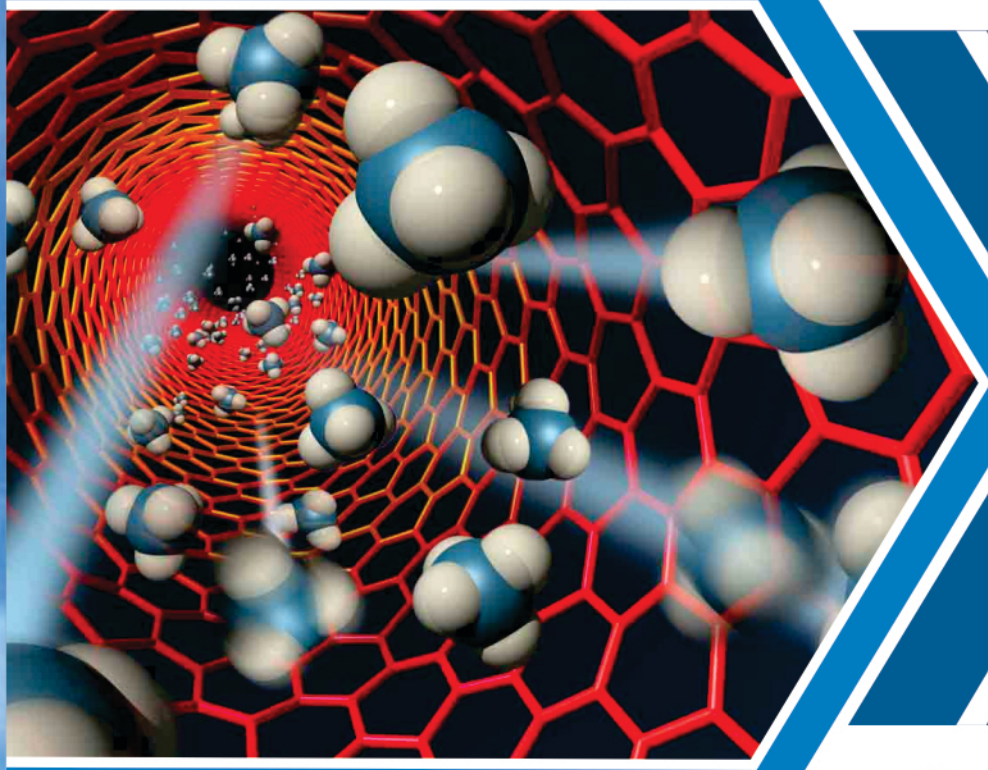
In celebration of the Golden Jubilee year

National Conference on

SEMICONDUCTORS, SURFACES, ALLOYS MODELING AND PREPARATIONS (SSAMAP - 2019)

6th December, 2019



SSAMAP - 2019

SOUVENIR

Editors

Dr. N. SOUNDARAM

Dr. R. MOHAN

Dr. J. YUVALOSHINI

Organized by

PG & Research Department of Physics

SREE SEVUGAN ANNAMALAI COLLEGE

(Accredited With 'B' Grade by NAAC & Affiliated to Alagappa University)

(Estd. 1970)

DEVAKOTTAI – 630 303, TAMIL NADU.

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PG & RESEARCH DEPARTMENT OF PHYSICS

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(Affiliated to Alagappa University, Karaikudi)

Devakottai - 630 303

Sivagangai District, Tamil Nadu

Preface

Materials play a major role in understanding our nature. Social and economic developments depend to a large extent on materials. Development of new and advanced materials and material processes are also critical to a nation's economy. New generation materials reshape our world and solve some of the planet's most pressing problems. Demand for new materials is constantly increasing due to the developments in technology and processes in the fields of Transportation, Bio-Engineering, Energy storage and conversion. Advanced materials offer exceptional properties enabling engineers to design novel and high quality products.

Nowadays, our society is facing challenges relating to energy, resources and environment. New materials should possess high performance, less manufacturing cost, less machining cost, less dependence on resource and energy and environmental friendly.

The National conference on Semiconductor, Surfaces, Alloys Modeling and preparation SSAMAP – 2019 covers all the major topics of advanced materials such as photonic materials, bio-sensors, superconductors, polymers, ferroelectric materials, semiconductors, catalytic-inorganic, composites, nano materials, thin films and non linear optical. This Souvenir book contains 75 abstracts of research submitted to the conference.

We wish to express our sincere thanks to our President, Vice-president, Secretary, Principal of Sree Sevugan Annamalai College, Devakottai. We would like to thank all key note, plenary, invited speakers and delegates for their contribution to this book. We also thank all the sponsors for their funding support. We would like to thank all committee members, students and volunteers involved in this editorial work.

Organizing Committee

(SSAMAP-2019)

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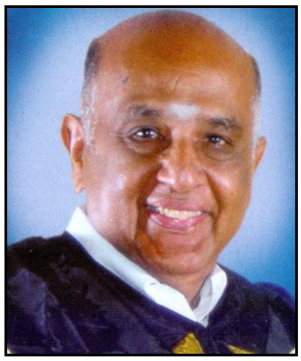
Personal : 04561 - 279066

Felicitation from the President's Desk



It gives me enormous joy to appreciate The Department of Physics for organizing A National Conference on Semiconductors, Surfaces, Alloys Modeling and Preparations (SSAMAP - 2019). I am happy that this conference will help many researchers in bringing out their innovative knowledge in concepts and concrete activities. I wholeheartedly congratulate the organizers for their strenuous efforts and wish all the stake holders a grand success of the event.

AN. LAKSHMANAN CHETTIAR
President

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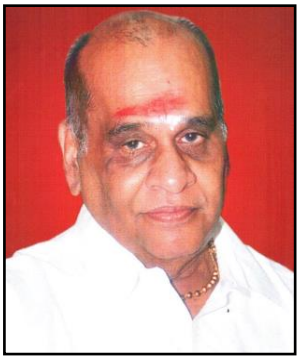
Felicitation from the Vice-President's Desk



In celebration of the Golden Jubilee year, it is a matter of rejoice to know the impressive academic performance of the Department of Physics in organizing A national conference - SSAMAP 2019. I am certain that SSAMAP will be a proof for the efficient teaching, training and learning processes that are mandatory in the field of Physics. I hope and pray that this will instill a strong sense of knowledge in the minds of faculties, research scholars and student fraternity.

I congratulate the sustained and the successful efforts of the organizers and the entire department in bringing out this Conference.

My Best Wishes!

A. S. Sevugan

A. S. SEVUGAN CHETTIAR
President

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Felicitation from the Secretary's Desk

I am delighted to appreciate the Department of Physics for successfully organizing the National conference SSAMAP 2019. The topic of the conference has so much practical values and the move at present is a reinforced focus towards the society-centric learning. The conference will certainly enchant the faculties, research scholars and the young students by providing many intellectual exercises.

I wholeheartedly congratulate the strenuous efforts of the organizers and the Department of Physics for organizing this conference with utmost perfection and precision.

All the Best!

A-S- Santhi

A. S. SANTHI ACHI
Secretary

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Felicitation from the Principal's Desk

Hearty Greetings to all!

I am immensely happy that the Department of Physics of our college is organizing a National Conference on Semiconductor, Surfaces, Alloys Modeling and preparation SSAMAP – 2019 on 06.12.2019. The Department of Physics continues the tradition of bringing together researchers, academics and scientist from all over India and Experts in physics since 2009. I strongly believe that this conference will enthuse the rural students and researchers and stand as a great source of knowledge.

I also congratulate the organizers for their effort in organizing this conference. May this conference be enriching, fruitful and memorable. I wish the conference all success.

Dr. S. CHINTHAMANI VASTHI RANI
Principal

SREE SEVUGAN ANNAMALAI COLLEGE
Devakottai - 630 303
Sivagangai District, Tamil Nadu

Mrs. R. MURUGESWARI
Convener

MESSAGE

The objective of this conference is to bring together eminent researchers from both academia and industry to discuss and share the latest research and developments in nanotechnology. I am sure that this conference would be a platform that will induce many young minds to do new things in almost every conceivable technological discipline.

I would like to express my heartfelt congratulations to my colleagues, research scholars and students, organizing this conference focusing on the two emerging areas of Materials Science. I hope all the distinguished invitees, delegates and scholars would feel benefited out of the academic deliberations in this one day and equally enjoy the visit and stay here. My best wishes for the success of the conference and hope this experience would be carried forward by all to enrich their scientific career.

(R. MURUGESWARI)

SREE SEVUGAN ANNAMALAI COLLEGE
Devakottai - 630 303
Sivagangai District, Tamil Nadu

Dr. N. SOUNDARAM
Organizing Secretary

MESSAGE

National conference on semiconductors, surfaces, alloys modeling and preparations (SSAMAP-2019) has been organized by the PG and Research Department of physics, S.S.A College, Devakottai on 6thDecember2019. It gives us immense pleasure to be a part of this significant event.

In the present scenario, Materials science is emerging as an excellent field of research attracting multi-disciplinary researches. The purpose of this conference is to bring together Scientists, Professors, Research scholars and Students who are interested in Materials science and Nanomaterials. Additionally, we are glad to inform that we have arranged 4 invited talks and more than 73 contributed research abstracts. We are glad that we have got full-fledged support from the Management and Principal who enabled us to organize this meet successfully. It is also obvious that this event would not have been possible without the support of all the participants who have promptly sent their papers and the Invited speakers who have readily consented to deliver the Inaugural, Valedictory and Special address besides Invited talks. I also would like to record the unstinted support from my Colleagues, Non-teaching staffs and students of the Department. Though we have taken extreme care in preparing the Souvenir, errors that might have gone unnoticed are regretted on our behalf. I take this opportunity to thank the Management and Alumni who have volunteered themselves to Co-sponsor this event. Finally, I wish the Delegates to have an enjoyable and memorable day at Devakottai.

(Dr. N. SOUNDARAM)

SREE SEVUGAN ANNAMALAI COLLEGE

Devakottai - 630 303
Sivagangai District, Tamil Nadu

Dr. R. MOHAN
Organizing Secretary

MESSAGE

We are very glad to present the souvenir of the *National Conference on Semiconductors, Surfaces, Alloys Modeling and Preparations* (SSAMAP – 2019) organized by the PG and Research Department of Physics, Sree Sevugan Annamalai College, Devakottai, Sivagangai held on 6th December 2019.

This conference brings together Patent officer**,** eminent scientists, researchers, academicians and research scholars from various colleges and universities who are actively involved in research in the areas of materials science. In total, 4 invited lectures, 73 contributed papers (30 oral presentations and 43 posters) are to be presented in this conference.

I would like to take this opportunity to thank our beloved President, Vice-President Secretary, Principal, Coordinator of our Department, Advisory committee members, Colleagues and Students who have given constant encouragement and invaluable support to organize this conference. It is a great pleasure to place on record my thanks to the management and alumni for the financial and technical supports, respectively. Finally, I thank all the participants who have submitted their research findings in time to bring this souvenir successfully.

My best wishes to all distinguished dignitaries and participants for fruitful deliberations during the conference.

(R. MOHAN)

Alagappa University
Karaikudi-630 003

Dr.G. RAVI, M.Sc., M.Phil., Ph.D., PDF (Japan), D.Sc.

Professor & Head
Department of Physics

MESSAGE

I am very much delightful to welcome you to the "**National Conference on Semiconductors, Surfaces, Alloys Modeling and Preparations (SSAMAP-2019)**" organized by Department of Physics on 6th December, 2019. Materials are fundamental for humans and their importance is such that the key stages of our civilization have been named after them, each new stage being brought about by a new material that revolutionized existing technologies. The objective of this conference is to provide a great opportunity for researchers and scientists to review recent trends and developments in the field of Materials Science, Energy and Sensors. This wonderful meet is to bring together people from academic, industry, and government organizations. Moreover, the aim is to exchange ideas and to strengthen cooperation among all dimensions of research people in the area of advanced material synthesis, energy and sensors applications. I wholeheartedly congratulate the organizing committee of this event. It is an honor and pleasure of appreciating the organizers who have been brought us together to discuss one of the main current challenges which rule the world in this modern era. On behalf of the Department of Physics, it is my great privilege to thank all the Alagappa University authorities, my colleagues, advisory committee members, reviewers, sponsors, invited speakers and participants from all over India for their contributions. Wish them all success.

(G. RAVI)

A.V.V.M. Sri Pushpam College (Autonomous)
Poondi – 613 503, Thanjavur (Dt), Tamil Nadu, India.

Dr. K.RAVICHANDRAN
Professor & Head
Department of Physics

MESSAGE

I am quite delighted to learn that the Department of Physics, Sree Sevugan Annamalai College, Devakottai, Sivagangai is organizing a "National Conference on Semiconductors, Surfaces, Alloys Modeling and Preparations" (SSAMAP – 2019) on 6th December 2019. It will provide a unique learning opportunity for academicians, researchers, technologist, students and industrial experts working in the field of advanced materials which has assumed great significance at the global level. Your endeavour for flow of the knowledge in the advanced field of Nanotechnology, smart materials, thin films etc. Among esteemed participants is a welcome step. I am sure that the lead speakers of various technical sessions will bring out scintillating ideas that will infuse into the minds of young scientists and participants. I wish all the delegates and dignitaries and participating in the National Conference deliberate for excellence. May this conference provide a healthy platform for the intellectuals working in this field. I extended may warm greetings to the organizers and the participants and wish a great.

(Dr. K.RAVICHANDRAN)

Vidhyaa Giri College of Arts and Science

Puduvayal, Karaikudi-630108

Dr. R. CHANDRAMOHAN
Research advisor
Department of Physics

MESSAGE

I am glad that our college P.G Research and Department of Physics is organizing National conference on "National Conference on Semiconductors, Surfaces, Alloys Modeling and Preparations" (SSAMAP – 2019) on 6th December 2019. The topic is most relevant in today's contest. I am overwhelmed on seeing the list of speakers including our Alumnus. This is a fitting tribute to our founder and his noble ideas. I congratulate the Principal and Department of Physics for conducting this part of Golden Jubilee Celebrations. I pray that the interaction lead to advances in topic.

(Dr. R. CHANDRAMOHAN)

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Dr. P. PERUMAL
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Alagappa Government Arts College
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ABOUT THE COLLEGE

Set in a quiet rural location 18 Kms from Karaikudi on Rameshwaram Road, the college came into existence in 1970 founded by the great Philanthropist Sri O.RM.M.SP.SV.AN. Annamalai Chettiar. This college is affiliated to Alagappa University, Karaikudi. It provides opportunities to the rural mass to pursue higher education in Arts and Science. The motto of the college is "Strive with Self Reliance". This college is one of the few colleges that is promoting higher education without capitation fees.

ABOUT THE DEPARTMENT

Department of Physics is functioning since inception of the college with B.Sc. Ancillary Physics. B.Sc. Physics major was started in 1982. The Department aims at the overall development of the students by involving them in programmes like seminars, cultural events, guest lectures by experts etc. The faculties are well experienced and well motivated researchers. Eighty percent of the faculties have completed Ph.D and two faculties are research supervisors. Inter collegiate meet and Workshops are the milestones of our Department.

ABOUT THE CONFERENCE

Material Science is an excellent field inviting inter disciplinary researchers. With the rapid advances in material characterization equipments, and materials with novel properties the material scientists are curious to invent the ultimate materials for every field of science. In this context the theme of this conference **Semiconductors, surfaces, and advances in Computations is very significant**. A special feature of this conference is lectures from Scientists and Professors from various Institutions

PROGRAM SCHEDULE

09.00 am – 10.00 am	Registration
10.00 am – 11.00 am	Inauguration
11.00 am – 11.15 am	Tea Break
Session - I 11.15am – 12.45 pm	**Invited Talk – I** **B. AHILAN** **Deputy Controller of Patents & Designs,** **Patent Office**, Government of India. **"Introduction to Intellectual Property Right (IPR) and Patent system"**
Session - II 12.45 pm – 1.00 pm	**Invited Talk – I** **Dr. R. MONIKA,** **Scientist,** Corrosion & Materials Production Division, CECRI, Karaikudi **"Introductory on Multi Physics modeling and simulation in science and engineering"**
1.00 pm – 1.45 pm	**Lunch break**
Session – III 1.45 pm – 2.45 pm	**Invited Talk - III** **Dr. BM. NAGABHUSHANA** **Professor,** HOD of Chemistry, Vice president of LSIKC, MS Ramaiah University of Technology, Bangalore "**Effect of Morphology on Properties oxide-Nano materials"**
Session – IV 02.45 pm – 03.30 pm	**Invited Talk - IV** **Dr. K. KUMAR, Post. Doc (Ireland)** Assistant Professor of Physics, Vidhyaa Giri College of Arts and Science, Puduvayal. "**Exploring Materials from Surface to Bulk by XPS and HAXPES"**
03.30 pm – 4. 30 pm	Oral & Poster Presentation
4.30pm – 5.00 pm	**Valedictory**

CONTENT

19	OP15	*Green synthesis and characterization of MgO nanoparticles using aerva lanata flower extract by solvothermal process* ***P. N. Nirmala***	*19*
20	OP16	*Preparation and characterization of ZnO thin films by SILAR method* ***G. Kavitha***	*20*
21	OP17	*Preparation of transition metal doped SnO_2 Nano Particles synthesized by co- precipitation method* ***Ragavi, S.Maheswari, M. Karunakaran and K.Kasirajan***	*21*
22	OP18	*Characterization of Silver nanoparticles synthesized using tridax procumbens and Ocimum sanctum (Tulsi) leaf extract and compare its antimicrobial activity* ***A. Ubaithulla Baig, N. Jabena Begum, R. Mohan, K. Ravichandran, R. Vadamalar***	*22*
23	OP19	*An Influence of Mn doping on ZnO Thin Films Prepared by SILAR Method* ***T. Sathya, M. Karunakaran, K. Radhi Devi and K.Kasirajan***	*23*
24	OP20	*Preparation and characterization of nickel oxide thin films using SILAR method* ***J. Nachammai, P. Perumal***	*24*
25	OP21	*Nebulizer sprayed NiO thin films for enhanced Room temperature Ammonia gas sensing: An effect of molar concentration* ***I. Loyola Poul Raj, S. Valanarasu***	*25*
26	OP22	*Synthesis of NiS/ZnS Bilayer Thinfilm by Chemical Bath Deposition Method* ***J.Yuvaloshini , P. Ramadevi and Ra. Shanmugavadivu***	*26*
27	OP23	*Preparation and characterization of Cd doped ZnS thin films using CBD method* ***P. Yogalakshmi***	*27*
28	OP24	*Synthesis and Characterisation of PEO/PVC based blend polymer electrolytes* ***C. Subbu , M. Sundrarajan, M.Karunakaran***	*28*

29	OP25	*Enhancement of silver doped zinc oxide nanopowder by handling the principle of green chemistry* ***R. Sujitha, A. Anusiyakani, R. Mohan, P. Ravikumar, P. Devendran, S. Snega***	*29*
30	OP26	*Effect of pure and co doped CuO thin films using spray pyrolysis technique* ***S.J. Helen***	*30*
31	OP27	*A First Principles Study on Rare Earth Nitride-ErN and phase transitions* ***A.Murugan, R.Chandramohan, K.Kumar R. Rajeswarapalanichamy and R. Swaminathan***	*31*
32	OP28	*Influence of Structural, Electrical, Surface Morphological, Gas Sensitivity, Surface Smoothness, Optical Properties And Anti Cancer (Hela cell) Activity of Sn doped CuO Nanostructure Films Prepared by Low Cost Method of SILAR Technique* ***Dr.K. Dhanabalan M.Revathi***	*32*
33	OP29	*Improving the photocatalytic efficiency of ZnO films through double doping (Sn+Mg) deposited using a nebulizer spray technique* ***R. Mohan, S. Srinivasan, J. Yuvaloshini, M. Karunakaran, S. Sudhahar***	*33*
34	OP30	*Synthesis and optical properties of Co doped ZnO thin film by chemical bath deposition technique* ***J.Yuvaloshini***	*34*
35	PP 1	*Structural, Optical and Biological Properties of Al + F Co-doped ZnO Nanoparticles Synthesized Via a Hydrothermal Method* ***K. Saravanakumar and R.K. Sankaranarayanan***	*35*
36	PP 2	*Incorporation of Marble and Granite Sawing Powder Wastes to Enhance the Processing of Clay Bricks* ***M.Shanthi***	*36*
37	PP 3	*Identification of irbesartan and its impurities using HPLC* ***V. Sathiyanarayanan, R.Jayaprakash and D. Easwaramoorthy***	*37*

74	PP 40	*High capable visible light driven photocatalytic activity of WO3/g-C3N4 hetrostructure catalysts synthesized by a novel one step microwave irradiation route* ***J.Revathi, Dr.Saravana Kumar***	*74*
75	PP 41	*Synthesis of self-assembled micro/nano structured manganese carbonate for high performance, long lifespan asymmetric supercapacitors* ***M. Karuppaiah, P. Sakthivel, S. Asaithambi, R. Yuvakkumar, Y.Hayakawa, G.Ravi***	*75*
76	PP 42	*Synthesis and Characterization of Cadmium Sulfide (CdS) Nano Thin Films Prepared by Chemical Bath Deposition Method* ***R. Premarani and R. Chandramohan***	*76*
77	PP 43	*Synthesize of Fe doped CuO Nanostructures for Sustainable Energy Harvesting Application* ***G. Udhaya Sankar, S.Asaithambi, M. Karuppaiah, G. RajKumar, G.Vijayaprasath, R.Yuvakkumar, G. Ravi***	*77*

B. AHILAN **IL-1**
Deputy Controller of Patents & Designs,
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Department of Industrial Policy and Promotion,
Ministry of Commerce and Industry,
Government of India.

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Intellectual Property Right and Patent System

Abstract

We encounter intellectual property at every step of our lives today. The vehicles, the mobile phones, the television, the computer, the refrigerator, the medicines, the books, the paints, the design of an article and practically everything we use is the product of human ingenuity, knowledge and skill, besides labour and capital and falls under some kind of Intellectual property that had to be respected before the item could be lawfully manufactured. The Intellectual property is created by the application of the human mind. It is non-physical, i.e. intangible and it derives its values from ideas. Different forms of Intellectual Property Rights are Patents, Industrial designs, Trademarks, Geographical Indications, Copyright, Trade secrets, Plant variety and Layout design of integrated circuits

Patents are one the oldest forms of Intellectual property protection. The aim of the patent system is to encourage economic and technical development by rewarding Intellectual creative. A patent is a statutory right granted for a limited period to an inventor in respect of an invention to exclude others from manufacturing, using or selling the patented product or from using the patented process, without due permission. Invention means a new product or process involving an inventive step and capable of industrial application.

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Effect of morphology on properties of oxide Nano materials

Abstract

Nano-materials are the foundation of major technological advances. The field of nano-structured materials is widening in several directions. Nano-materials are extremely important materials for a wide range of applications. Nanotechnology has the potential to change every part of our lives. Nanotechnology affects all materials: ceramics, metals, polymers, and biomaterials. In the coming decade nanotechnology will have an enormous impact Future advances could change our approaches to manufacturing, electronics, information technology and communications technology making previous technology redundant and leading to applications which could not have been developed or even thought about, without this new approach. The study of metal oxides has attracted the attention of materials scientists due to their optical, electrical, magnetic, mechanical, and catalytic properties, which make them technologically useful.

Synthesis of nano-metal oxides with tailored made *morphologies* has in recent times generated amongst *Material Chemists* because of the challenges addressed by the normal wet chemical routes over the sophisticated physical techniques. In wet chemical methods by changing the reaction conditions *as-synthesized* products with various representative morphologies could be obtained. The interest in nano materials stems form the fact that the new properties are acquired at this length scale and equally important that these materials change with *morphology*. Recently, there has been a growing interest in synthesis of efficient nano-materials with better properties. To achieve this, material must have fine size, narrow size distribution, non-aggregation, smooth surface and spherical morphology.

In this talk, the preparation of nano metal oxide materials with different morphologies through solution combustion and hydrothermal methods and effect of morphology on different properties will be discussed in detail.

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Introductory on multi physics modeling and simulation in science and engineering

Abstract

COMSOL Multiphysics is a powerful finite element analysis (FEA) software which creates a model work flow from defining the geometries and their material properties, add physics into the model for solver and finally postprocessing and visualization is done to produce accurate results in it. It provides ability to work on the cross-platform like Windows and Linux. The package uses for various disciplines in physics, mathematics and engineering applications. This software combines with eight add-on modules in the areas like: AC/DC Module, Acoustics, Chemical Engineering, Heat Transfer, Microelectromechanical systems (MEMS), Radio frequency, Earth Science and Structural Mechanics. It uses Application Programming Interfaces (API) with Java for application builder. It uses LIVELINK by combining MATLAB (Mathworks), CAD works, and Solidworks etc., Multiphysics module can be used in a single model builder. COMSOL version 5.0 uses physics-based applications without programming in COMSOL Desktop. It manages applications by COMSOL Server. It allows partial differential equations (PDE) and physics based interface.

The primary advantage of this software uses the modeler to try in a various approach and gives solution to solve a real problems before the material is fabricated and tested.

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Exploring Materials from Surface to Bulk by XPS and HAXPES

Abstract

In this work, economic way of preparing optical anti-refection (AR) window(pure IZO) thin films by low cost solution based techniques for commercial solar cells. This is a new feasibility study. The effects of optimization parameters on thin film growth, internal material properties, material characteristics such as structural, compositional, surface morphological, micro structural, and optical were studied in detail. The chemical and thin film strategies for the development of high quality optical AR applications using Chemical Bath Deposition, Spray Pyrolysis and Spin Coating are developed characterized and compared. To the best of our knowledge based on the literature survey this is the first time that we have got high quality pure IZO - AR thin films via novel solution based techniques for commercial solar cell windows. The visible transmittance is achieved is comparable to AR coatings developed by Physical techniques. The studies revealed the suitability of optimized conditions for preparing excellent AR thin films by each technique and the kinetics are discussed.

OP1

Certain crucial parameters that influence the photocatalytic dye degradation efficiency of semiconductor photocatalysts – A review

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Abstract

Purification of toxic effluents discharged from textile and leather industries is one of the foremost challenges now-a-days. As photocatalysis is considered as one of the best methods for the de-contamination of effluents, hectic research activities are going on for finding optimal values of the operational parameters of the photocatalytic dye degradation process to achieve maximum efficiency. In this review, the most important operational parameters and certain other factors *viz.* pH of dye solution, concentration of dye solution, dosage of photocatalyst, light intensity, dopants added, adsorption of dye molecules on the surface of the photocatalyst and bandgap which appreciably influence the degradation efficiency of semiconductor photocatalysts are discussed with the support of a plenty of reported data. In addition to the review on these parameters, a study on the effect of area of exposure on the photocatalytic degradation efficiency of ZnO was carried out. The results show that for any set of process parameters, a unique minimum area of exposure is needed to achieve maximum efficiency.

OP2

Development of zinc-halloysite nanotube/minerals substituted hydroxyapatite bilayer coatings on 316L SS for electrochemical applications

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Abstract

In the present investigation, the zinc-halloysite nanotubes (Zn-HNT)/strontium (Sr2+), samarium (Sm2+) substituted hydroxyapatite (M-HA) bilayer coating is obtained on 316L SS by electrodeposition and the Zn-HNT/M-HA bilayer coating can be successfully combined to produce the corrosion resistance for electrochemical applications. The existence the of the as-developed Zn-HNT/M-HA bilayer coating on 316L SS was confirmed by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), high resolution scanning electron microscopy (HRSEM), energy dispersive X-ray analysis (EDAX) and high resolution transmission electron microscopy (HRTEM). The effects of Zn-HNT/M-HA bilayer coating on anticorrosion property of 316L SS were also investigated using electrochemical studies in the simulated body fluid (SBF) solution. As a result of these investigations, it is revealed that the Zn-HNT/M-HA bilayer coating on 316L SS improved the anticorrosion performance and the combination of Zn-HNT and M-HA in the bilayer coating significantly enhanced the potential for corrosion resistance for electrochemical applications.

Keywords: Zinc-halloysite nanotubes, Substituted hydroxyapatite, Bilayer, Electrodeposition, Electrochemical studies.

OP3

Investigation of electrochemical and Photo catalytic properties of Nickel sulfide nanoparticles using single source precursor by microwave irradiation method

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Abstract

Nickel sulfide (NiS) nanoparticles (NPs) were synthesized by single pot microwave irradiation using $Ni(Ddtc)_2$ complex as single source precursor and Octadecylamine (ODA) as capping agent. The prepared NiS NPs were confirmed X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS) with mapping analysis. Optical studies showed that the synthesized NiS NPs are blue (lower wavelength) shifted relative to the bulk material. SEM image shows that the prepared nanoparticles were spherical in nature. The XRD patterns of the prepared NiS NPs revealed cubic crystalline phases. TEM images showed spherical morphological nature and the particle size was found around 23 nm. The elemental analysis and mapping spectra was confirmed to the formation of NiS NPs through the presence of Ni and S elements. And the prepared nanoparticles were examined to photocatalytic application and electrochemical studies.

Keywords: NiS Nano-catalyst, Single source precursor, Nano-catalyst, Microwave irradiation, Charge-discharge analysis, Photodegradation.

OP4

Synthesis, Characterization and Biological activity of Ni(II) and Cu(II) complexes with Mannich Base of 2-((4-methoxyphenyl) (morpholino)methyl) hydrazinecarboxamide

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Abstract

A mannich base lingand 2-((4-methoxyphenyl)(morpholino)methyl) hydrazinecarboxamide [MPMMHC] have been synthesized by using semicarbazide hydrochloride, Anisaldehyde, Morpholine and a few drops of liquor ammonia. The Ni(II) and Cu(II) complexes were prepared by using above said ligand. The ligand and the complexes have been characterized by various physical-chemical techniques such as elemental analysis, molar conductance, magnetic susceptibility, Infra-Red, Ultra-Violet, ^{1}H NMR and ^{13}C NMR spectroscopy. For all complexes the conductivity values are measure and this supports the non electrolytic nature of metal complexes. From the electronic spectra the above complexes forms octahedral geometry around the central metal ion. The biological activity of the ligand and its complexes were studied on microorganisms such as *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas aeruginosa* by disc-diffusion technique using DMSO as solvent. The values of zone of inhibition were found out at $37^{0}C$ for a period of 24h. The biological activity of the ligand and its Ni(II) and Cu(II) complexes are compared.

Keywords: Mannich base, semicarbazide hydrochloride, Anisaldehyde, Morpholine and antimicrobial activity.

OP5

Effect of La incorporation on the NH_3 sensing behaviour of ZnO thin films prepared using a low cost nebulizer spray technique

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Abstract

ZnO:La films (LZO) were deposited using a nebulizer spray technique. La concentration was varied as 0, 1, 3 and 5 wt.%. The structural, optical, morphological and gas sensing properties were studied for all the doping concentrations taken. All films exhibit considerable ammonia sensing characteristics. The optical studies show 82% transmittance in the visible region. The gas sensing results show that the LZO (3%) thin film shows high sensing response value and fast response/recovery time (28s/8s) for 100 ppm of NH_3 at room temperature. The reasons for the enhanced sensing ability of the doped films have been explained with the help of AFM, Raman studies and photoluminescence results.

Key words: zinc oxide, La doping, spray pyrolysis, ammonia sensor
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OP6

Effect of W doping on the ZnO thin film on the photocatalytic dye degradation of MB and RhB dyes

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Abstract

A series of W-doped ZnO nanocomposite with different W contents were deposited by nebulizer spray technique and characterized by X-ray diffraction (XRD), Photoluminescence spectroscopy (PL), Fourier transform infra-red spectroscopy (FTIR), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and diffuse reflectance spectroscopy (DRS). The XRD results revealed that all the W-doped samples showed a hexagonal wurtzite structure. The results of EDS spectra confirms W was doped into ZnO structure. The photocatalytic activity of undoped ZnO and W doped ZnO was evaluated by the photodegradation of methylene blue (MB) and rhodamine B (RhB) in aqueous solution. The results show that the photocatalytic activity of the W-doped ZnO is much higher than that of undoped ZnO and the optimum percentage of doped W is 3 wt%. The effect of pH on the degradation efficiency of the optimized sample ZnO:$W_{(3wt\%)}$ was analysed. The point of zero charge of the optimized sample was found to 7.2 using salt addition method. The enhanced photocatalytic activity of the W-ZnO samples may be related to the narrowing of the band gap and increase in the charge separation efficiency.

Keywords: W doped ZnO film; Nebulizer spray technique; stainless steel mesh substrates; Photocatalysis; point of Zero charge; Methylene blue; Rhodamine B; Reactive active species.

Acknowledgement: This work is financially supported by Department of Science & Technology, Science and Engineering Research Board (DST-SERB), Government of India, through the Major Research Project (EMR/2016/003326).

OP7

Effect of Zn doping level on the photocatalytic efficiency of SnO_2 thin films towards MB and MG dyes

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Abstract

This study focuses the effect of Zn doping level (2–8 at.% in steps of 2 at.%) on the photocatalytic efficacy of SnO_2:Zn thin film deposited using a nebulizer spray pyrolysis technique. The structural, surface morphological, photoluminescence studies were carried out for all the samples. The photocatalytic dye degradation study under visible light against the two different dyes viz methylene blue (MB) and malachite green (MG) revealed that SnO_2:Zn film doped with 6 at.% of Sn shows superior photocatalytic activity compared to other doped and undoped samples for both the dyes examined. The degradation efficiency of undoped SnO_2 is found to be 55 and 67% for MB and MG, respectively, whereas the Zn doped SnO_2 films (6 at%) exhibits enhanced photocatalytic activity against both the dyes and the degradation efficiency values for MB and MG are 88 and 97%, respectively. The reasons for this enhancement are addressed appropriately with the evidences obtain from photoluminescence and X-ray diffraction studies.

OP8

Effective growth of 6-Amino-2-Picolinium Veratriate single crystal for nonlinear optical applications

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Abstract

In the present work, new 6-amino-2-picolinium veratriate (6A2PV) organic single crystal was eminently grown by slow evaporation solution growth method with the dimensional value 20 × 4 × 10 mm^3. The grown 6A2PV crystal structure was confirmed by single crystal X-ray diffraction. It is revealed that synthesized 6A2PV compound crystallizes in a monoclinic crystal system with centrosymmetric space group $P2_1/n$. To find out the diffracting planes of the synthesized 6A2PV crystal by powder X-ray diffraction and it confirms the crystalline nature. ^1H NMR spectra was carried out to observe the various hydrogen exposen in 6A2PV structure and the series of functional groups were elucidated by FTIR spectral analyses. UV-Vis spectrometer clearly portrayed that the synthesized 6A2PV crystal has lower cut-off wavelength and good transmission. In PL studies the occurrence of high emission band at 383 nm with an excitation wavelength at 342 nm. In TG-DSC measurement to investigated the grown 6A2PV crystal thermal stability. The Vicker's microhardness test was arranged at room temperature and the gathered results were perceived under classical Meyer's law. The chemical etching was analysed and the results were expressed that growth feature of the crystal. Second order nonlinear optical property of synthesized 6A2PV crystal was conscious by Kurtz-Perry powder test. Density functional theory (DFT) computations were used by B3LYP/6-311++G (d,P) basis set to optimize molecular geometry and the HOMO-LUMO energies confirm the presence of charge transfer within the molecule, Mulliken population analyses to find out the charge distribution in the atomic level, molecular electrostatic potential to estabilished the electrophilic and nucleophilic reaction. NBO showed that the possible interaction between bonding and antibonding orbital molecular system with respect to the donor and an acceptor and first order hyperpolarizability also confirmed the nonlinear property.

OP9

Growth and Characterization of vanillin 5-chlorosalicylic acid nonlinear optical single crystal

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Abstract

An organic co-crystal vanillin and 5-chlorosalicylic acid (V5C) was grown by slow evaporation solution growth method. The V5C crystal belongs to orthorhombic crystal system with noncentrosymmetric space group $Pna2_1$ using single crystal X-ray study. The vibrational modes were confirmed through FTIR and micro raman spectral analyses. The optical studies of UV-Vis and PL spectrum showed cutoff wavelength at 360 nm and excitation wavelength at 350 nm. The thermal stability of V5C crystal is 150 ^{o}C was confirmed by TG-DSC analysis and the mechanical property also analyzed by Vickers microhardness tester. Second harmonic generation (SHG) efficiency was tested by Kurtz-Perry powder technique and found that high value of existing standard KDP crystals. The theoretical calculations were analyzed by DFT B3LYP method 6-311++G(d,p) as a basis set. The crystal structure of V5C was optimized and the geometric parameters were compared. The charge transfer properties were analyzed by HOMO-LUMO analysis. The Mulliken charge and molecular electrostatic potential (MEP) of the present molecule was theoretically analyzed.

OP10

Synthesis and characterization of sodium cobalt (II) phosphate ($NaCoPO_4$) cathode materials for energy storage application

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ABSTRACT

Energy storage plays an important role in the development of portable electronic devices, electric vehicles and large-scale electrical energy storage applications for renewable energy sources. Sodium-ion batteries (SIBs) have attracted the great attention recently, for these applications. They are considered to be one of the potential candidates to replace Lithium ion batteries (LIBs), due to its similar electrochemical properties. Sodium cobalt phosphate ($NaCoPO_4$) sample were successfully synthesized by sol-gel method. The thermogravimetric and differential thermal analysis (TG/DTA) cures of the material ($NaCoPO_4$) precursor, it is confirmed calcination temperature of 600°Cfor the prepared sample ($NaCoPO_4$). The structural properties analysis XRD pattern of the sample ($NaCoPO_4$) belongs to orthorhombic structure with space group Pnma. The presence of functional and vibrational groups of PO_4^{3-} polyanion types were ($NaCoPO_4$) identified using Fourier Transform and Infra-Red and Raman Spectroscopy. $NaCoPO_4$ was obtained non-uniform spherical like structure with porous morphology in Scanning Electron Microscopy. The presence elemental composites of the ($NaCoPO_4$) material from EDX and the chemical state can be obtained from X-ray photoelectron spectroscopy (XPS) measurement.

Key word: Energy, Sodium-ion batteries, Electrochemical, Sol-gel, Scanning Electron Microscope

OP11

The effect of samarium doping on PbS thin films fabricated using nebulizer spray technique for photosensing applications

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Abstract

High-quality samarium doped PbS thin films were fabricated through spray pyrolysis technique on glass slides. X-ray diffraction studies confirmed the single fcc phase of all the films. The crystallite size was found to increase from 21 to 29 nm for undoped to 5 wt.% Sm doping concentration. From the Raman analysis, the peaks observed at 192, 235 and 465 cm^{-1} confirm the presence of the PbS phase. The scanning electron micrograph revealed that the prepared films were highly compacted with an extremely fine nanostructure without any pinhole or crack. The EDAX analysis shows the existence of Pb, S and Sm. The energy gap was found to decreased from 2.15 to 1.58 eV when Sm doping concentration increases from 0 to 5 wt.%. The observed photocurrent is the highest for the 3 wt.% Sm doped PbS thin film sample. The photocurrent enhancement due to the samarium doping with PbS makes it a good contender for high quality photodetector applications

Keywords: Sm doped PbS film; X-ray diffraction; SEM; optical studies; Photosensitivity studies

OP12

Synthesis, growth and characterization of New Mannich base Nonlinear Optical Material

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Abstract

1-(phenyl(pyrrolidin-1-yl)methyl)naphthalen-2-ol (PPMN) Mannich base is a new nonlinear optical material is synthesized and grown as single crystal by slow evaporation technique at room temperature. Single crystal X-ray diffraction technique confirms the compound crystallized in the orthorhombic system with non centrosymmetric space group $Pna2_1$. The presence of functional groups, proton and carbon atoms are identified by FT-IR and NMR spectroscopic studies. The UV-Vis absorption spectrum shows the lower cutoff wavelength at 360.4 nm and optical band gap is found to be 6.34 eV. A peak observed at 415.5 nm in photoluminescence spectrum ensures the blue light emission property. The Kurtz and Perry powder technique confirms the second harmonic generation of PPMN and the efficiency is found to be 4.34 and 1.67 times than KDP and urea respectively. The laser induced damage threshold is measured as 2.1464 GW/cm^2. The dark current leads the photocurrent shows the negative photoconductivity effect of the crystal..

Keywords: Mannich base, Nonlinear optical, frequency conversion, Laser damage threshold, photoconductivity

OP13

Investigation of piperazinium orthophthalate single crystal yielding high second harmonic generation efficiency

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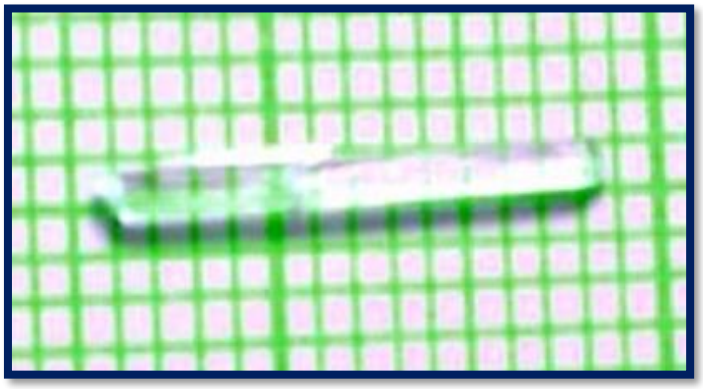
Abstract

The Piperazinium orthophthalate (PPA) single crystal was prepared in the room temperature by slow evaporation solution growth method using ethanol as a solvent. The single crystal X-Ray diffraction studies confirmed that PPA crystal belongs to the monoclinic crystal system with centrosymmetric space group $P2_1/c$. The Powder X-ray diffraction analysis confirms the crystalline perfection of the compound and nature of the crystal. The chemical composition and functional group of the PPA was confirmed by the FT-IR analysis. The optical absorption spectrum has the cut off wavelength at 330 nm and good transmission percentage in the range 390-800 nm. The band-gap energy was found to be 3.8 eV. PL spectral study of grown PPA showed one high intense blue emission peak at 364 nm and one medium intense peak at 533 nm for an excitation wavelength at 342 nm. Thermal stability of the material is confirmed by the TG-DTA analysis, the grown PPA crystal is stable up to 88°C and various endothermic peaks are appeared for various stages of decomposition. The mechanical stability of the crystal was analyzed by Vicker's microhardness test and Meyer's index is found to be 4.6. The grown PPA crystal has very high second harmonic generation efficiency compared to KDP Crystal.



Photograph of the grown PPA crystal

OP14

Structural and optical studies of CdO thin films using sol-gel dip coating for various molar concentrations

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Abstract

Cadmium oxide (CdO) thin films were deposited on glass substrates using sol-gel dip coating technique. CdO thin films were deposited by using various concentration of cadmium acetate solution such as 0.3M and 0.4 M. X-ray diffraction studies reveal that the films are polycrystalline in nature with cubic structure. The average crystalline size varies from 2 to 4 nm. Optical studies reveal that the films prepared from solution of 0.3M and 0.4M concentration have less transparency. Photoluminescence spectra of the CdO thin films recorded at room temperature under excitation wavelength of 290 nm. The emission peak is centered at 408 nm. Photoluminescence studies reveals that the optical quality of emission peaks which could be related to effective number of charge carriers resulting in the electrical conductivity of the films.

Keywords: Cadmium oxide, Sol-gel dip coating, X-ray diffraction, Optical studies, Photoluminescence.

OP15

Green synthesis and characterization of MgO nanoparticles using Aerva lanata flower extract by solvothermal process

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Abstract

Magnesium Oxide (MgO) was synthesized by hydrothermal precipitation method. The MgO nanoparticles were prepared by green synthesis method using aquous leaves extract of Aerva lanata, The particle Size, Characterization studies were carried out using XRD, FTIR, SEM and UV Spectrum. The XRD patterns were used for phase identification and showed impurities depending on the peaks present in the structure. The structure of the MgO nanoparticles were investigated with SEM and it indicates that the nanoparticles were bud-like in shape and it ranged from 9-27nm. FTIR spectrum confirms the existence MgO stretching .The absorption of the MgO nanoparticles were examined from UV-Visible spectrometer (SHIMADZU-UV-Vis) at room temperature. The absorption peaks appeared at 222nm for MgO nanoparticles and the band gap energy from UV spectrum was 5.58eV.

Keywords : Magnesium Oxide; Nanoparticles; XRD; FTIR; UV spectrum.

OP16

Preparation and characterization of ZnO thin films by SILAR method

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Abstract

Zinc Oxide thin films of two different molarities were deposited on the glass substrate by Successive Ionic Layer Adsorption and Reaction (SILAR) method. The effect of two different molarities of the deposited films was characterized by the structural, optical and morphological of the ZnO thin films were studied. The structural studies reveal that the deposited ZnO films polycrystalline nature with hexagonal structure. The optical studies carried out on the film shows higher morality of high transmittance and low absorption in nature. The morphological studies expose that smaller and bigger particles agglomerated randomly and found that there is no uniform shape.

Key words: Zinc Oxide, Structural studies, substrate, molarities, transmittance.

OP17

Preparation of transition metal doped SnO_2 Nano Particles synthesized by co-precipitation method

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Abstract

In this study we have reported the transition metal (Ni) doped SnO_2 nano particles were successfully synthesized by chemical co-precipitation method. The interaction of Ni doped SnO_2 nanoparticles characterized by X-ray diffraction pattern (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis diffuse reflectance Spectroscopy (DRS) and Photoluminescence Spectroscopy (PL). The XRD Pattern confirms the formation of tetragonal structure of SnO_2 and the peaks are identified with the JCPDS (88-0287). The SEM image indicates that the particles were irregular shape for all prepared samples. The SEM image showed that the agglomeration process is occurred slowly down with the addition of doping content. EDX studies conforms the presence of Sn, O and Ni elements. In FTIR studies the functional groups were identified based on Ni doped SnO_2. The minimum band gap value obtained for pure SnO_2. When the doping concentration increases band gap values also increases for 2% and 4% Ni doping. From PL studies strong band orientation was observed.

Keywords

Tin Oxide, Doping, Structural, Morphological and Optical Studies, band Gap.

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OP18

Characterization of Silver nanoparticles synthesized using *tridax procumbens* and *Ocimum sanctum (Tulsi)* leaf extract and compares its antimicrobial activity

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Abstract

An ecofriendly approach for green synthesis of nanoparticles using natural plant extracts is gaining a notable importance now-a-days which leads to the development of green nanotechnology. In the present study, two different leaf extracts *viz. Tridax procumbens and Ocimum sanctum (Tulsi)* leaf has been used to produce the silver nanoparticles (Ag NPs). The physico-chemical properties of silver nanoparticles were analyzed using different analytical techniques such as a UV–Vis spectrophotometer, Atomic Absorption Spectroscopy (AAS), Dynamic light scattering (DLS), X-ray diffraction and a Fourier Transform Infrared spectrophotometer. Synthesized nanoparticles are evaluated using its antimicrobial efficacy for different human pathogenic organisms by disk diffusion assay. Both the extracts exhibited significant results for the green synthesis of Ag NPs by using silver nitrate as a reducing agent, the synthesis of Ag NPs was determined by colour change from yellowish green to dark brown. X-ray diffraction pattern confirmed the presence of Ag nanoparticles which were crystalline in nature. Additionally, the functional metabolites were identified by the FTIR spectrum which results from presence of phytochemical compounds of leaf extracts. The reaction time (for both leaf extracts) to reduce silver ions into silver nanoparticles, was measured using AAS study. The nano size of the silver particles was confirmed using DLS technique. The screening study of antimicrobial activity confirms that the green synthesized Ag NPs will yields the possible application in medical industry.

OP19

An Influence of Mn doping on ZnO Thin Films Prepared by SILAR Method

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Abstract

Mn doped Zinc Oxide (ZnO) thin films have been successfully coated onto glass substrates at various Mg doping level such as 0%, 5%, 10% and 15% by Low cost SILAR coating technique. The film thickness was estimated using weight gain method and it revealed that the film thickness increased with Mn doping concentration values. The prepared film structural, morphological and optical properties were studied using X-ray diffraction (XRD), scanning electron microscope (SEM) and UV-Vis-NIR spectrophotometer respectively. The structure of the films were found to be hexagonal structure with polycrystalline in nature with preferential orientation along (002) plane. X-ray line profile analysis was used to evaluate the micro structural parameters such as crystallite size, micro strain, dislocation density and stacking fault probability. The calculated crystallite size values lies between 41 nm – 36 mn. The crystallite size values are decreased with increase of Mn doping concentration values and maximum value of crystallite size was estimated at 41 nm at doping concentration of 0%. Morphological results showed that the concentration of the Mn has a marked effect on morphology of the ZnO thin films. The optical studies revealed that the band gap can be tailored between 3.63 eV to 3.72 eV by altering doping concentration. EDAX studies showed that the presence of Zn, O and Mn content.

Keywords: Zinc Oxide, Thin Films, Structural Studies, Morphological Studies, Optical Properties.

OP20

Preparation and characterization of nickel oxide thin films using SILAR method

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Abstract

Nickel oxide (NiO) thin films have been prepared by SILAR method onto glass substrates and the as prepared thin films are annealed at 450 °C for 1 hour. The structural, optical and morphological properties of nano films are examined using X-ray Diffraction (XRD), UV-Visible and Photoluminescence (PL) studies and Scanning Electron Microscopy respectively. The thickness (t) of the films was calculated using weight gain method. The X-ray diffraction analysis revealed as the prepared thin films cubic structure with dominant (111) orientation. The crystallite size, microstrain and dislocation density were also calculated from XRD studies. The transmittance of the NiO thin films was found to be nearly 60% in the visible region. The room temperature PL spectrum of the NiO thin film showed dominant peak at 490 nm and other two shoulder peaks at 520 nm. The morphological studies showed that the prepared films were uniform, rough, large particles and agglomeration of particles.

KEYWORDS: Thin films, SILAR, transmission, excitation, thickness.

OP21

Nebulizer sprayed NiO thin films for enhanced Room temperature Ammonia gas sensing: An effect of molar concentration

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Abstract

In recent days hazardous gases like CO, CO_2, NO_2, SO_2 and NH_3 are released from various chemical industries due to rapid expansions of industrialization and growing population. Among them Ammonia (NH_3) is a highly toxic and it is used in many industries range from agriculture to petroleum industry. Hence it is very essential to develop highly selective and reliable ammonia gas sensor for safety and process control in detecting environmental pollution. Metal oxide semiconductor thin films have dragged attention of most researchers towards novel gas sensor. NiO is one of the universally recognized metal oxide materials due to its tunable transport properties together and it is a p-type material with outstanding properties, such as high chemical stability, good crystallinity, wide direct energy gap of 3.6–4.0 eV. In the present study Nickel oxide thin films were deposited by a simple and low-cost spray pyrolysis technique using two different molar concentrations 0.1M and 0.2 M respectively.X-ray diffraction show the Polycrystalline nature with simple cubic structure and high crystalline quality with dominant (111) plane orientation. Morphological studies show that the film appeared with porous nature. The gas sensing properties of NiO thin films for ammonia gas were investigated. The measurements revealed that the 0.2 M deposited film exhibit better gas sensing performance towards ammonia, due to its high surface area and maximum pore volume available for gas adsorption.

Keywords: NH_3sensor, Thin film, NiO, Molarity, XRD analysis, SEM analysis

OP22

Synthesis of NiS/ZnS Bilayer Thin film by Chemical Bath Deposition Method

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Abstract

NiS/ZnS thin films were grown by Chemical Bath Deposition (CBD) technique using eqimolar aqueous solutions of zinc chloride, nickel chloride and thiourea as precursor. Silicon glass substrates were placed in a beaker containing the precursors described above, and heated at 95°C for an hour. X-ray diffraction showed that the crystallographic phase present was the hexagonal wurtzite structure. The photoluminescence spectra of NiS/ZnS bilayer thin film exhibit an ultraviolet emission band centered at ≈ 3.87eV in the vicinity of the band edge, which is attributed to the well–known excitonic transition in ZnS. The optical transmission spectrum of the NiS/ZnS bilayer thinfilms shows good transmission of 60%, which is one of the prerequisites' for opto-electronics devices, especially for solar cell window layers. The band gap energy was determined as 2.45 eV. Scanning electron microscopy showed the formation of nanostructures, consisting of hexagonal structures. An EDAX spectrum confirms the compositional analysis of nickel, zinc and sulphur and it is found to be nominal composition. The diverse potential application in each areas as infrared detectors, window coatings, filters, photoconductors.

Keywords: NiS, ZnS, Bilayer, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Photoluminescence

OP23

Preparation and characterization of Cd doped ZnS thin films using CBD method

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Abstract

Cd doped Zinc sulphate (ZnS) thin films were deposited on glass substrates using Chemical Bath Deposition technique. The prepared ZnS thin films were characterized using X-ray diffraction, Optical studies and morphological studies. X-ray diffraction studies reveal that the films are polycrystalline in nature with hexagonal structure. Crystalline size varies from 9 to 5 nm. Optical studies reveal that the absorption spectrum of thin films shows that the absorption edges lies 300 nm and 400 nm believed that the blue shift in the absorption peak caused by the quantum confinement effect. Morphological studies, we can see the spherical shaped grains and some agglomeration clouds seen in the substrate.

Keywords: Zinc sulphate, Optical studies, X-ray diffraction, Morphological studies.

OP24

Synthesis and Characterization of PEO/PVC based blend polymer electrolytes

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Abstract

In this work, an attempt has been made to study the ionic conductivity variation, structural changes and morphological changes of PEO/PVC based polymer electrolyte membranes in accordance with the variation of blend ratio. Out of the four prepared samples, the sample with PEO(70wt%) and PVC (30wt%) exhibited a maximum value of ionic conductivity ($5.855 \times 10^{-5} Scm^{-1}$). The FTIR study of this sample also shows the appearance or disappearance of new peaks as well as shifts in the existing peaks and thus confirming the perfect blending. XRD study of this sample also confirms the less crystalline structure compared to the other samples. The SEM analysis of this sample also shows maximum number of micropores which are responsible for the better ionic conductivity. The temperature dependant ionic conductivities calculated from the AC impedance values too exhibit linear variation. Hence, such kind of polymer electrolyte membranes could be employed for lithium battery applications.

Key Words: Blend, Morphology, Micropores and Impedance.

OP25

Enhancement of Silver Doped Zinc Oxide Nanopowder by Handling the Principle of Green Chemistry

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Abstract

The green synthesis of Ag capped ZnO nano particles were using tridax Procumbers leaf extract has become low-cost and eco-friendly method. The XRD pattern of Ag capped ZnO nano particles were analysed. The typical ZnO hexagonal wurtzite structure conforms according to the JCPDS card no.36-1451. The preferential orientation is along the (101) plane observed in the present work and also that the pre-dominancy of the (101) peak is not affected by the Ag doping. UV- visible spectrophotometer we found that the band was observed around 370- 380 nm which was identified as “surface Plasmon resonance band” and this band is ascribed to excitation of valence electrons of ZnO arranged in the nanoparticles. SEM of the Ag/ZnO sample shows that agglomeration has been taken place. FTIR identified the possible biomolecules responsible for the reduction of ZnO and capping agent of bioreduced ZnO NPs through particular bond vibrations peaks coming at defined wave numbers. The antibacterial studies indicated that the nanopowder have the ability to destroy gram-positive bacteria and gram-negative bacteria. The bactericidal effects of nano composites are explained by the formation of highly reactive oxygen species (ROS) (OH^-, H_2O_2 and $O2^{2-}$) on the surface of the nanomaterial which causes fatal damage to the bacteria. Thus, it is concluded that Tridax Procumbers leaf leaves could be successfully used for the biosynthesis Ag/ZnO NPs which are multifunctional.

Keywords: Tridax Procumbers leaf, Green synthesis, biosynthesis Ag/ZnO NPs Antibacterial studies.

OP26

Effect of pure and Co doped CuO thin films using spray pyrolysis technique

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Abstract

Pure (undoped) and Zinc, Cadmium (Co) doped CuO thin films are prepared using spray pyrolysis technique on glass substrates. Influence of Zn & Cd doping on the structural, optical and electrical properties of CuO thin films is reported. XRD analysis reveals that the prepared pure and Zn & Cd doped CuO films show polycrystalline nature with face centered cubic structure. Also, Zn& Cd doping significantly increases the crystalline and changes the crystallite size. SEM images shows grains which are uniform and rod shaped grains. The transmittance of the prepared CuO films recorded in the UV visible spectra show 40 to 70% in the visible region. The estimated optical band gap values are blue shifted in Zn doped CuO thin films. Hall measurement shows that the films are n-type semiconductor. Also, it is observed that when the Cd doped, the electrical resistivity is high when compared to Zn doped CuO thin films.

Keywords:

Spray pyrolysis, XRD, UV visible spectra, Optical band gap, Hall measurement.

OP27

A First Principles Study on Rare Earth Nitride-ErN and phase transitions

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Abstract

The structural, electronic and mechanical properties of rare earth nitride ErN is investigated by the first principles calculations based on density functional theory using the Vienna *ab-initio* simulation package. At ambient pressure ErN is stable in the ferromagnetic state with NaCl structure. The calculated lattice parameters are in good agreement with the available results. The electronic structure reveals that ErN is half metallic at normal pressure. A pressure-induced structural phase transition from NaCl (B1) to CsCl (B2) phase is observed in ErN. Ferromagnetic to non magnetic phase transition is predicted in ErN at high pressure.

Keywords: Ab-initio calculations; Phase transition; Electronic structure; Mechanical properties.

PACS No.: 31.15.A- , 61.50.Ks, 31.15.ae, 62.20.-x

OP28

Influence of Structural, Electrical, Surface Morphological, Gas Sensitivity, Surface Smoothness, Optical Properties and Anti Cancer (Hela cell) Activity of Sn doped CuO Nanostructure Films Prepared by Low Cost Method of SILAR Technique

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Abstract

This study examined the influence of the Sn doping level on the structural, electrical, surface morphological, gas sensitivity, surface smoothness, optical properties and anticancer activity of Sn-doped cupric oxide (Sn:CuO) thin films synthesized on to glass substrates using low cost method of SILAR technique. The samples were characterized by X-ray diffraction, energy dispersive X-ray analysis, field emission scanning electron microscope, UV visible and Raman spectroscopy. The crystallite size of the films decreased with increasing Sn doping level from (2.5%, 5.0%, 7.5% and 10%). The band gap trended downward from 2.0 to 1.95 eV with increasing Sn doping level. The results showed that SnO2 doping strongly affects the structural, electrical, surface morphology, surface smoothness, gas sensitivity and optical properties and anticancer activity of the films. Finally, anticancer activity of the synthesized nanostructures has been determined against HeLa cancer cell line. Undoped CuO exhibited a stronger anticancer activity.

OP29

Improving the photocatalytic efficiency of ZnO films through double doping (Sn+Mg) deposited using a nebulizer spray technique

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Abstract

Undoped and Sn+Mg doped ZnO thin films were deposited onto glass substrates using a nebulizer spray technique. The optical, structural, photoluminescence, morphological and photocatalytic properties were investigated with various doping levels (2, 4, 6, 8 and 10 at. %) of Mg and constant doping level (6 at. %) of Sn. The XRD studies showed that all the films have hexagonal wurtzite structure of ZnO and the size of the films was found to be in the range of 60 – 90 nm. The optical transmittance in the visible region is desirably high (≈ 90 %) with significant enhancement in the optical band gap with Mg doping level. The blue shift of NBE emission peak is observed in the PL spectra with increase in the Mg doping level. From the SEM studies, it is clearly seen that there is a gradual decrease in the grain size with increase in the Mg doping level. The photocatalytic activity of the samples were evaluated by photodegradation of Methylene Blue dye and the results showed that the doping of Mg and Sn into ZnO lattice could enhance the photocatalytic activity which was attributed to increased band gap, decreased grain size and superior textural properties.

Keywords: doubly doped ZnO thin films, photocatalytic activity, nebulizer spray, Photoluminescence

OP30

Synthesis and optical properties of Co doped ZnO thin film by chemical bath deposition technique

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Abstract

Co doped ZnO thin films were prepared by Chemical Bath Deposition (CBD) method with the doping concentration of 0.01 M Co. The structural and optical properties of the as deposited films have been characterized using XRD, UV-Visible spectroscopy, Photoluminescence spectra and FESEM. The XRD results revealed the polycrystalline nature of the film with the presence of hexagonal wurtzite structure. The average crystalline size was calculated using Scherrer's formula and it is found to be in the range of 54 nm. UV-Vis absorption and transmittance spectra showed that the film is highly transparent in the visible region and in the case of doped ZnO thin films, d-d transition was observed in the violet region due to the existence of crystalline defects and grain boundaries. The energy band gap was found to be 3.74 eV. The photoluminescences (PL) spectra of the sample exhibited a broad emission in the visible range. The surface morphology of the thin films was investigated by FESEM and it revealed that they are homogeneously distributed. The energy dispersive X-ray analysis (EDX) confirmed the stoichiometric composition of the Co doped ZnO thin films. Its optical properties could be modified thoroughly by thermal treatment with hydrogen or by an appropriate doping process either by cationic or anionic substitution. ZnO doped with transition metals has been predicted theoretically to be very good candidates for room temperature ferromagnetism. As a consequence, transitional metal doped Zinc Oxide has found potential applications in spintronics. The growth processes of Co doped ZnO thin film is described the effect of cobalt doping on optical properties.

PP1

Structural, Optical and Biological Properties of Al + F Co-doped ZnO Nanoparticles Synthesized Via a Hydrothermal Method

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Abstract

Recent technology called nanotechnology allows the manipulation of materials at nanoscale level, which enables precision engineering to control nanoparticles (NPs') physicochemical properties, as well as their interactions with biological systems. Inorganic NPs, including metal oxides, are promising materials for applications in medicine, such as cell imaging, biosensing, drug/gene delivery, and cancer therapy. Metal oxides are particularly attractive with respect to applications in catalysis, sensing, energy storage, conversion optics, electronic devices memory arrays and biomedical applications. Zinc oxide (ZnO) nanoparticles (NPs) have received considerate attention recently due to their wide applications in a variety of areas, including chemistry, physics, materials science and the biomedical sciences. In particular, ZnO NPs have shown interesting antibacterial activities against both Gram-positive and Gram-negative bacteria such as spores. Co-doping doping of aluminium (Al) and fluorine (F) on ZnO NPs was successfully achieved by a hydrothermal method. The strong x-ray diffraction peaks revealed the high crystallinity of the synthesized nanoparticle and the XRD profiles showed that the material has hexagonal wurtzite structure. EDAX results confirmed the presence of Al and F and from the quantitative analysis it was observed that there was a systematic increase in both the dopants in the final product as they were included in the starting solution. The SEM images showed that the ZnO:Al+F NPs has nanorod structure with hollow hexagonal cross section. The co-doping enhanced the carrier concentration of the ZnO NPs indicated by the higher IR reflectivity. The small size and high surface-to-volume ratio of the ZnO NPs are believed to play a role in enhancing antimicrobial activity.

PP2

Incorporation of Marble and Granite Sawing Powder Wastes to Enhance the Processing of Clay Bricks

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Abstract

Accumulation of unmanaged wastes especially in developing countries like India have resulted in an increasing environmental concern. Recycling of such wastes as building materials appears to be viable solution not only to such pollution problem but also to the problem of economic design of buildings. The increase in the popularity of using environmentally friendly low-cost and light weight construction materials in building industry has brought about the need to investigate how this can be achieved by benefiting to the environment as well as maintaining the material requirements affirmed in the standards. Therefore, for the present investigation, sample of marble and granite sawing powder wastes were collected from companies located in Madurai District. Raw clay mixture and fired industrial brick were collected from a brick chamber located in the same District, Tamilnadu, India. Results obtained through chemical and mineralogical analysis (XRF and XRD), liquid and plasticity limit and plasticity index, particle size analysis, measurements of compressive and flexurural strength, water absorption, porosity and bulk density showed that marble and granite wastes can be incorporated into clay mixture upto 50 wt.%, with no determinal effect on the properties of the sintered brick products.

Keywords : Marble wastes; Clay Mixture; Mechanical Properties; Bricks.

PP3

Identification of Irbesartan and its impurities using HPLC

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Abstract

Anti-hypertension Irbesartan and its potential impurities were identified with the help of ICH guidelines through fabricated column using the different elution mixture instead of triethylamine. Nucleosil filled HPLC column of dimension C18 250mm, 4.0mm, 5 µ and make is Macherey-Nagel was used for the analysis of target molecules. The USP conditions such as wavelength-220 nm, buffer pH=3.2, 5.5 mL of Phosphate buffer with about 950 mL of water, and the pH adjusted to 3.2 using diluted ammonia. The mixture supplied to the column with the flow rate of 1.0ml/min. The validation conditions such as column temperature 30°C, cooler temperature 15°C, injection volume 20µl and the detection wavelength 220nm are modified in the waters instrument. The prepared stock solutions of drug and its impurities are injected and retention time's outcomes are observed likewise 9.3, 12, 19, 23, 26, and 29. Irbesartan exhibited the retention time of 18.79 and the results were almost linear with the pharmacopeia results.

Keywords: Irbesartan, HPLC, Reversed-phase, Stationary phase, Active content.

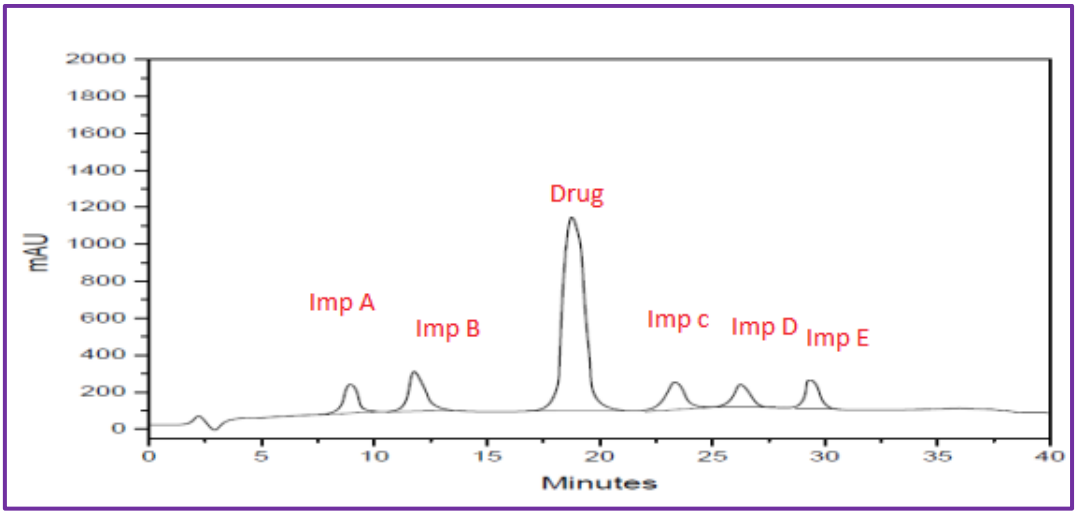

Fig.1. HPLC outcomes of the stock solution

PP4

Characterisation of Thiazole Derivative and Inhibition Study on *CANDIDA ALBICANS*

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Abstract

Identification of a new anti-fungal molecule is an important research due to contaminated food system and harmful pathogens. So, this work prepared 2-(Nicotinamido) Thiazole-4-Carboxylic Acid from Nicotinamide and Thiazole molecules. Then it is characterized by ^{1}H NMR spectroscopy and carried for the growth control ability study against Candida albicans. Zone of inhibition measured in millimeter for serially diluted solution of the compound. From the outcomes, 200 ppm showed very good inhibition and zone of inhibition is more than the standard 250 ppm concentration. The compound displayed 35mm of inhibition zone area but standard fluconazole showed 28mm for 250 ppm solution. The result revealed that the amide bond and acid group acts as an important pharmacophore and exposed the good inhibition behavior.

Keywords: Nicotinamide, Thiazole, Candida albicans, Amide Bond

PP5

Enhancing the photocatalytic efficiency of ZnO thin films under solar light irradiation by the addition of Mo and rGO

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Abstract

In the present study, ZnO:Mo/rGO thin films were deposited on stainless steel mesh substrates (SSM) using nebulizer spray method. The photocatalytic efficacy of the ZnO:Mo/rGO film were studied under solar light against two dyes *viz*. Methylene blue (MB) and Rhodamine B (RhB) and the results were compared with undoped ZnO films and Mo doped ZnO films. The band energy gap values are found to be 2.71 eV, 2.92 eV and 3.23 eV for ZnO:Mo/rGO, ZnO:Mo and ZnO films, respectively. Thus, ZnO:Mo/rGO photocatalyst is more responsive to visible light than the other two sets of samples. The PL, SEM, XRD and FTIR studies support the discussion on the mechanism behind this improvement.

Keywords: ZnO:Mo/rGO thin films; spray pyrolysis; stainless steel substrates; photocatalysis

Acknowledgement

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PP6

Electrochemical studies on $Co(OH)_2$/CNT composites for sustainable and environmental friendly supercapacitor device

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Abstract

Nanostructured electrode materials possess superior electrochemical properties in high performance supercapacitor applications. Cobalt hydroxide $Co(OH)_2$ nanosheets embedded on the surface of carbon nanotube was synthesised. Crystalline structure, functional groups, surface morphology and elements present in the composite were confirmed by using Powder X-ray Diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and EDX experiments respectively. The electrochemical performance of composite was observed by using cyclic voltammetry experiment and found higher specific capacitance about 1006.8 F/g in the scan rate at $0.5mVs^{-1}$. The charge-discharge curve reveals the specific capacitance at 432 F/g in 0.4mA. Electrochemical Impedance Spectroscopy (EIS) results gives the details about electrode/electrolyte interface properties. The higher specific capacitance was noted and its energy density, power density was measured for supercapacitor applications.

Keywords: Carbon nanotube, Supercapacitor, $Co(OH)_2$/CNT, Cyclic voltammetry, Energy storage devices

PP7

Role of source precursors of g-C_3N_4 on photocatalytic activity of ZnO/g- C_3N_4 thin film coated on stainless steel mesh substrates

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Abstract

In recent years, the environmental pollution has become one of the major problems worldwide as a result of rapid development of industrialization. Photocatalytic degradation of toxic dyes by semiconductor oxides such as ZnO, a low-cost metal oxide have been extensively studied and utilized because of its good electrons transfer ability can generate holes for strong oxidation under electromagnetic irradiation. It exhibits the poor photocatalytic response to visible light because of its wide bandgap (3.2 eV) and the fast recombination of photogenerated charge carriers. Graphitic carbon nitride, a narrow bandgap (2.7 eV) polymeric semiconductor can act as a desirable partner to ZnO to make a good visible light responsive photocatalytic composite.

In this study, four sets of film *viz.* ZnO/gU, ZnO/gTU, ZnO/gM and ZnO/gD are deposited onto stainless steel meshes using the source materials urea, thiourea, Melamine and dicyanamide, respectively with the help of tubular nebulizer spray pyrolysis technique. The structural, surface morphological, functional group and optical properties of the deposited films were examined using X-ray diffractometry (XRD), Scanning Electron Microscopy (SEM), FTIR spectroscopy, spectrofluorometry (PL) and diffuse reflectance spectroscopy (DRS) characterization techniques, respectively. The effect of precursor of graphitic carbon nitride on the photocatalytic activity of ZnO was investigated using the prepared film as catalyst for the degradation of methylene blue (MB) and malachite green (MG). It was found that the sample ZnO/gU exhibits superior photocatalytic activity compared to other samples. The degradation efficiency was found to be 98% and 97% for MB (75 min) and MG (45 min) dyes, respectively. The role of precursor for the enhancement of photocatalytic activity is analysed with supporting experimental evidences.

PP8

Perchlorate and Viton A as firework composition

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Abstract

Potassium Perchlorate ($KClO_4$) containing pyrotechnic mixtures is more sensitive to friction, electrical and impact. In this proposed study; pyrotechnic composition/formulation containing $KClO_4$ (oxidizer)-for the sensitivity (mechanical and electrical) study with different types of fuels is proposed, $KClO_4$ powder is treated with Viton A and the sensitivity study of pyrotechnic formulation contains sulphur and graphite powder also proposed.

The impact sensitivity, friction sensitivity and electrostatic sensitivity is to be studied by Bureau of explosives impact machine (BOE Impact Test), BAM Friction Test Apparatus and Electrostatic Discharge Test Instrument (ESD testing) respectively.

Keywords: Potassium Perchlorate, BAM Friction, Impact Test, Electrostatic Discharge

PP9

Preparation of Gd doped ZnO nanoparticles for visible light photocatalyst application

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Abstract

Zinc oxide is an attractive wide gap semiconducting material due to its multifunctional properties as well as high stable and nontoxic in nature. Due to its Excellency in catalytic activity widely used for treatment of wastewater. The Gd (1%, 2%, 3%) doped ZnO nano particles prepared by the nitrate citrate gel combustion method and samples were analysed through various analytical techniques such as XRD, UV and FTIR. The X-ray diffraction analysis clearly shows that there is no secondary phase up to 3% Gd doping. From the UV absorption, it is calculated that materials having the energy gap 3.283 eV, 3.283 eV, 3.296 eV respectively. The synthesized particle studied photocatalytic activity for methylene blue and against pure ZnO and Gd doped ZnO nano particles. Found better photocatalytic activity under visible region. This can be a potential candidate for the treatment of waste water in visible light itself.

Key Words: Doping, Photocatalyst, Visible Light, Water Treatment, Zinc Oxide.

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PP10

Docking studies on retro molecules derived from amoxicillin with 2MUV protein and active molecule identification

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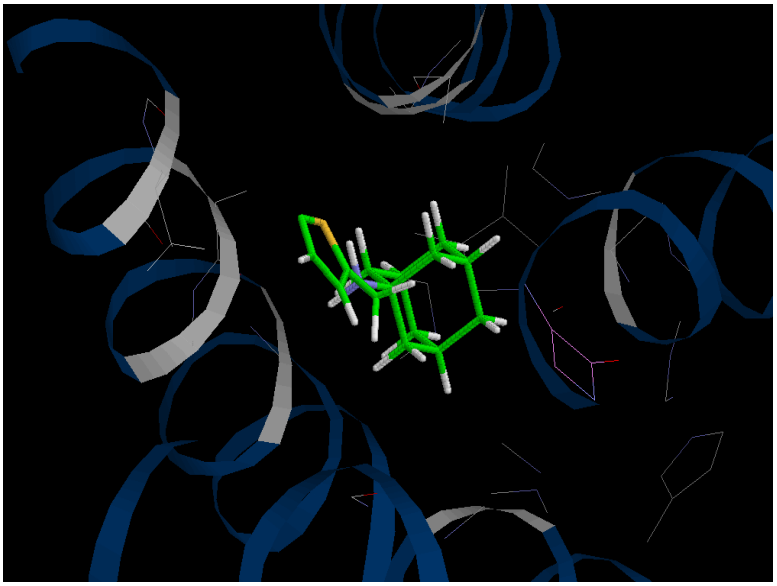
Abstract

Amoxicillin is a very good active commercial antibiotic which is used for cold and bacterial diseases. It contains the following functional groups such as free amine, hydroxyl group, secondary amide group, beta lactam, carboxyl group and Sulphur. Using retro, Amoxicillin has fragmented into 3-methyl-3-sulfanylbutanoic acid (MSA), amino (4-hydroxyphenyl) acetic acid (AHA) and 3-aminoazetidin-2-one (AAO) respectively. The pdb form of the amoxicillin and fragmented molecules were updated with influenza-A protein 2muv. The protein docked with the molecules using iGEMDOCK and docking energies were calculated for 13A^{o} radius. Amoxicillin, MSA, AHA, AAO are displayed the docking sore of -105.06, -72.02, -56.46, -45.53 respectively. From the outcomes this work concluded that the amoxicillin activity increased due to the free amine and lactam ring. The binding ability is higher if the molecule designed with secondary amide group and amine group due to hydrogen bond.

Keywords: Docking, Amoxicillin, 2mua, retro molecules



PP11

Effect of biosynthesis of ZnO nanoparticles via Cucurbita seed extract on Culex tritaeniorhynchus mosquito larvae with its biological applications

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Abstract

The biosynthesis of ZnO nanoparticles was synthesized by biogenic reduction of applied Cucurbita seed extract. The powder X-ray diffraction pattern displayed the high crystalline nature of synthesized ZnO nanoparticles and the crystallite size was calculated at 35 nm range. The Fourier Transform Infra-Red study revealed the functional groups of biogenic reduction and vibrational bands present in the synthesized nanoparticles. The UV–Visible analysis explained the SPR absorption peak at 371 nm. The Photoluminescence study revealed the strong red shoulder emission peak at 665 nm. The particle size analyzer displayed the particle size occupies majorly on 45–65 nm. The SEM analysis pointed the ZnO nanoparticles under rod, rectangular and hexagonal shapes were procured. The EDAX spectrum also mapping exposed the purity of formed ZnO nanoparticles with just Zn and O peaks. The HRTEM analysis exposed the hexagonal shape wurtzite structure ZnO particles formation. The physiochemical analysis revealed general nature of Cucurbita seed powder moreover which explained the phytochemicals involved in biogenic reduction of ZnO nanoparticles. The formed ZnO nanoparticles exhibited good antibacterial activity on E. coli, Bacillus pumilus, and Salmonella typhi bacteria. The cytotoxicity study stated the good toxicity on E. coli AB 1157. The antifungal activity showed a better effect on Aspergillus flavus and Aspergillus niger fungi. The antioxidant activity clarified the good free radical scavenging action. The anti lar-vicidal activity expressed a better impact on Culex tritaeniorhynchus mosquito larvae.

PP12

Structural, optical, vibrational and second harmonic properties of 6-amino-2-picolinium myristate single crystal

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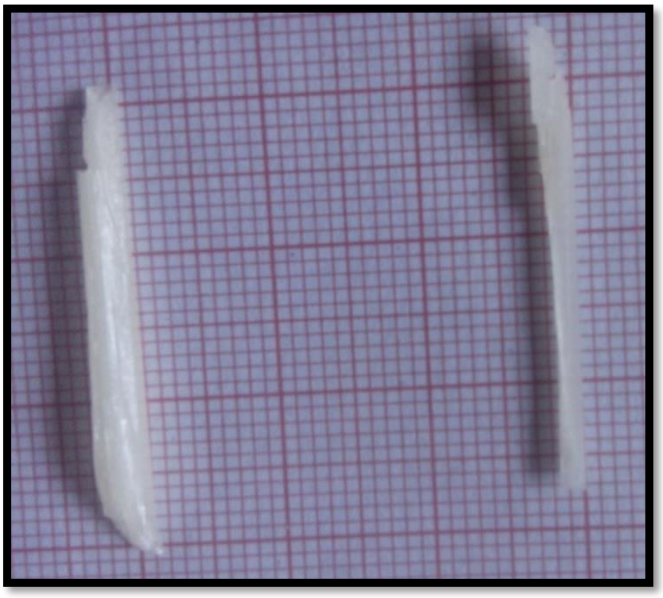
Abstract

An organic single crystal of 6-amino-2-picolinium myristate (6A2PM) has been grown by slow evaporation solution growth technique using ethanol as solvent. The crystal structure, lattice parameters and crystal perfection were confirmed by X-ray diffraction analysis. The functional groups and chemical composition of grown 6A2PM crystal was confirmed by FTIR analysis. UV-VIS spectrum reveals good transparency in entire visible region and the band gap energy of the grown 6A2PM crystal is found to be 2.9 eV. The photoluminescence spectrum gives the excited and emission spectra of 6A2PM grown crystal. Second harmonic generation confirms the non linear optical properties of grown 6A2PM crystal.



Photograph of as grown 6A2PM crystal

PP13

Effect of Temperature on Indium Tin Oxide Thin Films by JNS Pyrolysis Technique

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Abstract

Many techniques for thin films require high temperature (300°C to 550 °C) during deposition to obtain highly crystalline and transparent ITO films. These techniques may also need higher temperature post-deposition annealing treatment at 250 °C to 550°C to improve crystallinity or orientation, which generally damages the film surface and the underlying substrate properties during device fabrications. JNS pyrolysis technique is a new method that allows the large-scale deposition of high-quality films in a single-step heating and at low cost. ITO films with 5% Sn doping have been deposited on glass substrates by jet neubilizer spray pyrolysis by varying the substrate temperature. Amorphous to crystalline transition was observed and the dependence on substrate temperature of preferential orientation (222) at 350oC of ITO films was observed. The change of lattice parameter and the crystallite size values with substrate temperature are also studied. All the deposited films at various temperatures showed cubic nature with improved crystallinity. A mono dispersed uniform morphology with a bigger crystallite size of 37 nm (Smaller size 11.9 nm at 550°C) was observed at an increased temperature of 450oC. With a smaller variation in the band gap energy (0.39 eV) of the deposited films, a decreased resistivity of 4.4 x 10-3 Ω cm was observed for the ITO film deposited at 450oC. The irregular trend of the carrier concentration with respect to the substrate temperature was observed in two order variation. However, an increased mobility and concentration of carrier provides an avenue for tailoring the improved efficiency of solar cell. Keywords: JNSPT, Resistivity, Carrier Concentration, Mobility.

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PP14

Fabrication of Sputtered Vanadium pentoxide (V_2O_5) Thin films for Electrochemical Energy Storage Devices

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Abstract

Transition metal oxide based supercapacitors perform excellent charge storage capability and long life time stability. Among transition metal oxides, vanadium pentoxide is one of the best suited materials for supercapacitive applications, because it has wide range of oxidation states, layered structure, high energy density and low cost. The nanostructured vanadium pentoxide thin films are deposited onto Ni foam by a pulsed DC magnetron sputtering technique. The present study is focused on the highly improved V_2O_5 thin films. The microstructural characterization from X-ray diffraction (XRD) reveal peaks with predominant (0 0 1) orientation signifying orthorhombic phase. Raman studies confirmed the formation of V_2O_5 phase. X-ray photoelectron spectroscopy (XPS) was used to determine the surface compositions and confirmed the absence of impurities. The specific capacitance (Csp) of the electrode material was evaluated by cyclic voltammetry (CV). Galvanostatic charge–discharge (CD) test and the electrochemical impedance spectroscopy (EIS) measurements have been carried out for both annealed and as-prepared films. The annealed thin films exhibited a high rate pseudocapacitance of 137 $mFcm^{-2}$ at $1mAcm^{-2}$ of current density. The electrochemical impedance analysis revealed the films have a lower charge transfer resistance, resulting better capacitance.

Keywords: Transition metal oxide; V_2O_5; Supercapacitors; Thin films; Impedance analysis

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PP15

Enhanced photocatalytic activity of ZnO thin films and nanopowders through lattice compatible cobalt and Mg doping

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Abstract

The focus of this work is to study the effect of cobalt (Co) and Mg doping on structural, surface morphological and photocatalytic properties of ZnO thin films and nanopowders. The undoped and doped ZnO films and nanopowders were prepared using a cost effective jet nebulizer spray pyrolysis technique and simple, speedy and cost-effective microwave assisted synthesis, respectively. The XRD studies reveal that the Co doping only slightly degrade the crystalline quality of ZnO nanopowder whereas Mg doping causes a considerable degradation in the crystallinity. This result is interpreted on the basis of lattice compatibility theory. Surface morphological study shows that ZnO nanopowder exhibits hexagonal shaped grains. The Co doping results in well defined needle and disc shaped grains while spherical shaped ZnO nanopowders are observed for Mg doped ZnO nanopowders. The EDAX spectra affirm the presence of anticipated elements Zn, O, Co and Mg. Between the Co and Mg doped ZnO nanopowders, the former seem to be superior in photocatalytic and antibacterial activities. Moreover, between the two forms of the photocatalyts, viz. the thin film and nanopowder forms, thin film form is found to be superior considering the reusability as well as the efficiency.

PP16

Characterization of electroless Ni-P/Ni-B duplex coating on aluminium 7075 alloy

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Abstract

The present work deals with the preparation of Ni–P/Ni–B duplex coating by electroless nickel plating process on aluminium 7075 alloy and to analyse their wear resistance, microhardness and weight gain. The Ni–P/Ni–B duplex coatings were equipped using dual baths (acidic hypophosphite and alkaline borohydride) with nano TiC as reinforcement and cetyl trimethyl ammonium bromide (CTAB) as surfactant. The experimental results designated the approximate relation between the TiC content and the hardness of composite plating's. With the increasing of TiC content, wear resistance increases consistently. In particular, the influence of TiC content on 0.3% of CTAB (cationic surfactant) retain better wear resistance at 70^{o}C bath temperature. The duplex coatings are uniformly coated and compatibility between the deposits were appears to be good.

Keywords: Duplex coating, cationic surfactant, micro hardness, wear resistance.

PP17

Improving the Efficiency of Solar Flat Plate Collector Using Phase Change Material and Nano Fluid

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Abstract

In the present work, investigations are made to study performance characteristics of solar flat plate collector with PCM and nanofluids . Flat plate collector is one of the important solar energy trapping device which uses as air or water as working fluid.

In this project we designed and fabricated the flat plate collector for the commercial application.it is capable of using both the diffuse and the direct beam solar radiation . For residential and commercial use , flat plate collectors can produce heat at sufficiently high temperatures to pre heating water for boiler and to heat swimming pools , domestic hot water , and buildings , they also can operate a cooling unit , particularly if the incident sunlight is increased by the use of reflector .

Temperatures up to 45 ^{o}C are easily attained by flat plate collectors. We are going to test the performance of the flat plate collector with outlet temperature of water without using PCM and using PCM ($Zn(NO_3)_2.6H_2O$) and nano fluid (Al_2O_3).By obtaining the values and compare the rate of heat transfer.

PP18

Preparation of Eu-Doped Cu_2O Thin Films Using Different Concentrations by SILAR and Their Heterojunction Property with ZnO

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Abstract

Europium-doped Cu2O thin films were prepared by simple successive ionic layer adsorption and reaction (SILAR) with different Eu doping concentrations: 1%, 3% and 5%. The effect of doping level on structural, optical, surface morphological and electrical properties of the films were studied by x-ray diffraction analysis, UV–Vis spectroscopy, scanning electron microscopy and Hall effect measurements, respectively. Crystallite size, dislocation density, microstrain and texture coefficient of the films were estimated using x-ray diffraction data. The crystallite size was found to vary between 27 nm and 21 nm for the change of doping percentage 1–5%. Morphology of Eu:Cu2O and ZnO films had cauliflower and hexagonal shapes, respectively, without any cracks. Optical studies done on the films revealed an increase of band gap as 2.08 eV, 2.26 eV and 2.41 eV for Eu doping concentrations of 1%, 3% and 5%, respectively. The ZnO film showed a maximum of 80% transmittance and band gap of 3.20 eV. Photoluminescence (PL) studies revealed two emission peaks centered at 394 nm and 377 nm for the Eu:Cu2O and ZnO films, respectively. Eu:Cu2O/ZnO heterojunction solar cells were also prepared and their properties studied; they were found to show increased open circuit voltage and short circuit current for 5% Eu doping concentration. Key words: Eu-doped Cu2O, ZnO, heterostructure, solar cell efficiency, SILAR.

PP19

Annealing effect on physical properties of ZnO

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Abstract

ZnO thin films were deposited onto glass substrates using sol–gel spin coating technique from starting solutions having different precursor concentrations (0·1, 0·3 and 0·5M). The effects of precursor concentration and annealing temperature on the physical properties of the films were investigated. The X-ray diffraction studies confirm that all the films have preferential orientation along the (002) plane with hexagonal wurtzite structure. The optical transparency gradually decreases (from 95 to 80%) as the precursor concentration increases. The optical energy gap is in the range of 3·18–3·32 eV. The systematic study shows that the post-annealing process has significant impact on the quality of the films. The SEM images depict that the grain size decreases as the precursor concentration increases, and the AFM images show that the film annealed at 550°C has well defined uniform grains. The lowest dislocation density is observed for 0·3M annealed at 550°C.

Keywords: Thin films, ZnO, Spin coating, Annealing, Surface, Structural properties

PP20

Investigation of Iron vanadate nanoparticles prepared by chemical route for pseudocapacitor application

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Abstract

Iron vanadate nanoparticles were prepared by simple co-precipitation method and calcined at 650 °C. The crystal structure, composition of prepared material was confirmed using X-ray Diffraction analysis and Elemental Dispersive X-ray spectroscopic analysis. Morphology of the material was analyzed by Scanning Electron Microscopic techniques. Optical properties, functional group characteristics vibrations analysis was done by UV-Visible spectroscopy and Fourier transform infrared spectroscopy. Electrochemical behavior such as redox property, charge discharge mechanism and impedance analysis were examined with help of cyclic voltammetry, galvanostatic charge-discharge and electrochemical impedance spectroscopic studies and discussed.

Keywords: Iron vanadate, nanoparticles, cyclic voltammetry, charge-discharge, supercapacitor.

PP21

Synthesis and Characterization of CdS/ZnS and ZnS/CdS Thin films by Chemical Bath Deposition Method

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CdS/ZnS and ZnS/CdS thin films were successfully deposited on the glass substrate by chemical bath deposition method. The XRD pattern shows the major peak assigned to the ZnS phase of the peak at 33.03° with the diffraction plane (0 1 16). The average grain size of the film was found to be 56 nm. The band gaps of both the films are of 2.95 eV. The PL spectrum shows blue shift observed at 365 nm is due to excitonic emission of CdS-ZnS thin films and 497 nm is due to originated from the recombination of an electron from the shallow delocalized donor level. The FE-SEM micrographs of CdS/ZnS shows tightly adherent and are rarer composed of irregular-shaped grains and for ZnS/CdS films are homogeneous, denser and exhibit almost complete coverage of the substrate. The electrical conductivity for both the thin films has high resistivity and is constant with increase in temperature.

PP22

Kinetics and mechanism of oxidation of acidic amino acids by N-Bromophthalimide in aqueous acidic medium.

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Abstract

The kinetics of oxidation of acidic amino acids (glutamic acid,aspartic acid) with N-bromophthalimide has been investigated in aqueous perchloric acid medium potentiometrically. The rate shows first order dependence each on [NBP] and [amino acid] and negative fractional order dependence on[H^+].Addition of KBr(or) the reaction product phyhalimide had no significant effect on the reaction rate. The rate of reaction increased with decrease in dielectric constant of the medium. The rate remained unchanged with the variation in ionic strength of the medium. The thermodynamic parameters were computed by studying the reactions at different temperature. The rate laws derived are in excellent agreement with the experimental results plausible mechanisms were suggested.

Keywords:

Potentiometry, N-Bromophthalimide, Aspartic acid, oxidation, mechanism.

PP23

Green synthesis and characterization of Cd dopped ZnO nanoparticles using *calotropis gigantea leaf* Extract by solvothermal process

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ABSTRACT

Cd dopped Zinc Oxide was synthesized by hydrothermal precipitation method. The Cd dopped ZnO nanoparticles were prepared by green synthesis method using aquous leaves extract of Calotropis gigantea, The particle Size, Characterization studies were carried out using XRD, FTIR, SEM and UV Spectrum. The XRD patterns were used for phase identification and they showed impurities depending on the peaks present in the structure. The structure of the Cd dopped ZnO nanoparticles were investigated with SEM and it indicates that the nanoparticles were bud-like in shape and the particle size ranged from 9-27nm. FTIR spectrum confirms the existence Cd dopped ZnO stretching .The absorption of the Cd dopped ZnO nanoparticles were examined from UV-Visible spectrometer (SHIMADZU-UV-Vis) at room temperature. The absorption peaks appeared at 222nm for MgO nanoparticles and the band gap energy from UV spectrum was 5.58eV.

Keywords : Zinc Oxide; Nanoparticles; XRD; FTIR; UV spectrum.

PP24

Preparation and Characterization of Micro-Crystalline Cellulose Dispersed Poly (Vinyl Alcohol) Film

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Abstract

In the present work, the microcrystalline cellulose was synthesized by the jute fiber and was identified by Scanning electron microscopy. The synthesized microcrystalline cellulose was dispersed into the poly (vinyl alcohol) by simple ultra-sonication process and evenly coated into the food packaging sheets. The surface morphology of the synthesized microcrystalline cellulose dispersed poly (vinyl alcohol) film was studied by Scanning electron microscopy. The crystalline nature of the microcrystalline cellulose dispersed poly (vinyl alcohol) film was characterized by X-ray diffraction. The thermal properties of the synthesized microcrystalline cellulose dispersed poly (vinyl alcohol) film were investigated by Thermogravimetric analysis and Differential Scanning Calorimetry. The prepared microcrystalline cellulose dispersed poly (vinyl alcohol) film can be used as a promising candidate for food packaging applications.

Keywords: Micro-crystalline cellulose, Poly (vinyl alcohol), Ultra-sonication

PP25

Tuning the band gap of ZnO by suitably doping Cu and N for enhanced visible light responsive photocatalytic dye degradation

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Abstract

The ZnO, ZnO:N, ZnO:Cu and ZnO:Cu:N films were coated using nebulizer spray technique to decompose textile dyes photocatalytically. Among the different Cu doping concentrations tested (0.5, 1, 2, 3 and 5 wt %), 0.5 wt % showed superior photocatalytic efficiency whereas among the different N doping concentrations (1, 2, 3, 5 and 10 wt %) 3 wt % gave the best results. Therefore, these two optimum doping concentrations of Cu (0.5 wt %) and N (3 wt %) were chosen for the preparation of co-doped films. XRD, SEM, PL, optical and XPS studies were performed. The band gap values were found to be decreased from 3.28 to 3.01, 2.74 and 2.47 after N, Cu and Cu+N doping, respectively as observed from the optical study. The mechanism behind the enhancement of degradation efficiency has been addressed in the paper with the support of structural, compositional, optical and surface morphological analyses.

Keywords

Dye degradation, photocatalysis, spray pyrolysis, band gap tuning, co-doping

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PP26

Preparation and Antibacterial Activity of Seaweed Nanoparticle

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Abstract

At present, more synthetic antibacterial nanoparticles are developed and applied on textiles because of their novel properties and low material consumption of nanoparticles. To replace the synthetic chemicals from antibacterial finishing, research is ongoing to find bioactive agents from natural products. Recent research shows that seaweed can be used for isolation of antibacterial agents. Along with antibacterial activity, seaweed also is used for nutritional purposes and to remove metal ions from wastewater. In the present investigation, an attempt was made to extract bioactive substance using acetone as a solvent and characterized by Fourier transform infrared (FTIR) spectroscopy. Furthermore, the extracted bioactive substance was subjected to Atomic absorption spectroscopy (AAS) for heavy metal removal and applied on cotton fabric for antibacterial property.

Keywords: seaweed; bioactive agent; FTIR; AAS; antibacterial activity

PP27

Hydrothermal synthesis of $NiFe_2O_4$ and $CoFe_2O_4$ nanoparticles: structural, morphological and optical properties.

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Abstract

Cubic spinel structured nickel ferrite ($NiFe_2O_4$) and cobalt ferrite ($CoFe_2O_4$) nanoparticles were synthesized using hydrothermal method. The crystallinity, morphological and optical properties of the obtained samples were characterized by using powder X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) and UV–Visible diffuse reflectance spectra (DRS). The XRD analysis of the specimen confirmed the formation of single cubic spinel phase. Using the Scherrer formula, the crystallite size of the nickel ferrite and cobalt ferrite were found to be 36nm and 20nm respectively. SEM analysis revealed the presence of well grown agglomerated nanoclusters. The infra-red spectra showed the features of higher and lower energy bands corresponding to octahedral (O-band) and the presence of tetrahedral (T-band) complexes verified the creation of spinel ferrites. The UV– DRS study confirmed the samples were active in the visible region and the band gap values of the nickel ferrite and cobalt ferrite were 2 eV and 1.68 eV respectively.

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PP28

Effect of Substrate Temperature on Mn doped CdO thin films Prepared by Perfume Atomizer Spray Pyrolysis Method

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Abstract

Mn doped CdO thin films were deposited by perfume atomizer spray pyrolysis method on glass substrate by varying substrate temperature (T=200^0 C, 225^0 C, 250^0 C, 275^0 C, 300^0 C). The X – ray diffraction (XRD) analysis show that the prepared cadmium oxide thin films belongs to cubic structure with preferential orientation along with (111) direction. The thicknesses of the films were determined by Stylus profiler. The average optical transmittance of the CdO films in the range of 300 – 800 nm, is about 58%. Estimated band gap energy (E_g) is 2.65 eV and 2.5 eV. Photoluminescence (PL) spectra showed a strong emission peak around 523 nm. A systematic study on the influence of the substrate temperatures on the optical, electrical and structural properties of Mn doped CdO thin films deposited by perfume atomizer spray have been reported.

Key words: Thin films, X-ray diffraction, thickness, transmittance, Photoluminescence.
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PP29

Corrosion resistance of nanoparticle - incorporated nano coatings

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Abstract

Concrete admixtures can be prepared in various water samples such as rain water, well water, and sea water. These waters contain various types of ions. So corrosion behavior of mild steel immersed in simulated concrete pore solution prepared with the above water samples will vary. Corrosion resistance of mild steel in simulated concrete pore solution prepared with above water samples has been evaluated by polarization study. The corrosion resistance of mild steel in various samples of water is as follows: Rain water>Well water>Sea water. The corrosion resistance of mild steel in simulated concrete pore solution prepared in various water samples are in the decreasing order: Rain water>Well water> Sea water. This is revealed by the linear polarization resistance values and corrosion current values

Keywords: simulated concrete pore solution, mild steel, rain water, well water, sea water, polarization study.

PP30

Characterization of green synthesized silver nanoparticles doped ZnO nanostructures for health care applications

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Abstract

The growing need of environmental friendly nanoparticles provokes the researchers to use green methods for the synthesis of various metal nanoparticles for health related applications. Green synthesis includes synthesis through plants and microorganism. They allow large scale production of ZnO nanoparticles (NPs) free of additional impurities. The NPs synthesized from biomimetic approach show more antimicrobial activity and limit the use of expensive and toxic chemicals. In the present work, we discussed on characterization of green synthesized silver nanoparticles doped ZnO nanostructures. The silver (Ag) nanoparticles were synthesized using *Tridax procumbens* leaf extract. Then, the resultant green synthesized silver NPs were doped with ZnO nanostructures using simple soft chemical method. The resultant Ag doped ZnO nanostructures were thoroughly analyzed using different analytical techniques such as UV-Vis NIR spectrophotometer, photoluminescence spectrometer, Fourier Transform Infrared spectrophotometer, X-ray diffraction technique and Scanning electron Microscopy. The results showed that this green approach using *Tridax procumbens* leaf extract is optimum for the synthesis of Zinc Oxide NPs and it is also known to have the ability to inhibit the growth of various pathogenic micro-organism. The obtained antibacterial results of gram positive and gram negative bacterial strains, strongly evidenced, that these ZnO NPs can be used for various health related applications due to its eco-friendly, non-toxic and compatibility for pharmaceutical applications.

PP31

Effect of Solution Volume on Structural, Morphological and Optical Properties of CdO Thin Film Prepared by Perfume Atomizer Spray Pyrolysis Method

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Abstract

CdO thin films have been prepared using perfume atomizers spray pyrolysis method. CdO films have been deposited on glass substrates with different solution volume at 200˚C.X-Ray diffraction studies shows that the prepared thin film had cubic and polycrystalline nature. Scanning electron microscope shows the influence of solution volume on surface morphology of the CdO thin film. Optical studies show that in these films the electronic transition is of the direct transition type. The optical energy gap for the films of as deposited are vary from 2.34 – 2.51 eV with solution volume. Photoluminescence results analysis confirmed that the dependence of optical energy gap on solution volume.

Key words: Thin films, X-ray diffraction, thickness, transmittance, Photoluminescence.

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PP32

Structural, Electronic and Mechanical Properties of Rare Earth Nitride-XN (X = Tb,Tm): A First Principles Study

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Abstract

The structural, electronic and mechanical properties of rare earth nitride XN (X = Tb,Tm) are investigated by the first principles calculations based on density functional theory using the Vienna *ab-initio* simulation package. At ambient pressure XN is stable in the ferromagnetic state with RS structure. The calculated lattice parameters are in good agreement with the available results. The electronic structure reveals that XN is metallic at normal pressure. Ferromagnetic to non magnetic phase transition is predicted in XN at high pressure.

Keywords: Ab-initio calculations; Electronic structure; Mechanical properties; Charge Density; Magnetic Phase Transition.

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PP33

Effect of active sites in SILAR deposited nanostructured ZnO thin films for solar energy conversion

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Abstract

Pure and tungsten (W) doped zinc oxide (ZnO) thin films have been successfully deposited on a glass substrate by successive ionic layer adsorption and reaction (SILAR) method. Effect of W causes the change of strained stress in ZnO films, which subsequently affected the structural and optical properties. XRD patterns revealed that all the thin films possess a polycrystalline hexagonal wurtzite structure and W doped ZnO thin films (002) plane peak position is shift toward lower angle, which is due to the W doping. The SEM images show that W-doped ZnO thin films are exhibited uniformly coated and composed of nanostructured particles grown over the film. The transmittance spectra indicate that W doping can increase the optical band gap of ZnO thin films. The optical energy gap of the films was estimated from Tauc's law and observed to be an increasing tendency with the increment of the W doping concentrations. The optical constants such as reflectance, index of refraction, extinction coefficient, and optical conductivity were determined using the transmission at normal incidence of light in the wavelength range of 200-800 nm. In Photo Luminescence spectra, the band edge emission shifts to the blue with increasing amount of W doping.

Keywords: SILAR, Thin films, Transmittance, Reflectance.

PP34

Investigation of electrochemical and Photo catalytic properties of Nickel sulfide nanoparticles using single source precursor by microwave irradiation method

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Abstract

Nickel sulfide (NiS) nanoparticles (NPs) were synthesized by single pot microwave irradiation using $Ni(Ddtc)_2$ complex as single source precursor and Octadecylamine (ODA) as capping agent. The prepared NiS NPs were confirmed X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS) with mapping analysis. Optical studies showed that the synthesized NiS NPs are blue (lower wavelength) shifted relative to the bulk material. SEM image shows that the prepared nanoparticles were spherical in nature. The XRD patterns of the prepared NiS NPs revealed cubic crystalline phases. TEM images showed spherical morphological nature and the particle size was found around 23 nm. The elemental analysis and mapping spectra was confirmed to the formation of NiS NPs through the presence of Ni and S elements. And the prepared nanoparticles were examined to photocatalytic application and electrochemical studies.

Keywords: NiS Nano-catalyst, Single source precursor, Nano-catalyst, Microwave irradiation, Charge-discharge analysis, Photodegradation.

PP35

Synthesis and characterization of *calotropis gigantea* leaf extract capped ZnO based nanoparticles for environmental fortification

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Abstract

The concept of green chemistry and engineering has provided a new platform for the environmentally propitious synthesis, non-hazardous to the environment and human health. Now-a-days synthesis of nano-materials with plant extracts have been a source of brainwave in designing commercial products for promising applications like biosensors, photo catalysis, antimicrobial and antioxidant technologies, etc. In the present study, we reported for the synthesis of *Calotropis gigantea* (*C. gigantea*) leaf extract capped ZnO based nanoparticles (NPs) by a simple soft chemical route via green approach. The resultant products were thoroughly analyzed using different analytical techniques such as UV-Vis NIR spectrophotometer, photoluminescence spectrometer, Fourier Transform Infrared spectrophotometer and X-ray diffraction technique. The observed properties were compared with uncapped ZnO based NPs counterparts and reported. The XRD patterns reveal that the synthesized NPs exhibit clear crystallization with (101) as a growth direction. The optical studies indicate that the *C. gigantea* capped ZnO NPs show higher band gap when compared to the uncapped NPs. In PL spectra, both uncapped and *C. gigantea* leaf extract capped ZnO NPs showed two peaks at 395 nm and 426 nm corresponding to band edge and interstitial impurities emission, respectively. The synthesized NPs are evaluated using its antimicrobial efficacy for two different human pathogenic organisms such as *Escherichia Coli* and *Staphylococcus aureus*. It is shown that the *C. gigantea* leaf extract capped ZnO based NPs exhibit better antibacterial activity against human pathogens when compared to uncapped one.

PP36

Low cost economic routes for optical anti-refection (AR) window (pure IZO) thin films

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Abstract

In this work, economic way of preparing optical anti-refection (AR) window (pure IZO) thin films by low cost solution based techniques for commercial solar cells. This is a new feasibility study. The effects of optimization parameters on thin film growth, internal material properties, material characteristics such as structural, compositional, surface morphological, micro structural, and optical were studied in detail. The chemical and thin film strategies for the development of high quality optical AR applications using Chemical Bath Deposition, Spray Pyrolysis and Spin Coating are developed characterized and compared. To the best of our knowledge based on the literature survey this is the first time that we have got high quality pure IZO - AR thin films via novel solution based techniques for commercial solar cell windows. The visible transmittance is achieved is comparable to AR coatings developed by Physical techniques. The studies revealed the suitability of optimized conditions for preparing excellent AR thin films by each technique and the kinetics are discussed.

PP37

Growth and characterization of thiourea crystals

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Abstract

Non linear optical single crystals of Pottasium Chloride with Thiourea were grown from aqueous solutions by slow evaporation method at ambient conditions. The structure was confirmed by powder XRD. The functional groups have been confirmed by FTIR analysis. The density and melting point were measured for those PTC crystals. Their transmission was determined by UV- visible spectra and their hardness was found out increase with increase in load.

PP38

Fabrication of Hexagonal Disc Shaped Nanoparticles g-C3N4/NiO Heterostructured Nanocomposites for Efficient Visible Light Photocatalytic Performance

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Abstract

A hexagonal shaped nickel oxide/graphitic carbon nitride (NiO/g-C3N4) heterojunction composite was synthesized via a facile microwave irradiation route joint with succeeding calcination process. The structural, morphological and optical properties of the catalysts were characterized by XRD, TEM, Raman, UV–DRS, PL and BET analysis. XRD and TEM results exposed that cubic structure and with two dimensional hexagonal discs shaped morphology with sizes in the range of 30–40 nm. The incorporation of g-C3N4 caused a red-shift of the UV–Vis absorption edge of NiO. Moreover, exfoliation of bulk g-C3N4 into two dimensional g-C3N4 nanodiscs offers large surface area (102 m2 /g) and exposed active sites, which are beneficial for photocatalytic activity enhancement. The photocatalytic activity of the photocatalysts was analyzed by degradation of congo-red and malachite green (MG) under induced visible light irradiation. The results demonstrates that NiO/g-C3N4 with 1.2 mass ratios shows the optimal overall photocatalytic performance such as huge degradation efficiency (97%), high rate constant (0.02012 min-1) and high stability (only loss * 3.5) after 7 cycles test (for MG dye). The superior photoactivity of NiO–g-C3N4 photocatalysts possibly will be recognized to the successful interfacial charge transfer between NiO and g-C3N4, thus suppressing the recombination of the photoexcited electron–hole pairs.

Keywords NiO/g-C3N4 Microwave irradiation Visible light Electron–hole separation Congo-red

PP39

Construction of metal doped SnO_2 @MoS_2 composites with improved photo catalytic activities of methylene blue dye degradation

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Abstract

In this abstract, we report facile hydrothermal synthesis of Co, Mn and Ni doped SnO_2 @MoS_2 composite for photo catalytic degradation of organic dyes under visible light irradiation. The structural, optical, functional and morphological properties of the prepared material have been analyzed by using X-Ray diffraction, UV-Visible Spectroscopy, Fourier Transform Infrared Spectroscopy and Scanning Electron Microscope respectively. The average crystallite size was found in the range of 27.2 to 21.8nm The EDAX, Elemental mapping confirmed the presence of species of the prepared samples. SEM images revealed that the spherical morphology for the prepared samples. The XPS spectra revealed the binding energy and energy state of the Ni doped SnO_2 @MoS_2 samples. Further, the photo catalytic activities of metal (Co, Mn and Ni) doped SnO_2 @MoS_2 composite were analyzed by using methylene Blue as an organic dyes under visible light irradiation. The Ni doped sample has higher degradation efficiency (96%) compared to all other SnO_2 @MoS_2 samples after irradiation time of 90 min. The results will be discussed in detail.

Key Words: Methylene Blue, SnO_2 @MoS_2, Photocatalytic

PP40

High capable visible light driven photocatalytic activity of WO3/g-C3N4 hetrostructure catalysts synthesized by a novel one step microwave irradiation route

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Abstract

In this paper, WO3/graphitic carbon nitride (g-C3N4) composite photocatalyst were successfully synthesized using microwave irradiation method followed by annealing process at 400 °C for 2 h. Powder X-ray diffraction, Raman and transmission electron microscope results suggest that both pure and composite samples showed hexagonal-phase WO3 (JCPDS Card No. 83-950) with particle size around in 30–40 nm. The optical band gap and specific surface area of the g-C3N4/WO3 composites were in the range of 2.55–2.78 eV and 45–87 m2 /g, which is confirmed through UV–Vis diffuse reflectance (DRS) and N2 nitrogen absorption–desorption analysis. The photocatalytic activity of the photocatalysts was investigated by degradation of congo-red (CR) and malachite green (MG) under induced visible light irradiation. The results showed that WO3/g-C3N4 nanocomposite with a mass ratio of 1:3 (W1G3) showed the highest photocatalytic activity efficiency (93%) and high stability (only loss 3%) towards CR. The improved photocatalytic activity of the g-C3N4/WO3 composites is due to the synergistic effect of g-C3N4 and WO3 was considered to lead to improved photogenerated carrier separation. A possible degradation mechanism of CR over the g-C3N4/WO3 composite photocatalyst under visible light irradiation was also proposed.

PP41

Synthesis of self-assembled micro/nano structured manganese carbonate for high performance, long lifespan asymmetric supercapacitors

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Abstract

Recent advances in the development of manganese carbonate ($MnCO_3$) have opened up new attractive electrode material for supercapacitor applications. However, limited internal specific capacitance and long cycle stability of $MnCO_3$ due to its low electrical conductivity, poor interfacial properties and simple geometric configurations need to be further improved. Development of smart micro-nano architecture for electrode materials preparation is a critical challenge nevertheless it provides high specific capacitance, rich rate capability and long cycle stability. To achieve this, the facile strategy has been adopted to synthesis self-assembled micro-nano architecture of $MnCO_3$ via simple co-precipitation, microwave and hydrothermal-assisted methods. The optimized complex grain growth of 3D MS/NCs $MnCO_3$ electrode delivered an ultrahigh specific capacitance of 302.47 F g^{-1}, high rate capability and long cycle stability. Moreover, an asymmetric supercapacitor is employed in as-prepared 3D MS/NCs $MnCO_3$ as positive electrode and activated carbon as negative electrode which exhibits high energy density of 18.07 W h kg^{-1}, power density of 7498 W kg^{-1} and superior capacitance retention of 98.79% even after 10000 cycles. From these results, we concluded that the self-assembled micro-nano structures are preferred as the future promising electrode architecture for supercapacitors.

Keywords: $MnCO_3$, Morphologies, Efficient electrode properties, Asymmetric Supercapacitors.

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PP42

Synthesis and Characterization of Cadmium Sulfide (CdS) Nano Thin Films Prepared by Chemical Bath Deposition Method

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Abstract

In this work, thin CdS films have been deposited onto glass substrate using the chemical bath deposition technique (CBD). Different synthesis parameters, such as deposition temperature, deposition time, and post annealing temperature, were studied and optimized in order to avoid the super saturation phenomenon and to achieve a low-temperature growth. Structural identification was done by XRD method at 2θ lying between 0º and 80º. The XRD results showed that the deposited films were polycrystalline with cubic structure having the plane as preferred growth. SEM was utilized in the morphological study of the films. In addition, deposited films exhibit an optical transmittance ranging from 60 to 85% depending on the synthesis parameters, with band gap energy around 2.42 eV. Further, optical constants were studied using UV-Visible absorption spectrum. CdS films with excellent structural quality and a controllable thickness are obtained when the deposition bath temperature is fixed at 80 °C. The process developed in this work might be useful for depositing CdS films on flexible substrates.

Keywords: annealing, deposition, diffraction, scanning electron microscopy.

PP43

Synthesize of Fe doped CuO Nanostructures for Sustainable Energy Harvesting Application

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Abstract

The Fe doped CuO nanoparticles was synthesized through Co-precipitation method at 440℃ by using Copper Acetate and Iron Chloride anhydrous as starting materials with the presence of NaOH as stabilizing agent. The impact of doping on the structure and morphology was examined by X-ray diffraction (XRD) and Scanning Electron Microscope (SEM). No secondary segment was observed on monoclinic phase of Fe doped Copper Oxide. The carrier concentration and resistivity of the pelletized (7*14mm-diameter) Fe-CuO were determined through Hall measurements. The Hall coefficient confirms the p-type nature of Fe-CuO. Thus, the overall discussions of Fe-CuO deal with sustainable energy harvesting application.

Keywords: Hall measurement, Sustainable energy harvesting material, P-type Fe-CuO.

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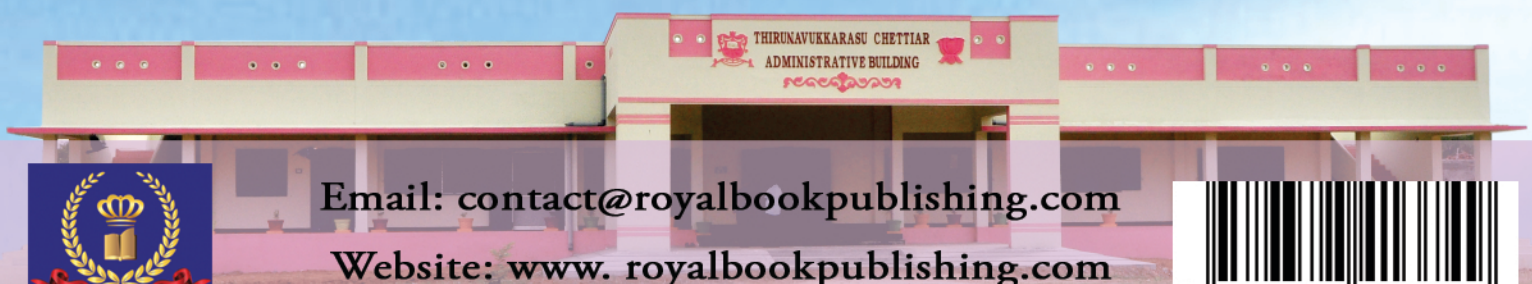

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