A substantial part of current research on biomaterials is focused on the design and preparation of blood contacting devices with perfect bio-compatibility. Currently, most common approaches to increase the blood and cell compatibility of the polymeric materials are by solvent and co-solvent composition of the coating fluid, the use of corona pre-treatment or low-pressure plasma technology. The conventional modification techniques could not be able to produce the products on industrial scale and requires huge amount of chemicals for processing, which affects the overall performance of the materials.

However, in the era of sustainable development, most of these techniques have several drawbacks such as cost, safety, energy consumption and/or environmental concerns. This talk focuses specifically on ecofriendly nonthermal plasma technology which is well recognized surface tailoring methods and has demonstrated to be successful for different application related to biomedical applications.

INV-05

Mesocrystals: New materials design for different applications

Dr.Rajaboopathi Mani

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Abstract

The classical and non-classical crystallization will be discussed. The mesocrystal comes under non-classical crystallization, which is formed by spatially separated, self-assembled and crystallographically oriented nanoparticles [1]. The internal structural features of mesocrystals have different advantage and thus the mesocrystals materials design strategy can be utilized to enhance the properties of different functional materials [2]. The application of mesocrystals as electrodes for batteries, photocatalyst, in concrete materials and in drug development will be discussed.

Reference

1. Marie Jehannin, Ashit Rao, and Helmut Cölfen, J. Am. Chem. Soc. 2019, 141, 10120 –10136.

2. Lei Zhou and Paul O'Brien, J. Phys. Chem. Lett. 2012, 3, 620 – 628.

Acknowledgement

The research project is funded by European Union (H2020-MSCA-IF-2018) under Marie Skłodowska-Curie Individual Fellowship, Grant Number: 842140.

INV-06

Current Technological Understanding of Potential Materials Design for Li-Ion Batteries

Dr. R. Muruganantham

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Abstract

Electrochemical energy storage devices are crucial role of increasing importance of sustainability and environmental anxieties. Rechargeable batteries serve as a variety of electrical energy storage applications such as portable electronic devices to electric and hybrid electric vehicles. Li-ion batteries have great predictable choice as the power storage device for transport-sector and large-scale smart grids storage applications. Hence, the significant research exertions are keen to perceiving materials that offer higher capacity, higher energy density, longer cycle life, facile synthesis, cost - effective, and / or better safety compared to those of the conventional intercalation-type electrodes such as lithium cobalt oxide and graphite. The progress of high-capacity electrode materials in commercial applications is challenging and affects several factors.

This talk highlights the selection of energy efficient electrode materials, construction of electrode for batteries, fabrication of Li-ion coin cell and current developments scenario of batteries in large-scale applications.

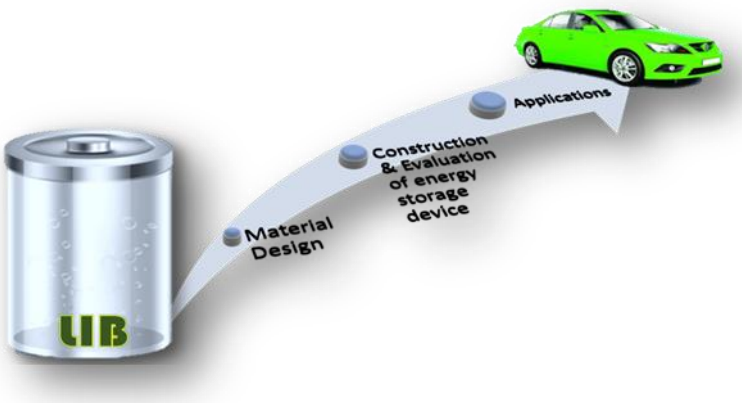

Figure. Shows a schematic represents of this report in Li-ion energy storage device.

INV-07

Materials for Non-Volatile Memory Application and Probing Fundamental Electron Transport Mechanism

Mr.Chandrasekar Sivakumar

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Abstract

One of the promising non-volatile memories of the next generation is Resistive Random-Access Memory (ReRAM). It has vast benefits in comparison to other non-volatile memories (e.g. DRAM, PCRAM, CBRAM, etc.). After the first resistive switching phenomenon observed by Hickmott in 1962, the Resistive Random Access Memory (ReRAM) has attracted a wide attention from the researchers and scientist for the next generation high density nonvolatile memory [1]. The ReRAM usually consists of simple Metal-Insulator-Metal structure (MIM) and the resistive switching refers to changes in the resistance of an insulating layer, such as a metal oxide substrate with two metal electrodes under a strong electric field and this phenomenon has attracted considerable interest for applications in electronic devices and semiconductor industries [2-3]. In 2013, owing to the reduced cost per bit and easy to incorporate chips as 3D crossbar provisions ReRAM memory technology was accounted by International Technology Road Map For Semiconductors (ITRS).

Owing, to their sub-ns operation speed (< 10 ns), lower power consumption (<0.1 pJ), long retention time (< 10 years), high endurance cycle (>1012 cycles), excellent miniaturization potential down to <10 nm and compatibility to the existing CMOS technology for integration with current solid state devices make them potential candidate for future semiconductor applications [4-7].

The resistive switching behaviour was observed in much class of materials such as binary metal oxides (SiO_x, NiO_x, TiO_x, GaO_x and ZnO_x, etc.,), Perovskites and organic compounds and it works with the variation of

resistivity with low and high current states with respect to the applied electric field. In this talk, I will focus on resistive switching of NiO_x synthesised by hydrothermal method and β-Ga_2O_3 nanowires grown by VLS (CVD) method. In addition to this, will share some of research works to probe the origin of resistive switching in TiO_2 material via Molecular dynamics simulation [8-10].

Keywords: Resistive switching, Transition Metal Oxide, Molecular dynamics

References

1. Hickmott T W, Low frequency negative resistance switching in thin anodic oxide film *J. Appl. Phys.* 1962 33 2669-2682
2. Chen Y L, Balraj B, Chung P F, Sivakumar C, Lee W J, Ho M S, Impact of Lattice Plan Orientation in TiO2 based Resistive Switching Memory: A Computational Approach, *Appl. Phs. Lett.* 2021 118 083202
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10. Bharathi M, Balraj B, Sivakumar S, Wang Z, Shuai J, Ho M S, Guo D, Effect of Ag doping on bipolar switching operation in molybdenum trioxide (MoO3) nanostructures for non-volatile memory, *J. Alloys Compd.* 2021 862 158035

ORAL POSTER CONTRIBUTIONS

OP-01

Green and Chemical Routes for the Synthesis of Vanadium Pentoxide Nanostructures: Energy Storage Applications

V. Divya , K. Shireesha , V. Shireesha , CH. Shilpa Chakra *

Center for Nano Science and Technology, Institute of Science and Technology, JNTU Hyderabad, India-500085

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Abstract

Metal oxides play an important role in energy storage devices, while vanadium pentoxide is most promising due to variable oxidation states, wide potential window, unique layer structure etc. In general, specific capacitance of a vanadium pentoxide is very low due to poor ionic diffusivity and electrical conductivity but can improve drastically by encapsulating vanadium pentoxide with metals or carbonaceous materials or by decreasing the size to nanoscale or by modifying the morphology. On the other hand, the methodologies employed play a crucial role in increasing specific capacitance of a particular compound. Here we report a microwave assisted synthesis of vanadium pentoxide nanoparticles by green and chemical synthetic approach.

The prepared samples were characterized by various spectroscopic, microscopic and electrochemical methods. The major peak in Uv-vis spectra confirms six-fold coordination state of V+5 with square pyramidal configuration.

FTIR and XRD analysis concludes orthorhombic structure of synthesized nanoparticles with crystal size ranging from 20-25 nm.

The anions and cations of an electrolyte is also play a crucial role in determination of specific capacitance of a particular materials and is in the order of 2M KOH > 2 M LiOH > 2 M Na_2SO_4 > 2 M NaOH and are in accordance

with hydration sphere radius, solvated ion size, ion shape and conductivity of particular ion. On the other hand calcinations temperature and concentration of specific electrolyte play a crucial role in determination of specific capacitance of a particular materials and is as follows 6M KOH (600 °C) > 6M KOH (400 °C) > 2M KOH (600 °C) > 2M KOH (400 °C). The V_2O_5 -green modified electrode is showing excellent electrochemical performance than V2O5-chemical modified electrodes due to less agglomeration of oxide, high percentage of vanadium over the surface leads high intercalation and de-intercalation of K+ ions from electrolyte into V_2O_5 lattices.

OP-02

Synthesis and characterization of tin sulphide (SnS) over FTO substrates

Aaron Kevin Cameron Theoderaj[1], Kauviah. R[1] and M. Chitra[1*]

[1]Department of Physics, Anna University, Chennai- 600 025

[*]Corresponding author: chitrashadrach@annauniv.edu

Abstract

Eco-friendly tin sulphide (SnS) thin films are deposited on FTO (Fluorine doped tin oxide) glass substrate by chemical bath deposition (CBD) method. X-ray diffraction (XRD) analysis, Scanning Electron Microscope (SEM) images, Energy Dispersive X-ray (EDX) analysis and UV-Visible absorption spectrum are used to characterise the synthesised SnS films. The X-ray diffraction (XRD) analysis is used to study the structure and the crystalline size of the SnS tin films. XRD analysis confirmed that all the deposited films exhibited polycrystalline nature with a predominant plane (040). The surface morphology is studied using the Scanning Electron Microscopy (SEM). It revealed nano-flower morphology of the coated SnS. EDX compositional analysis revealed that thin film has a stoichiometric composition (Sn/S, 54.13/45.8) of ~SnS. The optical properties are studied using the UV-Visible absorption spectrum.

Keywords: Thin films, SnS, FTO glass, Chemical bath deposition, XRD, SEM, EDX, UV-Visible

OP-03

A thermodynamic approach to adsorption of methyl orange from aqueous solution using a low cost activated carbon prepared from waste biomass

Rimene Dhahri[1*], K Venkateshwarlu[2], Younes Moussaoui[3]

[1]Materials, Environment and Energy Laboratory (UR14ES26), Faculty of Sciences of Gafsa, University of Gafsa, Tunisia.

[2]Telangana University, Nizamabad, India

[3]Organic Chemistry Laboratory (LR17ES08), Faculty of Sciences of Sfax, University of Sfax, Tunisia.

Corresponding author E-mail: dhahririmene@gmail.com

Abstract

In this paper, thermodynamic parameters of the methyl orange adsorption process on active carbon was evaluated by using a batch system. Experiments were performed as a function of pH (2, 4, 6, 8 and 10), temperature (15 °C, 30 °C and 40 °C) and initial concentration (20, until 200 $mg.L^{-1}$). The obtained adsorbent was analyzed using FTIR (Fourier Transform Infrared Spectroscopy), SEM (Scanning Electron Microscope) and Brauner Emmet and Teller (BET) analyzer. The Langmuir and Freundlich isotherms were used to describe the adsorption equilibrium studies at different temperatures.

Langumir is otherm shows better fit than other is otherm in the temperature range studied. Maximum adsorption occurred at pH 2. Thermodynamic parameters like the change in enthalpy (ΔH_0), entropy (ΔS_0) and Gibbs free energy (ΔG_0) were evaluated and the adsorption process was found to be endothermic and spontaneous.

The results show that prickly pear seed cake biomass is an appropriate precursor for the preparation of adsorbent which has specific affinity for removal of Methyl Orange from aqueous solutions.

Keywords: Prickly pear seed cake, Activated carbon, Adsorption, Methyl Orange.

POSTER CONTRIBUTIONS

PP-01

Facile Synthesis of Mesoporous Rare-Earth Metal Oxide (Gd_xO_y) Electrodes for Electrochemical Capacitors

I. Manohara Babu[1]

[1]Advanced Energy Materials Laboratory (AEML), Korea Institute of Energy Research, Daejeon, Republic of Korea

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Abstract

Rapid utilization of renewable energy sources has urged the research community to fabricate a novel energy storage device without any issue to environment. Of course, electrochemical capacitors (ECs) have ruled the energy domain for the past few decades on account of their salient features like ultra-fast rate characteristics, excellent cycle life, exceptional energy and power density.

In this perspective, we have devised to engineer an electrode using rare-earth element (Gadolinium oxide) via one-pot hydrothermal approach by the aid of anionic surfactant. The as-synthesized electrode shows good electrochemical characteristics (redox behaviour) with cyclic stability (low degradation) and this could be attributed to the presence of mesoporous rod like morphology.

This facile architecture provides plenty of directions for the electrolyte ions during the electrochemical reaction that results in notable electrochemical performance. The highlights of the present study has opened new way for electrodes in EC world.

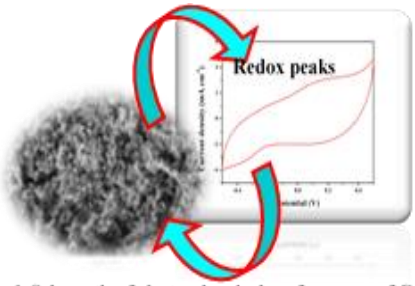

Figure 1. Schematic of electrochemical performance of Gd_xO_y

Reference

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PP-02

Oxadiazole Based Dyes as Photosensitizers for Dye- Sensitized Solar Cells- A Density Functional Theory Study

Shipra Bhati[1]

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Abstract:

Global energy demand is expected to more than double by 2050 due to the growth in population, industrial growth, and economies. Renewable energy resources have much higher potential than the current global energy demand. Solar energy conversion approaches are considered potentially the leading way to resolve the world energy crisis. The present research work focuses on the design and study of geometry and electronic structure of oxadiazole-based dye-sensitized solar cells (DSSCs) using density functional theory. A series of D-π-A oxadiazole-based organic dyes possessing electron-rich fragments were designed and simulated using DFT/TD-DFT. The electronic properties, absorption spectra, and light harvesting efficiency (LHE) were theoretically studied.

The HOMO-LUMO energy gaps of the designed oxadiazole photosensitizers indicated that the dyes are capable of injecting electrons into the conduction bands of TiO_2. The dye (2)/ TiO_2 system showed the highest red shift value in the series. The free energy of electron transition (ΔG^{inject}) for systems 1 to 6 were found to be negative and thus favoring electron injection. The results indicate that system 2 with 1,3,4-oxadiazole has the highest incident photon to conversion efficiency (IPCE) and is expected to be a promising photosensitizer in the DSSC field.

Keywords: Renewable energy, dye-sensitized solar cells, oxadiazole, density function theory.

PP-03

Facile Route to Obtain novel Dy/TiO_2 mesoporous nanoparticles modified by salicylic acidas efficient photocatalysts with high specific surface

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Abstract

The development of active semiconductor photo catalysts with desirable material properties and efficient carrier transformation is indispensable for better photo catalyst utilization and performance optimization. Here, we demonstrate the synthesis of novel mesoporous salicylic acid/Dy-TiO_2nanoparticles through a modified sol–gelfollowed by impregnation method for enhancement of the photocatalytic properties under visible light irradiation.Contrary to the usual practice using saturated solution of (water/ SA) the SA complexing/sensitizing molecules were mixed directly into suspension ofhexane (nonpolar solvent) containing Dy-TiO_2 powders.

The crystallography and grain size have been studied using XRD and TEM Analysis. The development of the anatase phase TiO_2 is affirmed by XRD and FT-IR.With the doping of Dysprosium ion, the grain size increases.

UV–Visible Spectra reveals the optical properties and the optical band gap calculated using Kubelka- Munk plot wasfound to be 3.12 eV for TiO_2 and 2.95 eV for Dy-TiO_2abruptly decreased to 2.26 eV and 2.24 eV for TiO_2/SA and Dy-TiO_2/SA, respectivelydue to formation of defect states and atomic structural disordering.The surface modification of Dy-TiO_2 powders with salicylic acid induced significant shift of absorption to the visible spectral region due to charge transfer complex formation.

PP-04

Highly selective and sensitive detection of Cu^{2+} by colorimetric method using organic probe

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Abstract

A new synthesized organic compound, selectively detect Cu^{2+} ion. It is one of the most important transition metal for humans, excess of copper ion can act as environmental pollutants and an essential trace element in various biological systems. Cu^{2+} shows high selectivity organic probe gives rise to a great red-shift during the study of the photophysical properties. The synthesized organic compound (Probe) comfirmed by the H^1 and C^{13} NMR spectroscopy. The selective detection can be declared by absorption, colorimetric and test trip method.

Keywords: Cu^{2+}, colorimetric, test trip, and organic compound.

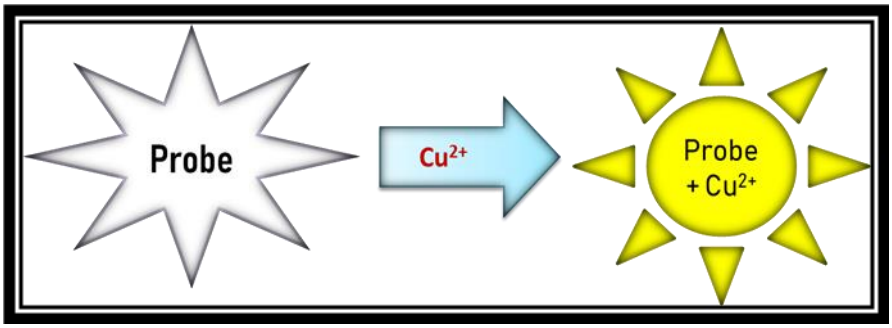

Figure:1

PP-05

A fluorescent probe of 3-acetylcoumarin fluorophore for detection of opd and opp

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Abstract

A chromogenic and fluorogenic active coumarin based chemodosimeter (DP21) has been synthesised. It promotes absorption and emission at 335, 425 and 475 nm respectively.

In the presence of phenylenediamineisomers such as ortho-phenylenediamine and para-phenylenediamine showed a red shift. The color of the probe solution changed from light yellow to reddish brown and dark yellow by naked eye. The fluorescence microscopy experiments divulge that probe DP21 may be used in the detection of PDA isomers in the henna products of cosmetics.

Keywords: Skin cancer, Cosmetics, Phenylenediamine, Fluorimetric, Colorimetric, Sensors.

PP-06

Optical investigation of NaO_2 loaded phosphovanadate glass system

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Abstract

Sodium superoxide loaded phosphovanadate based glass systems were prepared from a mixture of vanadium pentoxide (V_2O_5), phosphorus pentoxide (P_2O_5) boric acid (H_3BO_3) and sodium superoxide (NaO_2) using a melt-quenching method. Amorphous phase of as-prepared glass system confirmed using X-Ray Diffraction technique. Surface morphology of glass system studied using scanning electron microscope. Ultraviolet-visible spectroscopy was employed to extract complex optical parameters like direct and indirect optical band gap, Urbach energy, refractive index, complex dielectric constant and optical conductivity.

This primary report on sodium superoxide loaded phosphovanadate based glass systems opens wide avenue for battery and super-capacitor applications.

PP-07

Co-precipitation Synthesis and Characterization of Sn doped α-Fe_2O_3 nanoparticles with enhanced Photo catalytic activities

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Abstract

In this study, Sn-doped hematite (α-Fe_2O_3) nanoparticles with various dopant concentrations ranging from 3 to 12 mol% were prepared successfully using a simple co-precipitation technique. The effects of Sn doping on the structural, morphological, optical, and magnetic properties were determined using X-ray diffraction (XRD), Raman spectroscopy, transmission electron microscopy (TEM), UV-visible diffuse reflectance spectroscopy, and a superconducting quantum interference device. XRD analysis showed that all of the samples had a typical hematite-type hexagonal structure of Fe_2O_3 without any additional peaks due to Spurious phases. The cell parameters *a* and *c* decreased monotonically as the Sn content increased, thereby indicating that Sn ions were substituted into the α-Fe_2O_3 lattice.

These results and the TEM analyses showed that the size of the nanoparticles decreased to 10 nm as the Sn doping concentration increased. UV-visible absorption measurements showed that the decrease in particle size was accompanied by a decrease in the band gap value from 2.07 eV for α-Fe_2O_3 to 1.87 eV with 12 mol% Sn doping.

Furthermore, the magnetic properties demonstrated that all of the samples exhibited ferromagnetic behavior at room temperature. The photocatalytic activities of the samples were studied based on the degradation

of methylene blue as a model compound, where the results showed that an appropriate amount of Sn dopant could greatly increase the amount of hydroxyl radicals generated by α-Fe2O3 nanoparticles, which were responsible for the obvious increase in the photocatalytic activity.

Keywords*:* Co-precipitation, Hematite (α-Fe_2O_3), Nanoparticle, Photocatalysis, Sn-doped α- Fe_2O_3.

PP-08

Studies of additive properties of some simple heterocyclic Drugs in different solvent by Ultrasonic studies

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Abstract

Ultrasonic velocity and density measurements of 3-phenyl-1-(3'-Aminophenyl) prop-2-en-1-one substituted in methanol and Benzene have been carried out at 303K in the concentration range in 0-100% ethanol. Different acoustic properties like apparent molal volume, apparent molal compressibility, intermolecular free length, specific acoustic impedance and relative association have been determined. The results of the present study suggest the presence of molecular interactions in Methanol and Benzene mixtures.

These parameters have been interpreted in terms of solute-solvent and solute-solute interactions, which provide important and valuable information regarding internal structure, molecular association, complex formation and stability of complexes.

The effect of different substituents in this solvent i.e. Methanol+Benzene and effect of dilution on **3-phenyl-1-(3'-Aminophenyl) prop-2-en-1-one** were investigated.

Keywords: Ultrasonic velocity, acoustic parameters, interferometric measurements, solute-solvent interaction.

PP-09

Synthesis and acoustical studies of some chalcones in different solvents at 305.15K

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Abstract

Some new chalcones have been synthesized and their characterization was done by IR, ^{1}H NMR, and mass spectral data. Ultrasonic velocities of various solutions of different concentrations of these synthesized compounds in DMF, THF and $CHCl_3$ have been measured at 308.15 K by using single crystal interferometer at a frequency of 2MHz. The density and viscosity have also been measured by pycnometer and Ubbelohde viscometer. Using these experimental data, variation of adiabatic compressibility (β), acoustic impedance (Z) and relaxation time (□) with concentration and temperature have been studied.

Acoustical parameters provide important information in understanding the solute-solvent interaction for reported compounds in DMF, THF and $CHCl_3$. Which are interpreted in terms of solute-solute and solute-solvent interactions in different solutions.

Keywords: Chalcone, Ultrasonic velocities, Density, Viscosity, DMF, THF, $CHCl_3$.

PP-10

Synthesis and charterisation of Eu^{3+} activated Calcium Tungstate Phosphor

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Abstract

In this research paper we report the synthesis of $CaWO_4$ pure and doped by different concentrations of Eu^{3+} by using advanced solid state reaction method. The samples were characterized by X-ray diffraction (XRD), scanning electron microcopy (SEM) and photoluminescence analysis. The crystal structure and luminescence properties were investigated by X- ray diffraction patterns, photoluminescence excitation and emission spectra. The results indicate that CaWO4:xEu^{3+} phosphors can be excited by ultraviolet wavelengths 254 nm and a strong orange red emission located at 611, 616 nm ($^5D_0$-$^7F_2$) corresponding to the characteristic emission of Eu^{3+} ions was observed in all the samples. Scanning electron microcopy (SEM) images revealed that the replacement of Ca^{2+} by Eu^{3+} ions changed the particles' shapes, resulting in different morphologies of the micro crystals.

The $CaWO_4$:Eu^{3+}phosphor shows great potential for applications in white light-emitting diodes and field-emission displays as an excellent red-emitting phosphor.

Keywords: Photoluminescence, Rare Earth ions, X-ray diffraction, Solid State Reaction.

PP-11

Dyeremoval from aqueous solution using Adsorbent derived from Tinospora Cordifolia

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Abstract

Water pollution cause by dyes has become the major issue for plant and human being.In the present study eco-friendly, highly efficient, low cost adsorbents has been derived from locally available plant Tinospora cordifolia. The efficiency of prepared adsorbent was investigated for adsorption of Victoriablue (VB) and RhodamineB (RhB) dyes from aqueous solution at different time, with different dose of adsorbent etc. Adsorptive removal for VB and RhB dyes was observed 76% and 56% respectively after10 min.

PP-12

Excellent spinal $LiMn_2O_4$ Cathode materials for lithium-ion batteries

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Abstract

Lithium Manganese ($LiMn_2O_4$) spinal is a most promising cathode material for lithium-ion batteries. The spinal $LiMn_2O_4$ with uniform morphology, high crystallinity, increasing batteries performance and discharge capacity for a very long time. The discovery of nanostructured electrode materials is the topmost attractive approach to improved battery performance such as capacity, cycling life and rate capability.

$LiMn_2O_4$ synthesised by using sol-gel technique. The cubic structures of a single phase of $LiMn_2O_4$ are confirms X-ray diffraction (XRD spectrum investigation), and also structural morphology investigated by scanning electron microscope [SEM]. FT-IR and Raman spectroscopy is used to analyse the molecular structure of a compound.

Thermal analysis, thermogravimetric analysis and differential thermal analysis (TGA/DTA) measuring carried out for the $LiMn_2O_4$ samples.

Keywords: Sol-gel technique, Batteries.

PP-13

Antibacterial Activities : Synthesis And Characterization

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Abstract

The development of environmental friendly prototypes for antibacterial agents and an alternative to antibiotics is a necessary step towards the control of infections. With this in mind, the production of composites based natural and synthetic materials have been successfully explored. These composites are characterized by biological and physical methods, viz., FTIR, XRD, UV-Vis, PL, SEM. XRD spectrum confirmed the existing nature of semi crystalline peaks. Further, the existence of high dislocation density in the phthalic acid provides clear evidence to the antibacterial activities while compared to other acid doped polyaniline. The angular intensity profile is used to estimate the % of crystallinity of the polymer system.

SEM studies reveal a new aspect of morphological growth and demonstrate rock-like structure which was derived from the aggregation of small granules. Band gap energies (using UV visible spectrum) for the Phthalic, Calotropis and Oxalic acid, doped PANIs were calculated as 2.1, 2.72 and 2.82eV respectively. Antibacterial analysis exhibits better results for the Calotropis doped Polyaniline compared with phthalic acid and oxalic acid.

Keywords: Polyaniline; Calotropis; Antibacterial activity.

PP-14

MoO3 Nanoparticles / Manganese - Doped Graphene Hybrid Composite For Electrochemical Application

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Abstract

MoO3, MoO3/GO and MoO3/GO/Mn composites have been prepared by hydrothermal technique. The samples are characterized by various performances such as structural, morphological, elemental, surface area analysis. XRD data reveals that the MoO3 nanoparticles showed orthorhombic crystal structures and their miller indices are in good agreement with the standard values (0 2 0), (1 1 0), (0 4 0), (0 2 1) crystalline planes of MoO3. The crystalline nature of the nanocomposite enhanced with the increase in annealing temperature.

SEM images show the formation of stacked Graphene Oxide (GO), and spherical nano-crystallites are observed. The presence of the molybdenum (Mo), oxygen (O) and manganese (Mn) are confirmed from the EDS spectrum. Electrochemical analysis reveals the capacitance behavior for MoO3/rGO/Mn nanocomposite. BET reveals the specific surface area, pore volume, and pore size values are 85.81 m2/g, 0.2475cm3/g, and 11.75nm for the optimized samples.

Keywords: Hydrothermal method; Molybdenum oxide; Manganese; Graphene

PP-15

Highly efficient and selective detection of Alanine by organic fluorophore

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Abstract:

Imine based sensor for the detection of alanine have been synthesized and characterized. It shows remarkable fluorescent intensity towards alanine through ICT mechanism. Alanine involved physiological functions like energy storing and protein synthesis in human body. The abnormal level (>5.5mg) of alanine leads to liver disease and jaundice. Hence, the probe applied for the alanine detection using colorimetric and fluorimetric experimental techniques at neutral pH. Selectively detect the analyte by probe in the presence of interfering other biomolecules such as, leucine, asparagine, urea, creatinine, ascorbic acid, cysteine, tryptophan, alanine, glutamine and albumin. In which, the real sample analysis were performed for alanine by the probe.

PP-16

Clitoria ternatea Nanoparticles: Synthesis, Characterization, and Pharmacological Study

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Abstract

The aim of the present study was to develop a method for the preparation of gold nanoparticles of *Clitoria ternatea* flower with a view to improve its aqueous-phase solubility and examine the effect on its Pharmacological properties. Transmission electron microscopy (TEM) revealed the formation of monodispersed spherical shape with a mean diameter of 18 ±2 nm. The CTF-AuNPs synthesized through this biological approach were relatively stable up to 4 months after synthesis.

A minimum inhibitory concentration of CTF-AuNPs was determined for a variety of bacterial and fungal strains and was compared to that of *Clitoria ternatea* flower.

It was found that the aqueous dispersion of nanocurcumin was much more effective than *Clitoria ternatea* flower extract against Staphylococcus aureus, Bacillus subtilis, Escherichia coli and Pseudomonas aeruginosa, The results demonstrated that the water solubility and antimicrobial activity of *Clitoria ternatea* flower markedly improved by particle size reduction up to the nano range. For the selected microorganisms, the activity of nanocurcumin was more pronounced against Gram-positive bacteria than Gram-negative bacteria.

The mechanism of antibacterial action of *Clitoria ternatea* nanoparticles was investigated by transmission electron micrograph (TEM) analysis, which revealed that these particles entered inside the bacterial cell by completely breaking the cell wall, leading to cell death.

Keywords: Clitoria ternatea, Gold nanoparticles, antimicrobial, antioxidant, anti-inflammatory activity.

PP-17

Growth, spectral and thermal properties of inorganic material – tetraethyl ammonium tetrabromonickelate complex $[N(C_2H_5)_4]$ $NiBr_4$

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Abstract:

Studies at high pressures and temperatures are helpful for understanding the physical properties of the solid state, including such classes of materials as, metals, semiconductors, superconductors, or minerals. Resources in good crystalline form are needed in modern technologies using semiconductors, magnetic garnets and ultraviolet and infrared solid-state lasers. Numerous surveys have been then done with respect to their magnetic properties and magnetic phase transitions both experimentally and theoretically. Attributable to their fascinating physical properties like ferro elastic, ferroelectric and commensurate – incommensurate phases at low temperatures, the importance of this type of complex (A=univalent cation, $NH_4^{(+)}$ and its alkyl derivatives; B= divalent transition metal cation and X=halogen) has been lingering more attention in recent years.

The TEATBr-Ni complex type ABX_4 was grown by a slow evaporation process at room temperature.

Tetraethyl ammonium tribromo nickelate compound was prepared by mixing tetraethyl ammonium bromide and Nickel bromide in 1:1 molar ratio respectively using triple distilled water.

The synthesised complex is characterised by an elementary analysis, powder X-ray diffraction, thermogravimetric and differential thermal analysis. The synthesised complex is analysed by FTIR (The absorption at 3171.92 cm^{-1},

a broad envelop represents O-H frequency due to moisture in the compound). proton and carbon-13 NMR spectrally. Elemental analysis data obtained for the complex confirm the molecular formulae $[N(C_2H_5)_4]$ $NiBr_4$. The IR spectrum of the complex confirms the presence of methyl and methylene groups in the complex. The IR spectra also confirm the presence of C-C and C-N bonds. The NMR spectra suggest the presence of N-ethyl group in the complex. TG-DTG thermogram indicates that the final decomposition of the complex starts from 827°C to form the end product. The spectral studies may be helpful to design new metal complexes with technical applications.

PP-18

Synthesis of flower-like Molybdenum disulfide nanoparticles by simple hydrothermal method

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Abstract

In this work, the nanostructured Molybdenum disulfide (MoS_2) nanoparticles were successfully synthesized for various temperatures like 140, 160, 180 and 200 ^oC by facile hydrothermal method. The prepared nanoparticles have been studied systematically by the various advanced techniques such as X-Ray diffraction (XRD), Fourier Transform Infrared Spectra (FTIR), and Scanning Electron Microscopy (SEM). The structural analysis of the prepared nanoparticles was observed from XRD Spectrum.

From FTIR, the functional groups of the synthesized nanoparticles have been studied. The surface morphology of the prepared nanoparticles was captured through SEM.

Keywords: Molybdenum disulfide; Hydrothermal method, Flower-like, XRD.

PP-19

Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis of 0D antimony single crystals

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Abstract:

The title compound $[C_3H_5N_2S]SbCl_4$ prepared by the reaction of 2-aminothiazole with antimony (III) oxide in ethanol and HCl, was crystallized the triclinic symmetry with P ī space group (Z = 2).

The revision of intermolecular interactions using Hirshfeld surface analysis established that the most important role in the stability of crystal structure was provided by hydrogen bonding interactions. The vibrational spectrum measured at room temperature by FT-IR and Raman spectroscopy shows the presence of organic and inorganic cations.

The number of ^{13}C is in full agreement with the crystallographic data. The optical properties of the compound were investigated in the solid-state at room temperature

Keywords: $[C_3H_5N_2S]SbCl_4$, X-ray single crystal diffraction, hydrogen bonds, vibrational spectrum, optical properties.

PP-20

Fabrication and Electrical Characterization of CdTe Screen-Printed Thick Films for Photovoltaic Applications

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Abstract

The II-VI semiconductors are of great importance due to their applications in optoelectronics, solar cells, integrated optics and electro-optic devices. Cadmium telluride is a suitable material for the fabrication of photovoltaic devices. We have prepared cadmium telluride films in air atmosphere by screen-printing method and studied their applications in photovoltaic devices. The energy band gap of these films was found to be 1.76 eV by absorption spectra in wavelength range 675-875 nm. The X-ray analysis of these films confirms the polycrystalline nature of prepared films having wurtzite (hexagonal) structure. The Schottky junction of cadmium telluride using silver was made and the photosensitivity and photoresponsitivity of it were determined by using current-voltage characteristics. The DC conductivity and activation energy of films were also measured in vacuum by two-probe technique. Screen-printing followed by sintering is a very simple and viable technique compared to other costly methods.

It is less time consuming, less pollutant and ensures maximum material utility and offers a suitable method for preparing films on large area substrates.

Keywords: CdTe; Sintering; Screen printing; Conductivity.

PP-21

TiO_2 thin films: Impact of substrate temperature on structural and morphological properties

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Abstract:

Smooth and white spherical shaped TiO_2 thin films are effectively deposited by Nebulizer Spray Pyrolysis (NSP) technique. The prepared films are characterized by DRS, PL, XRD, SEM and I-V analysis. The expansion and contraction of Ti-O bonds leads to a high crystalline nature with its purity at 289 nm. The absorbance increases with substrate temperature due to the decrease of film thickness, packing density and shrinkage of spray droplets. Anatase phase polycrystalline tetragonal structure with preferred orientation along (1 0 1) direction obtained from XRD.

TiO_2 thin films indicate that the film is made up of small granules having slab like particles with some voids at lower temperature.

The tiny particles are combined together to form white spherical shaped flower particles with pinholes at 450°C. A room temperature resistivity of the film deposited at 400°C is found to be in the order of 10^5 Ω/cm, which decreases to 10^3 Ω/cm for the films prepared at 450°C.

Keywords: TiO_2; Anatase; Tetragonal, DRS, NSP

PP-22

SrO nanoparticles: Impact of annealing temperature on the properties

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Abstract:

Strontium oxide (SrO) nanoparticles are prepared by chemical precipitation method. The SrO nanoparticles are characterized by UV-DRS, XRD and I-V characteristics. Strontium oxide nanoparticles would allow more light for absorption in UV region due to its rough surface while the same would allow moderate light absorption in visible region due to its high packing density. The expansion and contraction of Sr-O bonds leads to a high crystalline nature with its purity at 322 nm. It is proposed that strain and surface defects in SrO nanocrystal take place due to different absorption edge.

X-ray diffraction peaks reveal the single-phase polycrystalline tetragonal structure with dominant orientation along (2 0 2) direction.

Influence of annealing temperature strongly induce the growth of peak which indicates the increased intensity of (202) peak.

The heat treatment strongly distresses the growth of triplet peaks (002), (101) and (110) whereas the same augment the growth of (202) and (310).

Keywords: SrO; Tetragonal structure; XRD, DRS

PP-23

Srtuctural,Photocatalytic and Anticancer properties of Polyaniline/Vanadium pentoxide (V_2O_5) nanocomposites

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Abstract

In this present work, Polyaniline/ V_2O_5 nanocomposites were developed with different V_2O_5 loadings (20%, 40%, 60% and 80%) through in situ chemical polymerization method.

In order to study the impact of V_2O_5 on the photo catalytic properties of the prepared composite samples were characterized by Fourier infrared spectroscopy (FT-IR), X-ray Diffraction (XRD), Photo Luminescence (PL) Photocatalytic properties, Anticancer activity and UV-Vis spectrum. The FT-IR spectrum confirms the presence of functional groups in the composite structure. The intensity of polyaniline is found to increase with increasing metal oxide ratio.

The promotions of electrons from ground state to excited state of composites were confirmed by UV - Vis studies. Photocatalytic and Anticancer activity analysis exhibits a better result for the composites.

Keywords:PANI/V_2O_5**,**Nanocomposites, Transition metal oxide, Structural, Photo-catalytic property, Anticancer activity.