# SRINIVAS INSTITUTE OF TECHNOLOGY

(UNIT OF A. SHAMA RAO FOUNDATION)

VALACHIL, MANGALURU

NAAC ACCREDITED

# INTERNATIONAL CONFERENCE ON RECENT TRENDS IN APPLIED SCIENCES

## ICRTAS- 2022

ISBN: 978-81-956922-0-0

AUGUST 3rd & 4th 2022

# ABSTRACTS

ORGANIZED BY

DEPARTMENTS OF BASIC SCIENCE

## Building and Infrastructure Lab

## Founders Day


## Building and Infrastructure Library & Hostel

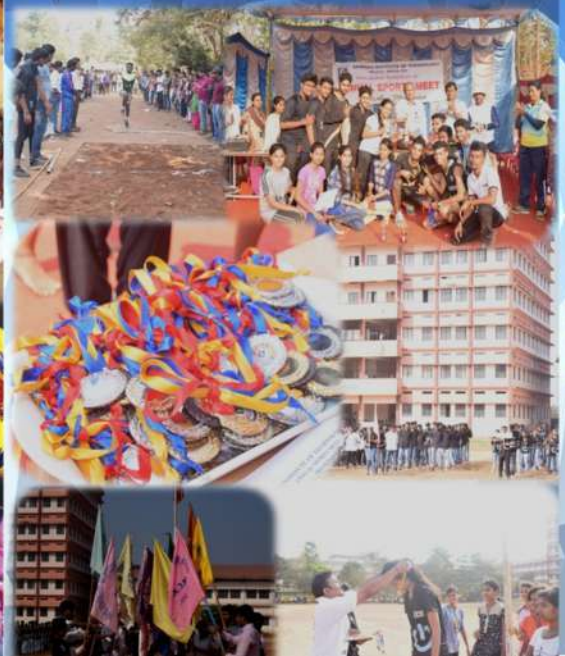
## Abhiyana

## Prathibha The talent show




## College Day

## Sports Day



## Graduation Day

*VISION*

*To be a premier institute of professional education and research, responsive to the needs of industry and society.*

*MISSION*

*To achieve academic excellence through innovative teaching-learning practice, by providing conducive research environment, industry-institute interaction and skill development, leading to professionals with ethical values and social responsibilities.*

## About Srinivas Group

Srinivas Group of colleges sponsored by A. Shama Rao foundation was established in the year 1988, with a vision of fastering excellent education. The group provides quality professional education in Medical, Allied Health Sciences, Pharmacy, Hotel Management, Business Management, Engineering, Education etc. Srinivas Group is well known for imparting innovative education and has state of the art facilities for education and training and also recognised as center of excellence in research across disciplines. The dedicated faculty believes in and works towards materializing the adage of "Education is our passion but not profession".

Srinivas Group of colleges is located in Mangaluru, the coastal city of Karnataka situated on the West Coast of India. It is ensconced between the Western Ghats and the Arabian Sea. Mangaluru well connected by air, road and rail. It is 342 Kms from Goa, 1050 Kms from Mumbai, 45Kms from Cochin on NH17 and Bangaluru is 380Kms on NH 48.

## About Srinivas Institute of Technology

Srinivas Institute of Technology (SIT) is one of the premier engineering colleges of the coastal region aiming towards high standards of education with holistic approach.SIT is recognised by AICTE, affiliated to VTU and accredited by NAAC. The Institute started in the year 2006, is a unit of A. Shama Rao Foundation, Mangaluru, and is located at the Srinivas Campus spread over 15 acres of land at Valachil, Arkula Village, about 10kms from Mangaluru city, adjacent to NH66. The institute hosts 3000 plus students studying under 12 UG, 5 PG programmes and 6 Research Centers

## About the Basic Science Departments

The Department of Physics, Chemistry and Mathematics is started in 2006. It has well-established laboratories equipped with sophisticated instruments, which fulfill the needs of UG and Ph.D. students. Now, the Department is offering Ph.D. in Physics and Chemistry. Based on the facilities available, the Department had been recognized as a Ph.D. research center by Visvesvaraya Technological University, Belagavi**.**

## About the Conference

The Conference is intended in bringing out the innovative ideas of academicians in science, Research scholars and students shall disseminate their original ideas and results to promote research and development activities, professional interaction and lifelong learning. Conference provides a platform to bridge the gap between industry and Academia. It also focuses on networking people with similar interests to have a collaborative work and to have better solutions to societal problems. The conference will be conducted in online mode.

**Best wishes from**

Dr. CA A Raghavendra Rao,

Chancellor, Srinivas University,

President, A Shama Rao Foundation

**Best wishes from**

Dr. A Srinivas Rao

Pro-Chancellor, Srinivas University,

Vice-President, A Shama Rao Foundation

# From the principal's desk


Dr. Shrinivasa Mayya D
Chairman ICRTAS-2022, Principal

Srinivas Institute of Technology

I am very happy to announce that the departments of basic science organizing two day International Conference on Recent Trends in Applied Science ICRTAS-2022 in Srinivas Institute of Technology.

I am sure that this conference provides a platform to receive ample information by the budding research scholars from international speakers of scientific community to explore their innovative ideas and keep in pace with emerging technological developments.

I extend my good wishes to the organizers and all the participants, for the grand success of the conference.

# PREFACE

**Recent Trends in Applied Sciences** is the international conference (ICRTAS-2022) organized by the departments of basic science of SRINIVAS INSTITUTE OF TECHNOLOGY. The conference has received an overwhelming response from scientists, academicians, industrialists and research scholars from various part of country, which is being indicated by the number of research papers received. In addition there are invited talks by eminent personalities from foreign countries. This souvenir contains the abstracts of various research papers reviewed by expert referees and selected for virtual oral presentation during the two days conference.

The main objective of the conference is to bring together scientists, academicians, industrialists and research scholars from various fields of science and technology to discuss modern developments in the field discussed in ICRTAS. This provides an opportunity for teachers and research scholars to interact with experts of their areas of interest, which will promote research activity.

This conference would not have become a reality without the encouragement and financial support of our management, Dr. CA A Raghavendra Rao, Chancellor Srinivas University, President A Shama Rao Foundation, Dr. A Srinivas Rao, Pro-Chancellor Srinivas University, Vice-President A Shama Rao Foundation and Directors of Srinivas group of colleges and Srinivas University. I am extremely grateful to each and every one. I also thank Sri Durga Laboratory Equipment Supplies for co-sponsoring the event

I am indebted to our beloved principal Dr. Shrinivasa Mayya D for the constant support and encouragement extended in organizing the conference. Strong support for the conference has come from all the participants who have promptly sent their papers and the invited speakers who have readily consented to deliver the inaugural and keynote address. I also should on record with gratitude, the unstinted support from members of various committees, my colleagues, nonteaching staff and students of SIT

I wish the conference would turn out to be a memorable event.

**Conveners**

# Organizing Committee

**Chief Patron**

Dr. CA A Raghavendra Rao

Chancellor, Srinivas University

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**Patron**

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Prof. Sadana, Assistant Professor, Department of Mathematics

# SRINIVAS INSTITUTE OF TECHNOLOGY

Valachil, Mangaluru 574 143

Accredited by NAAC

## Departments of Basic Science

*Cordially invite you to the Inaugural function of*

*A* ***Two day International Conference on***

# RECENT TRENDS IN APPLIED SCIENCE (ICRTAS) - 2022

*Wednesday, 3rd August 2022 at 9:30 am*

Presided by

**Dr. CA. A. Raghavendra Rao**

*Honourable Chancellor, Srinivas University &*
*President, A Shama Rao Foundation, Mangaluru*

Chief Guest:

**Dr. Vishnumurthy Hegde, Ph.D.**

*Group Leader, Adesis Inc (Universal Display Company)*
*Deleware, US*

Guest of Honour

**Dr. A. Srinivas Rao**

*Honourable Pro-Chancellor, Srinivas University &*
*Vice President, A. Shama Rao Foundation, Mangaluru*

**Dr. Shrinivasa Mayya D**

Principal

**Dr. Anant Kumar Kulkarni**
**HOD, Dept. of Mathematics**

**Dr. Suryanarayana K**
**HOD, Dept. of Physics**

**Dr. Gopalakrishna Bhat**
**HOD, Dept. of Chemistry**

**Faculty & Staff, Departments of Basic Science**

# A Two day International Conference on
# RECENT TRENDS IN APPLIED SCIENCE (ICRTAS) - 2022

DAY -1

Key Note Speaker:

**Dr. Vishnumurthy Hegde, Ph.D.**
Group Leader, Adesis Inc (Universal Display Company)
Deleware, US

**Dr. Ismail Naci Cangul, Ph.D.**
Bursa Uludag University, Bursa, Turkey.

DAY -2

Technical Talk:

**Dr. Subramanya Herle, Ph.D.**
CTO of Energy Storage & Sr. Director,
Applied Materials, Global Leader in semiconductor & Display equipment company,
Headquarters, California, US

Programme Schedule:

| Day/Date | Time | Activity/Topic |
|---|---|---|
| 3/8/2022 Wednesday | 9.30 AM - 10.30 AM | Inaugural and Keynote address by Dr. Vishnumurthy Hegde, Group Leader Adesis Inc (Universal Display Company) Delware, USA |
| | 10.45 AM- 12 Noon | Chemistry paper presentation by participants From C-1 to C-8 |
| | 12 Noon – 1.00 PM | Physics paper presentation by participants From P-1 to P-7 |
| | 2 PM- 3 PM | Keynote address by Dr. Ismail Naci Cangu Bursa Uludag University, Bursa, Turkey |
| | 3 PM - 4.15 PM | Maths paper presentation by participants From M-1 to M-8 |
| 4/8/2022 Thursday | 9.30 AM - 10.30 AM | Technical talk on Fostering innovation for a better world with materials engineering by Dr Subramanya Herle, CTO of Energy Storage & Sr. Director, Applied Materials, Global Leader in semiconductor and Display equipment company Headquarters, California. |
| | 10.45 AM- 12.15 PM | Chemistry paper presentation by participants From C-9 to C-17 |
| | 12.15 PM – 1.00 PM | Physics paper presentation by participants From P-8 to P-11 |
| | 2 PM- 3.30 PM | Maths paper presentation by participants From M-9 to M-18 |
| | 3.45PM- 4.15 PM | Feedback session |

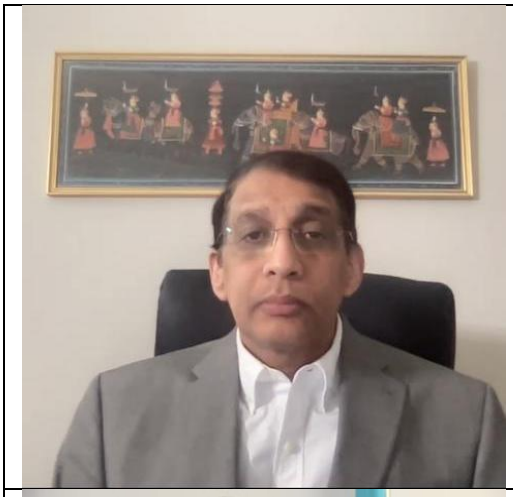
# INDEX

**CHEMISTRY**

**MATHEMATICS**

**PHYSICS**

# KEYNOTE SPEAKERS



## Prof. Dr. Vishnu Murthy Hegde

Group leader, adesis inc. (a universal display company)

Delaware, US

## Prof. Dr. Ismail Naci CANGUL

Uludag University

Faculty of Arts and Science

Department of Mathematics, Office No: 154

Gorukle, 16059

Bursa/Turkey

## Dr. Subramanya Herle, PhD

CTO of energy storage and Sr. Director**,**

Applied Materials, global leader in semiconductor & Display equipment company, Headquarters, California, US

# INAUGURAL ADDRESS

Vishnu Murthy Hegde, Ph. D.

Group leader, Adesis Inc. (A Universal Display Company), Delaware, US

## OLED TECHNOLOGY

Chemistry and Engineering

OLED (Organic Light Emitting Diodes) is a light emitting technology, made by sandwiching organic thin films between two conductors. When electrical current is applied, a bright light is emitted. OLEDs are emissive displays that do not require a backlight and so are thinner and more efficient than LCD displays (which do require a white backlight). The OLED display is based an organic substance used as the semiconductor material in light-emitting diodes (LEDs).

## KEYNOTE ADDRESS


# Prof. Dr. Ismail Naci CANGUL

Uludag University, Faculty of Arts and Science, Department of Mathematics, Office No: 154

Gorukle, 16059, Bursa/Turkey


Dear Organizers and Participants of the International Conference on Recent Trends in Applied Sciences (ICRTAS-2022) organized by Srinivas Institute of Technology Mangaluru. I am very happy, honored and excited to be a part of this International Conference. I especially thank to the Head of Department of Mathematics, Dr. Anantha Kumar Kulkarni for the kind invitation.

Mathematics is the most eminent and trustable science. A theorem does not loose its truth in years. It is timeless. It does not depend on the place where it has been proven. There is a book of Springer-Verlag. It is called Proofs from the Book. It is about the beautiful proofs which are appreciated by the genius mathematician Paul Erdos who lived in the 20th century. The very first proof is about the infiniteness of the prime numbers. It was proven in the third century BC. After 2300 years, it is still valid and it is still appreciated. It will be the same after thousands of years. This shows the power of mathematics. There is no other science where the information keeps its beauty and truth for such a long time. A chemical theory like atom theory keeps changing every five to ten years due to technological developments such as the electron microscope. In medicine, every 2-3 years, techniques change and the old techniques are

demolished. In social sciences, the situation is worse. There could be more than one theory on the same subject by more than one academician and you have to decide which one to support and use keeping in mind that many other wise people will be supporting other theories.

In the history, the development of mathematics depended on the civilization. In some civilizations, mathematics is done for purely theoretical purposes and in some of them, for applications in real life. For example, in Ancient Indian and Egyptian Mathematics, all mathematics problems were about the daily life. But in Roman Empire, most of the mathematics was dealing with abstract equations without any particular applications. That is why the equations having all the coefficients and all the roots as integers are today called as Diophantine equations after the famous mathematician Diophantus.

The last century was the golden age for pure mathematics. Many mathematicians freely involved in pure mathematical theories without worrying about their applications. But in the last 30-40 years, with the advances in technology, governments started to ask to scientists to produce some practical applications out of their scientific works. This mostly affected mathematicians. To get their papers published, to be involved in scientific projects, to get appointed, etc., mathematicians need to concentrate on applications more than theory. I think this is a very serious problem. Without theory, no applications are possible. Without research and development, no new applications can be obtained. We must involve good students in Mathematics research.

These kind of meetings are very important to share our findings¸ to learn from each other, to get motivated by what the others doing. Each time I come back from a meeting, I feel like I know nothing. I learn a lot from every talk. I suggest the young mathematicians to attend as many meetings as possible and to listen all the talks. Even if a talk is not related to your study area, it is likely that you will learn something from that talk, a formula, a technique, a different view of looking, a newidea…

So once more, I would like to thank the staff of Mathematics Department at Srinivas Institute of Technology in Mangaluru for organizing such a nice meeting and inviting me. I sincerely hope that it will be a fruitful meeting to all participants and everyone will benefit from it.

# *CHEMISTRY*

**C-01**

# SYNTHESIS OF (2-(4-HALOSUBSTITUTED PHENYL) QUINOLIN-4-YL)(5-(4-HALOSUBSTITUTED PHENYL)-3-PHENYL-1H-PYRAZOL-1-YL)METHANONE AND IT'S PHARMACOLOGICAL ACTIVITY

Venuprasad K.D[1*], Balakrishna Kallauraya[1] Alphonsus D'Souza[2], Gururaja .R [3]

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[2] Department of Studies in Chemistry St.Philomenas College(Autonomous) Mysuru .570015.Karnataka, India

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Synthesis of hitherto unreported title compound was prepared as outlinein the scheme (2-(4-halosubstituted phenyl)quinolin-4-yl)(5-(4-halosubstituted phenyl)-3-phenyl-1H-pyrazol-1-yl)methanone was prepared according to literature method. The 2 phenyl Quinoline -4-carbohydrazide was prepared by using hydrazine hydrate in the presence of alcohol medium and 1-(3- halosubstituted phenyl)-3-(4-halosubstituted phenyl)prop-2-yn-1-one was synthesised by Bromination of chalcone in the presence of drybenzene and $Et_3N$, finally it is coupled with hydrazide in the presence of sodium acetate and triethylamine under alcoholic medium, it was refluxed for 6hrs to obtain desired compounds, and these compounds were Screened for pharmacological activities but all compounds are potent antifungal agent and not antibacterial.

KEYWORDS: antifungal agent, non antibacterial.

**C-02**

# SYNTHESIS, CHARACTERIZATION AND FLUORESCENCESTUDY OF METHOXY NAPHTHALENE CHALCONE

Priyanka Mahesha[1] , Nitinkumar S. Shetty[1]*, Suresh D. Kulkarni [2]

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In the present scenario, fluorogenic compounds get more attention in the field of optoelectronics, sensors, bioimaging probes, etc. Hence researchers were more interested in the facile synthesis of these types of fluorophore materials. Hereby we report new fluorophore (2E)-3-(4-fluorophenyl)-1-(6- methoxynaphthalen-2-yl)prop-2-en-1-one(**MNC**) synthesized from methoxy naphthalene ketone. Thiscompound was characterized by IR, 1H, and 13C NMR. The emission behavior was studied at differentconcentrations. The emission maxima were centered at 432nm with the slight shoulder at 455nm. The 0.1mM concentration was more emissive than any other lower and higher concentration. The quantum efficiency of the molecule was also distinct. The Commission Internationale de l'Elcairage(CIE) color coordinates showed violet emission in the solution state(0.15.0.06).

KEYWORDS: Emission, Naphthalene, Fluorophore, CIE.

**C-03**

# ELECTROCHEMICAL INVESTIGATION OF AN ECO-FRIENDLY IONIC LIQUID AS CORROSIONINHIBITOR ON 6061Al-10(VOL.%) SiC(P) COMPOSITE IN HCl

Namitha K[1], Padmalatha Rao[1], and Suma A Rao[1]*

[1] Department of Chemistry, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal,
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In this study, the corrosion inhibition efficiency of ionic liquid 1, 3 dimethyl imidazolium dimethyl phosphate (DIDP) on 6061Al-10 vol% SiC(P) composite material was studied in 0.05 M HCl. Electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) techniques were adopted for corrosion rate measurements. Conditions were optimized to achieve maximum inhibition efficiency by varying inhibitor concentration and temperature. Kinetic parameters were calculated using the Arrhenius rate law equation and the transition state equation. Results were fitted into various adsorption isotherms from which thermodynamic parameters were evaluated. Surface morphology studies like SEM, AFM, and XRD were performed before and after the addition of DIDP. With the increase in DIDP concentration, inhibition efficiency increased. Maximum efficiency of about 90% was shown at 1000 ppm of DIDP concentration at 303 K. Inhibition efficiency decreased with an increase in temperature, accounting for physical adsorption of DIDP. DIDP behaved as a mixed type of inhibitor. Surface morphology results showed more roughness in 6061-aluminum composite material immersed in 0.05 M HCl in the absence of DIDP compared to composite material in the presence of DIDP inhibitor. DIDP emerged as an efficient, eco-friendly green inhibitor.

KEYWORDS: Corrosion; electrochemical studies; adsorption; 6061Al-SiC composite; ionic liquid; surface studies.

**C-04**

# PREPARATION AND CHARACTERISATION OF ARECA CELLULOSE -G- POLY (N, N- DIMETHYLACRYLAMIDE) HYDROGELS INCORPORATED WITH MAGNETIC NANOPARTICLES

Smitha Rai[1], Vishalakshi B[2], K.M. Usha[1]

[1] Department of Studies in Chemistry, University College, Mangalore -575001.

[2] Department of Post Graduate Studies and Research in Chemistry, Mangalore University,Mangalagangotri-574199.

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Cellulose, a major part of all plants is not utilized at its best. Areca nut husk fibers are easily available and are abundant agricultural waste, whose utilization needs more attention. Hence the present study involves the potential use of cellulose fibres from the husk of *Areca catechu.* Hydrogel system composing of areca cellulose and N, N'-dimethylacrylamide (DMA) was prepared using ammonium peroxodisulfate (APS) as an initiator under microwave irradiation condition in the presence of N, N-methylenebisacrylamide (MBA) as a crosslinker. The magnetic nanoparticle incorporated hydrogels (CF-g-PDMA/Fe O ) was incorporated into grafted hydrogel (CF-g-PDMA). The magnetic nanoparticle incorporated hydrogels were then characterised using Fourier transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA), Powder X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM). The swelling behavior of the hydrogel was studied under different pH conditions and the swelling parameters were evaluated.

KEY WORDS: Cellulose Fibres, Hydrogel, Magnetic nanoparticles.

**C-05**

# BIOSYSNTHESIS OF SILVER NANOPARTICLES USING MUSA PARADISIACA (KADALI)AND ITS ANTIMICROBIAL ACTIVITES

Crystal Menezes[1], Minolin Pinto[1]

[1]Department of Chemistry, St Aloysius College (Autonomous), Mangaluru

Nanotechnology is a new and emerging technology with wealth of applications. It involves the synthesis and application of materials having one of the dimensions in the range of 1-100 nm.. Nanobiotechnology is a field that interrelates both biological sciences and nanotechnology. It provides a platform for the development of eco-friendly and the green synthesis of nanoparticles with the help of biological sources like plants and microorganisms.
Nanoparticles exhibit completely new or improved properties based on specific characteristics, such as size, distribution and morphology.

Metal nanoparticles have been of great interest due to their distinctive features such as catalytic, optical, magnetic, and electrical properties. Nanoparticles of noble metals, such as silver, gold and platinum, are widely applied in products that directly come in contact with the human body, such as shampoos, soaps, detergent, shoes, cosmetic products, and toothpaste, besides medical and pharmaceutical applications. The silver nanoparticles have various important applications. Historically, silver has been known to have a disinfecting effect and has been found in applications ranging from traditional medicines to culinary items. It has been reported that silver nanoparticles are non-toxic to humans and most effective against bacteria, virus and other eukaryotic microorganisms at low concentrations and without any side effects.

Silver nanoparticles were produced by the direct interaction of silver nitrate with peel extract in aqueous media without the intervention of any external man-made chemicals. Therefore, this reaction pathway satisfies all the conditions of a 100 % green chemical process. The amount of plant material is found to play a critical role in controlling the size and size

dispersity of nanoparticles. The methodology employed here is very simple, easy to perform, inexpensive, and eco-friendly. The colloidal solutions are stable, suggesting that CBPE can

be used as both reducing and stabilizing agent for the preparation of Ag nanoparticles. High pressure or temperature is not required for the green synthesis of NPs, and the use of toxic and hazardous substances and the addition of external reducing, stabilizing, or capping agents are avoided. Detection and characterization of biosynthesized NPs are conducted using different techniquessuch as UV-visible spectroscopy, FT-IR, XRD, BET.

KEY WORDS: Silver Nanoparticles, Biosynthesis, Musa paradisiacal, anti microbial

**C-06**

# SYNTHESIS, GROWTH AND CHARACTERIZATION OF NONLINEAR OPTICAL CRYSTALS OF GLYCINE SUCCINATE AND HISTIDINE SUCCINATE

Sahana A[1], Sahana Devadiga[2]

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[2]Assistant Professor of Chemistry, St Aloysius College (Autonomous), Mangalore

Nonlinear optical crystals of Glycine Succinate and Histidine succinate were grown from a mixed solvent of water, ethanol and methanol. Since amino acid exhibits nonlinear optical property, it is of interest to dope them in glycine and Histidine. The overwhelming success of molecular engineering in controlling nonlinear optical properties in last decade has prompted better initiative in crystal engineering.

In the present crystals of glycine and histidine doped with succinic acid have been grown by slow evaporation method. Grown succinate crystals were subjected to FTIR analysis. To confirm the synthesized compound and the functional groups of Glycine and histidine succinate crystal were identified from FTIR analysis.

KEYWORDS: Non linear optic crystals, amino acids, Glycine succinate, Histidine succinate, slowevaporation, crystal growth method, Seed crystal growth method, IR spectroscopy.

**C-07**

# EFFECTUAL INHIBITION OF MILD STEEL BY N-SUBSTITUTED SULFONAMIDEDERIVATIVE: EXPERIMENTAL AND COMPUTATIONAL TECHNIQUES

Pramila D'Souza[1], Jyothi Kudva[1], Sunil Kumar[2] & Prathima Shekara[1]

[1]Department of Chemistry, St Joseph Engineering College, Mangaluru, India

[2]Unichem Laboratories, Goa, India Corresponding

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N-(pyridin-2-yl)-4-[(quinazoline-4-yl)amino]benzene-1-sulfonamide (NPQS) was investigated as a corrosion inhibitor on mild steel in 0.5M HCl solution. The experimental techniques used are potentiodynamic polarization, electrochemical impedance spectroscopy, SEM and EDS. The efficacy of inhibition rises with inhibitor concentration but declines with the ascent in solution temperature. The thermodynamic parameters have been evaluated and the adsorption study of NPQS heeded Langmuir adsorption isotherm. A computational investigation was probed on NPQS using density functional theory (DFT) at the B3LYP/3-21G basis sets level to evaluate the association of their molecular and electronic structure. The calculated quantum chemical parameters comprise of $E_{HOMO}$ (highest occupied molecular orbital), $E_{LUMO}$ (lowest unoccupied molecular orbital), $\Delta E$, absolute electronegativity, softness, global hardness, binding energy, molecular surface area and fraction of electrons transferred from the inhibitor molecule to the metal surface. The results of experimental and computational techniques affirm NPQS as an effectual corrosion inhibitor.

KEYWORDS: Sulfonamide derivative, Mild steel, Corrosion inhibition, Electrochemical techniques, Density functional theory

**C-08**

# SYNTHESIS, CHARACTERIZATION AND DFT STUDIES OF 1,3-THIAZOLE DERIVATIVES

Sheethal Fernandes[1], Jyothi Kudva[1], and Smitha D'Souza[1]

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Thiazole is one of the most versatile scaffolds which display a diverse range of pharmaceutical and chemical applications. The extending applications of thiazole derivatives have drawn interest to synthesize thiazole derivatives. In the present study, ethyl 4-methyl-2-(phenylsulfonamido)thiazole-5-carboxylate (Compound **1**) and 4-methyl-2-(phenylsulfonamido)thiazole-5-carboxylic acid (Compound **2**) were synthesized. The synthesized derivatives were characterized for their physiochemical data and the structures were validated by FT-IR, $^{1}H$, and $^{13}C$ NMR spectroscopy techniques. The interpreted IR data was compared with theorical dataobtained from density functional theory (DFT) calculations. Frontier molecular orbitals HOMO-LUMO gap and electron densities of the compounds have been conducted by DFT methods with B3LYP/3-21G basis sets level. The nucleophilic and electrophilic sites were analysed from Mulliken charges. The study presents the efficient synthesis of thiazole derivatives using mild reagents in higher yields and the properties are supported by the computational studies. Consequently, present work offers significant insights empirically and theoretically to develop thiazole analogues

KEY WORDS: Synthesis, Thiazoles derivatives, Characterization, Density Functional Theory calculations

**C-09**

# SYNTHESIS OF FUSED PYRAZOLE AND THIAZOLE DERIVATIVES AS ANTIMICROBIAL CANDIDATES WITHMOLECULAR DOCKING STUDIES

Nagma Banu H A[1*] Balakrishna kalluraya[1]

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Heterocyclic compounds containing thiazole embedded with pyrazole moieties were designed viaclaisen schmidth reaction and the condensation reaction with substituted phenacyl bromide. Their structures were confirmed by FTIR,$^{13}$C-NMR,$^{1}$H-NMR and mass spectral analysis. All the compounds were screened for their antimicrobial activity. Molecular docking studies were performed to check the insights of the activity experimentally and theoretically.

KEYWORDS: Thiazole, Pyrazoline, Antimicrobial, molecular docking.

**C-10**

# SYNTHESIS CHARACTERIZATION AND QUANTUM CHEMICAL CALCULATION OF SULFONAMIDE QUINAZOLINE DERIVATIVE

Smitha Maria D'Souza[1], Jyothi Kudva[1], Sheetal Tresa Fernandes[1]

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Email ID: smithamaria05@gmail.com

In view of the significant biological activities of quinazoline derivatives, one such compound has been synthesized and characterized by FT-IR, 1H and 13C NMR, HRMS and mass spectra. The synthesis involves the reaction of N, N-2-chloro-4-amino-dimethylformamidine with commercially available sulfa drug. The obtained compound is 4-[(7-chloroquinazolin-4-yl)amino]-N-(pyrimidin-2-yl)benzene-1-sulfonamide (CNPS). A computational investigation was probed on CNPS using density functional theory (DFT) at the B3LYP/3-21G basis sets level to evaluate the relation of molecular and electronic structure. The quantum chemical parameters calculated consists of the following study: ΔE, absolute electronegativity, softness, EHOMO (highest occupied molecular orbital), ELUMO (lowest occupied molecular orbital), global hardness, binding energy and molecular surface area. The data proves that this derivative is well capable of exhibiting exuberant properties as antimicrobial, anticancer, antitubercular, antimalarial and many other biological activities.

KEY WORD: Quinazoline-sulfonamide, DFT, quantum chemical parameters.

**C-11**

# SYNTHESIS AND CORROSION INHIBITION STUDIES OF A NEW PYRAZOLINE DERIVATIVE

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A new methyl phenyl and carbothiamide based pyrazoline derivative (MMCP) was synthesized and the compound was confirmed by the spectral analysis using FT-IR, mass, $^{1}H$ and $^{13}C$NMR spectra. The electrochemical studies consisting of electrochemical impedance spectroscopy and Tafel polarization techniques were carried out to evaluate MMCP as corrosion inhibitor on mild steelin 0.5M HCl solution. The concentration of the inhibitor was varied from 10ppm to 40ppm at the temperature range from 303K to 323K. The change in the free energy of the adsorption and slopes of Tafel plot reveal mixed type corrosion inhibition of MMCP. The theoretical analysis of the inhibition effect was performed with quantum chemical calculations using density functional theory (DFT). The scanning electron microscopy with EDX studies and UV-Visible spectroscopy study confirmed the formation of the metal-MMCP complex. The experimental and theoretical data proved MMCP as a potent corrosion inhibitor ata considerably low concentration.

KEY WORDS: Pyrazoline derivative, Electrochemical studies, Inhibitor, Complex

**C-12**

# EFFECTUAL INHIBITION OF MILD STEEL BY N-SUBSTITUTED SULFONAMIDE DERIVATIVE: EXPERIMENTAL AND COMPUTATIONAL TECHNIQUES

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N-(pyridin-2-yl)-4-[(quinazoline-4-yl)amino]benzene-1-sulfonamide (NPQS) was investigated as a corrosion inhibitor on mild steel in 0.5M HCl solution. The experimental techniques used are potentiodynamic polarization, electrochemical impedance spectroscopy, SEM and EDS. The efficacy of inhibition rises with inhibitor concentration but declines with the ascent in solution temperature. The thermodynamic parameters have been evaluated and the adsorption study of NPQS heeded Langmuir adsorption isotherm. A computational investigation was probed on NPQS using density functional theory (DFT) at the B3LYP/3-21G basis sets level to evaluate the association of their molecular and electronic structure. The calculated quantum chemical parameters comprise of $E_{HOMO}$ (highest occupied molecular orbital), $E_{LUMO}$ (lowest unoccupied molecular orbital), $\Delta E$, absolute electronegativity, softness, global hardness, binding energy, molecular surface area and fraction of electrons transferred from the inhibitor molecule to the metal surface. The results of experimental and computational techniques affirm NPQS as an effectual corrosion inhibitor.

KEYWORDS: Sulfonamide derivative, Mild steel, Corrosion inhibition, Electrochemical techniques, Density functional theory

**C-13**

# REMOVAL OF BASIC DYE FROM AQUEOUS MEDIUM USING A NOVEL AGRICULTURALWASTE MATERIAL: ANNONA SQUAMOSA PEEL POWDER

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In the present study Annona Squamosa peel powder (ASPP), a agricultural waste, was activated by carbonizing in a Muffle Furnace to improve its surface adsorption capacity and used as an adsorbent for removal of Rhodamine Blue (RhB) from aqueous solution. Carbonization of the bioadsorbent plays a key role in efficient adsorption which is proved by surface analysis of the bioadsorbent by Scanning Electron Microscope before and after adsorption. The color removal performance of ASPP has been investigated using parameters such as initial dye concentration (10-40ppm), pH (3-7), time of contact (15-90 min) and adsorbent dosage (0.1-0.6 mg/50ml). Adsorption was favorable at slightly acidic condition and the maximum removal was obtained at pH 6. Percentage of dye removal was maximum when the contact time was 75 min (81.5%) and adsorbent dosage of 0.3mg/50ml (85.3%). The kinetic studies revealed that the kinetic data fitted well with pseudo first order model. The isotherm study indicated that RhB adsorption on ASPP is in agreement with Langmuir Model. The results show that ASPP can be a promising alternate for the removal of RhB from aqueous solutions and effluents.

KEYWORDS: Rhodamine Blue, Annona Squamosa Peel Powder, Langmuir isotherm,Pseudo first order Model.

**C-14**

# FORMULATION AND EVALUATION OF CURCUMIN, HONEY AND SILVER NANOPARTICLES FOR ANTIBACTERIAL AND BURN WOUND HEALING

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Wound healing is a complex and active mechanism that involves restoring the skin and tissue after an injury itself. There are a number of factors that would affect wound healing, including oxygenation, sex, age, nutrition, hormones, drugs, diabetes, eating habits, smoking, and alcoholism. Nanotechnology is on the verge of offering a range of innovative technologies and methods that would revolutionize the medical and pharmaceutical sectors. The present study was aimed to assess the antibacterial and wound healing activity of curcumin, honey, hydrogel embedded silver nanoparticles in experimental animal rat. Six formulations i.e., F1, F2, F3, F4, F5 and F6 of Silver nanoparticles embedded hydrogels were prepared and were subjected for characterization using UV Spectroscopy, Scanning electron microscopy (SEM) and X-ray diffraction analysis. SEM clearly showed the presence of synthesized nanoparticles. F2 formulation showed the maximum zone of inhibition which is a clear indication of the antibacterial activity. F2 formulation was found to be very good as compared to all other formulation. All the evaluation parameters shows good activity but formulation F2 was found to be the optimum and a very good antimicrobial agent. In the rat model silver nanoparticles hydrogel was more successful in burn wound healing than the commercially available brand of Silver sulfadiazine gel which was taken as standard.

KEYWORDS: Wound healing, Nanotechnology, Hydrogel, SEM, X-ray diffraction, UV Spectroscopy.

**C-15**

# DESIGN, SYNTHESIS AND ANTIDIABETIC EVALUATION OF SOME NEW COUMARININCORPORATED 1,3,4-OXADIAZOLE DERIVATIVES

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Objective: *In-silico* analysis of some new coumarin incorporated 1,3,4-oxadiazole derivatives as potential α-glucosidase and α-amylase enzyme inhibitors were designed and synthesized for antidiabetic activity.

Methodology: A series of coumarin incorporated 1,3,4-oxadiazole derivatives (No. 1-10) were synthesized and were subjected to in-silico analysis against human α-glucosidase (PDB ID: 5NN8) and α-amylase (PDB ID: 2QV4) enzymes. The GLIDE module of Schrodinger suite 2020-4 was employed in the molecular docking studies. The Prime MM-GBSA tool wasused in determining the free binding energies while the QikProp tool was employed in screening of the ADME properties of the designed compounds. Structural characterization of the synthesised compounds was done by IR, $^{1}$H NMR and mass spectroscopy. Invitro antidiabetic studies were done against α-glucosidase and α-amylase enzyme inhibition assays with acarbose as the standard.

Results: The compounds No. 8 and No. 7 showed significant antidiabetic activity compared to acarbose, against α-glucosidase and α-amylase respectively, which was also incorrespondence with the results of the molecular docking studies. Compound No. 4 was found to be effective against both the target enzymes. The in-silico studies showed that the designed compounds followed the Lipinski's rule of five and the values of different ADME parameters studied were within the acceptable range.

Conclusion: All the compounds showed moderate to good target enzyme inhibition. Compounds No. 7, No. 8 and No. 4 can be considered as lead molecule in further development of potential α-glucosidase and α-amylase inhibitors to reduce postprandial hyperglycaemia in the treatment of type II Diabetes.

KEY WORDS: Molecular docking , Coumarin, Oxadiazole, Antioxidant, Antidiabetic,

**C-16**

# DESIGN AND ANTIBACTERIAL EVALUATION OF BENZOPYRAN-2-ONE DERIVATIVES

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Background: The overuse and misuse of marketed antimicrobial agents had developed drug resistance which became a major problem faced today worldwide. With different pharmacological traits of oxadiazole and coumarins derivatives, a new series of coumarinyl -oxadiazole Schiff base derivatives were designed and synthesized. All these synthesis molecules FP1-FP7 were characterized using IR, $^{1}$H NMR and mass spectroscopy and evaluated for their antibacterial potential against Gram-negative (*E. coli, P.aeruginosa*) and Gram-positive (*B. subtilis, S. aureus*) bacterial strain by measuring Minimum Inhibitory Concentration values.

Result: Among all synthetic's compounds, FP6 was found to be the best antibacterial agent having concentration values of 3.12 and 6.25 µg/ml against Gram-negative bacteria and Gram-positive bacteria respectively. Compounds FP1-FP7 binding interaction with receptor Staph Gyrase B 24kDa (PDB code: 4URM) were also studied and docking score was in the range of -5.18 to -3.87 kcal/mol. Compounds FP6 and FP5 showed the best interaction with docking scores -5.18 and -5.17 kcal/mol respectively.

Conclusions: The antibacterial result showed satisfying structure-activity states the antibacterial potential was highly influenced by electron density of coumarinyl -oxadiazole moiety. Also, the binding affinity with Staph Gyrase B 24kDa during molecular docking promote the synthetic research work. Hence, coumarinyl -oxadiazole Schiff base derivatives could be a satisfying lead molecule as an antimicrobialagent.

KEYWORDS: coumarin, oxadiazole, antimicrobial activity, drug resistance, molecular docking. Minimum inhibitory concentration

**C-17**

# COMPARISON OF PHOTOCATALYTIC ACTIVITY OF ZnO NANOPARTICLES FOR THEREDUCTION OF $Cr^{+6}$ TO $Cr^{+3}$

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ZnO nanoparticles (ZnO NPs) were successfully synthesized by the simple and low-cost solgel and surface directing agent (SDA) Hi-AL N-Cetyl–NNN-Trimethyl ammonium bromide (Hi-AL) assisted sol-gel methods for the first time for photocatalytic reduction of $Cr^{6+}$to $Cr^{3+}$.Physico-chemical properties of the obtained photocatalysts were investigated via thorough characterizations. The crystalline structure and phase purity of the prepared photocatalysts were established by X-ray diffraction (XRD). XRD pattern reveals hexagonal wurtzite structure with higher phase purity and crystalline structure. Fourier transform infrared (FTIR) spectrum indicates the presence of ZnO stretching vibration. UV-Visible spectra of the ZnO nanoparticle by Sol-Gel method (ZnO sol-gel) and Surface Directing Agent Assisted Sol-Gel method of ZnO nanoparticles (ZnO SDA sol-gel) shows a maximum absorbance at 330 nm corresponding to a band gap of 3.460 eV which was blue shifted compared to that of bulk ZnOnanoparticles (3.370 eV).The blue shift may be due to quantum size effects. . UV-Visible spectra of SDA sol-gel method shows the maximum absorbance at 360 nm corresponding to a band gap of 3.100 eV, which was red shifted compared to ZnO sol-gel as well as bulk ZnO. This indicates that ZnO SDA sol-gel have much stronger absorption than that of Zn nanoparticles by Sol-Gel method, i.e., ZnO nanoparticles possess higher photo catalytic activity than ZnO nanoparticles by Sol-Gel method. Scanning electron microscope (SEM) image of ZnO nanoparticles by Sol-Gel method shows that the nanoparticles are agglomerated during the formation stage itself to form very tiny crystals. ZnO nanoparticles by surface directing agent assisted sol-gel

method shows porous network with lot of voids this kind of morphology this kind of morphology is because of addition Surface Directing Agent is very useful during the adsorption and absorption of water or $K_2Cr_2O_7$ solution during the photocatalytic reduction of $Cr^{6+}$ to $Cr^{3+}$. Energy dispersive X- ray spectroscopy (EDS) clearly shows the presence of Oxygen and Zinc in the the prepared photocatalysts. Transmission electron microscopy (TEM) image of ZnO nanoparticles by Sol-Gel method shows particles are almost irregular sized with lot of aggrication with average size ~ 40nm, whereas TEM image of ZnO by Surface Directing Agent assisted Sol-Gel method shows spherical particles with less agglomeration as compared to that of ZnO nanoparticles by Sol-Gel method this is because addition of Surface Directing Agent which reduces the surface tension,increase the solubility of the reactants and reduce the self assembling process. ZnO by surface directing agent assisted sol-gel method exhibited good photocatalytic reduction of $Cr^{6+}$ to $Cr^{3+}$ than the normal sol-gel method in both visible and UV-light sources, this is because of porous network with lot of voids, lower band gap, 2% higher quantum yield than ZnO by sol-gel method. Effectof $Cr^{6+}$ concentrations (Fig 1), effect of catalytic loads (Fig 2), effect of pH (Fig 3) and effect of recycle on the photocatalytic reduction of $Cr^{6+}$ to $Cr^{3+}$(Fig4) were explore.

KEY WARDS: ZnO nanoparticles; sol-gel; surface directing agent; photocatalytic reduction of $Cr^{6+}$ agglomeration.

**C-18**

# ELECTRODEPOSITION METHOD FOR THE DEVELOPMENT OF A PT-RH ALLOY COATING: AN EFFICIENT MATERIAL FOR THE PHOTOCATALYTIC APPLICATION

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A method of electroplating a platinum-rhodium(Pt-Rh)alloy coating with a specified composition on a metal substrate stainlesssteel(SS304) is presented in this article.The Pt-Rh bath consists of $[Pt(NH_3)_2]HPO_4$, $H_2SO_4$ and $Rh_2(SO_4)_3$. The Pt-Rh alloy electrodeposition coatings were characterized by different analytical methods such as Scanning Electron Microscopy(SEM) and X-raydiffraction(XRD). SEM images justifies that coating is uniform in 75% dutycycle. XRD confirms that crystalline size was reduced from 75% dutycycle to the rest of the PC's coating sand DC(Directcurrent).Incorporation of the Pt-Rh metal ions was verified by EDX analyses. A photocatalytic degradation study of Pt-Rh coating was conducted for Methylene Blue(MB)dyes under UVlight radiation.PC 75% duty cycles showed an exceptional dye degradation percentage compare to DCcoating source. All photocatalytic behaviour was controlled by using UV–Visspectrophotometer.

KEYWORDS: Platinum-Rhodium, SS304, SEM, XRD, Dye degradation.

**C-19**

# DEVELOPMENT OF PLATINUM COATING BY ELECTRODEPOSITION TECHNIQUE AND APPLICATION IN HYDROGEN GENERATION

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A thin layer of platinum coating (0.5 µgcm$^{-2}$) on stainless steel surface was deposited by direct current (DC) and pulse current (PC) electrodeposition method for hydrogen evolution reaction (HER) application. Scanning electron microscopy (SEM), atomic force microscopy (AFM)and X-ray diffraction (XRD) analysis were used to characterize the coatings. Linear sweep voltammetry (LSV) and cyclic voltammetry (CV) studies were carried out to know the over potential values for hydrogen evolution reaction (HER) on these coatings. The optimization of catalytic activity for hydrogen evolution using different coating methods helps in reducing the overall cost. Tafel polarization experiments were conducted for DC and PC platinum coating to know hydrogen generation trend. Cathodic slope and HER current values revealed that, coatings obtained at 75% duty cycle by PC method exhibit lower cathodic slope, high current density of 150 mA/cm $^2$ and more corrosion current with highest hydrogen evolution. Chronopotentiometry experiments showed that 20 ml of hydrogen collected by for 75% sample.

KEYWORDS: Electrodeposition, Platinum, HER, LSV, Chronopotentiometry.

**C-20**

# HIGHLY EFFICIENT MOLYBDENUM OXIDE NANOFLAKES FOR LITHIUM ION STORAGE

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Solution based combustion method synthesis of porous $MoO_3$ nanoparticles in one step by using ammonium heptamolybdatepentahydrate as a precursor with novel areca seed powder as green fuel. The analytical techniques like PXRD, FTIR, SEM, HRTEM, SAED were recorded in order to detect morphology, structure and composition of synthesised material. The obtained average crystalline size from XRD analysis was found to be 20nm with TEM analysis of particle size ranging from 2-10nm. As prepared material shows high specific capacity of 980 $mAhg^{-1}$and excellent run of about 400 cycles with extraordinary cycling performance of 652 $mAhg^{-1}$ after 200 cycles including enhanced rate capability of 564$mAhg^{-1}$ even at high current rate and thereby proving the auspicious anode material for lithium ion batteries.

KEY WORDS: Areca seed; Li-ion: Anode; Charge-discharge: Chronopotentiometry

**C-21**

# SUSTAINED DRUG RELEASE STUDIES OF GUAR GUM/CARBOXYMETHYL CELLULOSE BLEND - ZINC OXIDE NANOCOMPOSITES

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Zinc oxide (ZnO) nanoparticles were synthesized by green chemistry approach. The obtained zinc oxide nanoparticles were confirmed using UV-Vis spectroscopy. The prepared zinc oxide nanoparticles were used as a compatibilizer to biocompatible polymer blend system of guar gum (GG)/carboxymethyl cellulose (CMC). The miscibility/compatibility was studied using density, ultrasonic velocity, and adiabatic compressibility methods in aqueous solution. Solution studies confirmed that GG/CMC blends were compatibilized by ZnO nanoparticles when the composition of GG is more than 50% in the blend. Further thin films of GG/CMC blend-ZnO nanocomposites were prepared. The morphology studies (FESEM) confirms the uniform distribution of GG and CMC in the blend when GG content is more than 50% in the blend. To assess the physical stability of the thin films thickness, weight, folding endurance (FE), % moisture absorbance (PMA), and % moisture loss (PML) were measured as per the standard procedures. The drug release studies were performed using a sample drug metoprolol succinate. The diffusion study showed that the drug release from CMC-ZnO nanocomposite thin film patch was immediate compared to that of GG-ZnO nanocomposite thin film patch. The 70/30 GG/CMC blend-ZnO nanocomposite thin film patch showed sustained release of the drug, metoprolol succinate.

KEYWORDS: Drug release, biocompatibility, nanocomposites, guar gum, zinc oxide nanoparticles

**C-22**

# SUSTAINED DRUG RELEASE STUDIES OF XANTHAN GUM/CARBOXYMETHYL CELLULOSE BLEND - ZINC OXIDE NANOCOMPOSITES

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Zinc oxide (ZnO) nanoparticles were synthesized by green chemistry approach. The obtained zinc oxide nanoparticles were confirmed using UV-Vis spectroscopy. The prepared zinc oxide nanoparticles were used as a compatibilizer to biocompatible polymer blend system of xanthan gum (XG)/carboxymethyl cellulose (CMC). The miscibility/compatibility was studied using density, ultrasonic velocity, and adiabatic compressibility methods in aqueous solution. Solution studies confirmed the compatibility of all compositions of XG/CMC blend-ZnO nanocomposites. Further thin films of XG/CMC blend-ZnO nanocomposites were prepared. The morphology studies (FESEM) confirms the uniform distribution of XG and CMC in the blend. To assess the physical stability of the thin films thickness, weight, folding endurance (FE), % moisture absorbance (PMA), and % moisture loss (PML) were measured as per the standard procedures. The drug release studies were performed using a sample drug metoprolol succinate. The diffusion study showed that the drug release from CMC-ZnO nanocomposite thin film patch was immediate compared to that of XG-ZnO nanocomposite thin film patch. The ZnO nanocomposite of XG/CMC blends showed sustained release when compared with their pure polymer.

KEYWORDS: Drug release, biocompatibility, nanocomposites, xanthan gum, zinc oxide nanoparticles

**C-23**

# SUSTAINED DRUG RELEASE STUDIES OF GUAR GUM/HYDROXYPROPYLMETHYL CELLULOSE BLEND - ZINC OXIDE NANOCOMPOSITES

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Zinc oxide (ZnO) nanoparticles were synthesized by green chemistry approach. The obtained zinc oxide nanoparticles were confirmed using UV-Vis spectroscopy. The prepared zinc oxide nanoparticles were used as a compatibilizer to biocompatible polymer blend system of guar gum (GG)/hydroxypropylmethyl cellulose (HPMC). The miscibility/compatibility was studied using density, ultrasonic velocity, and adiabatic compressibility methods in aqueous solution. Solution studies confirmed the compatibility of all compositions of GG/HPMC blend-ZnO nanocomposites. Further thin films of GG/HPMC blend-ZnO nanocomposites were prepared. The morphology studies (FESEM) confirms the uniform distribution of GG and HPMC in the blend. To assess the physical stability of the thin films thickness, weight, folding endurance (FE), % moisture absorbance (PMA), and % moisture loss (PML) were measured as per the standard procedures. The drug release studies were performed using a sample drug metoprolol succinate. The diffusion study showed that the drug release from HPMC-ZnO nanocomposite thin film patch was immediate compared to that of guar gum. The blend-ZnO nanocomposite thin film patches showed sustained release when compared with their pure polymer.

KEY WORDS: Drug release, biocompatibility, nanocomposites, guar gum, zinc oxide nanoparticles

**C-24**

# AGRICULTURAL MICRONUTRIENT RELEASE STUDIES OF GUAR GUM/METHYL CELLULOSE BLEND - ZINC OXIDE NANOCOMPOSITES

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Zinc oxide (ZnO) nanoparticles were synthesized by green chemistry approach. The obtained zinc oxide nanoparticles were confirmed using UV-Vis spectroscopy. The prepared zinc oxide nanoparticles were used as a compatibilizer to biocompatible polymer blend system of guar gum (GG)/methyl cellulose (MC). The miscibility/compatibility was studied using density, ultrasonic velocity, and adiabatic compressibility methods in aqueous solution. Solution studies confirmed that the GG/MC blend – ZnO nanocomposites are compatible when the composition of GG is more than 50%. Further thin films of GG/MC blend - ZnO nanocomposites were prepared. The morphology studies (FESEM) confirms the uniform distribution of GG and MC in the compatible blend. Potassium chloride (KCl) was used as the source for $K^+$ ions. Thin film patches were prepared by solution casting-solvent evaporation method. Distilled water (pH 7) was used as the medium of release. After each 10 minutes the samples were taken out from the set-up and dried, and studied for the $K^+$ ion release. UV-Vis spectroscopy at $\lambda$max. 515 nm was used for this study. The average release of $K^+$ ion from 1 $cm^2$ patch is found to be 0.07 mg/50 mL. The total amount of $K^+$ ions released from 30/70 GG/MC blend-ZnO nanocomposite for five release-dry-release cycle is 0.36 mg/50 mL. Hence it can be proposed that 50 pouches (of 1 $cm^2$) of $K^+$ ion loaded 70/30 GG/MC blend-ZnO nanocomposite can release the required amount of micronutrient potassium every day for five days.

KEYWORDS: Micronutrient release, biocompatibility, nanocomposites, guar gum, zinc oxide nanoparticles

**C-25**

# AGRICULTURAL MICRONUTRIENT RELEASE STUDIES OF XANTHAN GUM/METHYL CELLULOSE BLEND - ZINC OXIDE NANOCOMPOSITES

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Zinc oxide (ZnO) nanoparticles were synthesized by green chemistry approach. The obtained zinc oxide nanoparticles were confirmed using UV-Vis spectroscopy. The prepared zinc oxide nanoparticles were used as a compatibilizer to biocompatible polymer blend system of xanthan gum (XG)/methyl cellulose (MC). The miscibility/compatibility was studied using density, ultrasonic velocity, and adiabatic compressibility methods in aqueous solution. Solution studies confirmed that the blends are compatible when the XG content is below 70% in the XG/MC-ZnO nanocomposites. Further thin films of XG/MC blend - ZnO nanocomposites were prepared. The morphology studies (FESEM) confirms the uniform distribution of XG and MC in the compatible blend. Potassium chloride (KCl) was used as the source for $K^+$ ions. Thin film patches were prepared by solution casting-solvent evaporation method. Distilled water (pH 7) was used as the medium of release. After each 10 minutes the samples were taken out from the set-up and dried, and studied for the $K^+$ ion release. UV-Vissible spectroscopy at λmax. 515 nm was used for this study. The average release of $K^+$ ion from 1 $cm^2$ patch is found to be 0.254 mg/50 mL. The total amount of $K^+$ ions released from 30/70 XG/MC blend-ZnO nanocomposite for five release-dry-release cycle is 1.27 mg/50 mL. Hence it can be proposed that 10 pouches (of 1 $cm^2$) of $K^+$ ion loaded 30/70 XG/MC blend-ZnO nanocomposite can release the required amount of micronutrient potassium every day for five days.

KEYWORDS: Micronutrient release, biocompatibility, nanocomposites, xanthan gum, zinc oxide nanoparticles.

**C-26**

# POLY (VINYLIDENE FLUORIDE) AND GAUR GUM BLEND POLYMER ELECTROLYTE FOR SUPERCAPACITOR

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In the present work, gel polymer electrolyte (GPE) a novel gel composite was prepared using poly(vinylidene fluoride) (PVdF) and guar gum (GG). Combined DSC-TGA data for GPE showed that PVdF provides the mechanical support and jelly guar gum occupies the interstitial spaces. The ionic conductivity, activation energy, dielectric studies were studied to understand the electrode/electrolyte interface mechanism. Dielectric studies revealed that the unique pathway of proton transfer within the guar gum structures reduces the charge transfer resistance significantly at the interface. Optimized GPE was used in the fabrication of supercapacitor and specific capacitance was found to be 237 Fg -1. The time constant was 0.4s and showed consistent cyclic pattern during galvanostatic charge/discharge studies with 97% Columbic efficiency.

KEYWORDS: gel polymer electrolyte, PVdF-guar gum, supercapacitor.

# *MATHEMATICS*

**M-01**

# EXTREME ISOLATE GEODESIC GRAPHS

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Here we study the new concept of extreme isolate geodesic graph in a connected graph G = (V (G), E(G)). The geodetic set S ⊆ V (G) is called an isolate geodetic set, if the induced sub graph < S > has atleast one isolate vertex. The cardinality of an isolate geodetic set which is minimum is the isolate geodetic number and is denoted as go(G). The extreme order ex(G) is the number of extreme vertices in a connected graph G. If go(G) = ex(G) then the graph G is an extreme isolate geodesic mgraph. Here we investigate general properties of some graphs. A positive integers n, d and k can be obtained for the graph G and also we proved go(G) = k = ex(G) with r ≤ d ≤ 2r. Also we find the extreme isolaten geodesic graph in G = Cn by adding the k leaf vertices vi to each vertex in G.

KEYWORDS: geodetic set, extreme geodesic graph, isolate geodetic number, ex- treme vertex.

**M-02**

# FIBONACCI WAVELET COLLOCATION SCHEME FOR THE NUMERICAL SOLUTION OF NONLINEAR ORDINARY DIFFERENTIAL EQUATIONS

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Wavelets analysis is a relatively new developed important tool of mathematical analysis for many problems. In this paper, scheme is based on collocation points with Fibonacci wavelets, an efficient and new numerical scheme is developed for the solution of nonlinear ordinary differential equations. The proposed scheme is developed by using the Fibonacci wavelets. It has been presented here that the proposed scheme can be very easily implemented and the Fibonacci wavelet solutions are most accurate. Hence the Fibonacci wavelet collocation scheme (FWCS) has a clear benefit over the classical methods. Numerical test equations declare that the outer performance of convergence of Fibonacci wavelet scheme over Taylor Matrix method, Matrix method and Homotopy perturbation method.

KEYWORDS: Wavelets; Fibonacci wavelet approximations; Fibonacci wavelet collocation scheme; nonlinear ordinary differential equations.

**M-03**

# RESULTSONCOMPACTNESSANDCONNECTEDNESS

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In general topology, as well as all generalised forms of topologies, the concepts of compactness and connectedness play an important role.The main goal of this present study is to introduce the concept so f*gpα*-compactness, *gpα*-connectedness and *gpα* paracompactness using *gpα* opensets. Further, the properties of the sespaces have been studied.

KEYWORDS: gpα-closed set, gpα-open set, gpα-compact space, gpα-connected space, gpα-paracompact space.

**M-04**

# RESULTS ON BINARY SOFT TOPOLOGICAL SPACE

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In this paper, we study the concept of binary soft topological spaces defined on two universal sets and a parameter set. The binary soft nowhere dense, binary soft dense, binary soft Gδ, binary soft first and second category sets are defined and studied their properties. Also, we introduced binary soft baire spaces and studied their characterizations.

KEYWORDS: Binary soft set, binary soft nowhere dense set, binary soft dense set, binary soft Gδ-set, Baire space.

**M-05**

# TOPOLOGICALINDICESFORCENTRALGRAPHOFAGRAPH

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Topology is the investigation of the properties of mathematical figures that are invariant (don't change) while going through changes. In this paper we obtain value of degree based topological indices for central graph of a given graph G. Central graph is obtained by subdividing a graph *G* and joining al lnon adjacent vertices. Also we find the graphs whose central graph has maximal and minimal values for each index.

KEYWORDS: Degree of a vertex, Central graph, zegrab index.

**M-06**

# TERMINAL STATUS CONNECTIVITY INDICES OF SOME CLASS OF TREES

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The terminal status of a vertex and terminal status connectivity indices of a connected graph have been introduced by Ramane et. al. In this paper we have studied theses indices for some class for trees, also obtained maximal and minima values. Further we have obtained few more results regarding the same.

KEYWORDS: Status of a vertex, terminal status of a vertex, terminal status connectivity indices of graph

**M-07**

# NEW GENERALIZED OPERATIONAL MATRIX OF INTEGRATION USING CLIQUE POLYNOMIAL OF COMPLETE GRAPHS TO SOLVENONLINEAR SINGULAR INITIAL VALUE PROBLEMS

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The main objective of this paper is to generate new operational matrix by making use of the graph theoretic polynomials for solving numerical problems. We generate new operational matrix of integration by making use of clique polynomials of one of the standard class of graphs called complete graph, in its generalized representation. Using these, clique polynomial operational matrix method (CPOMM) is proposed to solve second ordered nonlinear singular initial value problems, in which given differential equation is transformed into a system of algebraic equations that can be solved efficiently with the help of suitable solvers. Efficiency of the developed method is revealed by considering illustrative numerical problems and the obtained results are comparing favorably with the corresponding exact solution and errors.

KEYWORDS: Non-linear singular initial value problems, graphs, clique polynomial, operational matrix, collocation method.

**M-08**

# REGULAR GENERALIZED FUZZY B- CONTINUOUS IN FUZZY TOPOLOGY

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To introduce a new type of generalized function that is ‘rgfb-continuous’, strongly ‘rgfb-continuous’, perfectly ‘rgfb-continuous’ is aim of this article. Some of their characteristics and attributes have been verified. Interrelation between existing functions is studied.

KEYWORD: ‘rgfb-continuous’, strongly ‘rgfb-continuous’, perfectly ‘rgfb-continuous’ and fuzzy topological space (fts).

**M-09**

# NUMERICAL SOLUTION OF DERIVATIVE DEPENDENT DOUBLY SINGULAR BOUNDARY VALUE PROBLEMS BY USING LEGENDRE WAVELETS

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Different class of derivative dependent doubly singular boundary value problems exist in many areas of science and engineering such as heat distribution in a steady state, fluid dynamics, mechanical engineering, aerospace engineering and medical science etc. It is a familiar fact that the solutions of boundary value problems have singular nature near the corners and edges of the domain. The singularities are of type's vertex, edge, vertex-edgesingularities. Due to the presence of singularities the classical numerical methods are unable to yield accurate numerical solutions and the rate of convergence of these methods degrades.

This is due to the fact that, in particularly finite element method discretized equations results ill-conditioned matrices which leads to small change in the system or forcing function will make large difference in the solution. In order to reduce the condition number, improve efficiency of computations and accuracy of the solutions; it is desirable to find efficient methods along with standard numerical techniques such as finite difference method, FEM, multigrid, wavelet multigrid methods and so on. In this paper, we have developed the Legendre wavelet technique for the numerical solution of derivative-dependent doubly singular boundary value problems. The present technique is developed by using the Legendre wavelets. It has been shown here that the present technique can be easily implemented and the results obtained are most accurate. Hence the present method has a clear advantage over the classical methods. Numerical order of convergence of the proposed technique is calculated. The results show the better accuracy of the proposed method, which is justified through the illustrative examples.

KEYWORDS: Wavelets; Legendre wavelet technique; Derivative dependent; Doubly singular, Boundary value problems.

**M-10**

# SEPERATION AXIOMS THROUGH Š $\alpha*$ - OPEN SETS IN SOFT TOPOLOGICAL SPACES

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In this paper, we introduce the concept of Š T α* - space and also discuss their relationship with other soft mappings, Counter examples are given to show the non – coincidence of these functions.

KEYWORDS and phrases: Š T α*- space.

**M-11**

# CLASSIFICATION OF COMPACT CONNECTED CONTACT TORIC MANIFOLDS(C.C.C.T)

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In this paper we will give the complete proof of classification theorem for compact connecte contact toric manifolds and some of its applications by recalling some concepts , basic definitions that arise from contact geometry such as Contactomorphism,Lens spaces etc.

KEYWORDS: Contact toric manifolds, Good cone and Orbital moment maps and Contactomorphism,.

**M-12**

# SOFT NANO FEEBLY GENERALIZED CONTINUOUSFUNCTION

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The present paper deals with the new sets in soft nano topology called the soft nano feebly open sets. With the help of soft nano feebly open sets we introduce soft nano feebly generalized closed sets in soft nano topological spaces. Union and intersectin of soft nano feebly generalized closed sets and their various properties are studied. Composition of soft nano feebly genralized continuous functions and soft nano continuous functions are dealt with 2010 AMS Classication: 54A05, 54C05

Keywords: soft nano feebly open sets, soft nano feebly generalized closed sets, soft nano feebly generalized continuous functions.

**M-13**

# A NEW CRITERIA ON OSCILLATION OF LINEAR DELAY DIFFERENTIAL EQUATIONS

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In this article, we shall particularly deal with oscillation criteria for the linear delay diferential equation. We discuss the oscillation criteria for the equation of the type* $\chi^{l}(\nu) = \chi(\nu) + p(\nu)\chi(\nu - \tau) = 0$, $\nu \geq \nu 0$ where the function $\tau \in C([\nu 0, \infty], (0, \infty))$. We provide modern adequate status carry out oscillation of the solution for these kind equations.

**M-14**

# A NEW CLASS OF MAC ROBERT TYPE INTEGRALS INVOLVING GENERALIZED HYPERGEOMETRICFUNCTIONS

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Masjed-Jamei and Koepf [12] established interesting and useful generalizations of various classical summation theorems for the generalized hype rgeometric series ${}_2F_1$, ${}_3F_2$, ${}_4F_3$, ${}_5F_4$ and ${}_6F_5$. By employing these summation theorems, in this paper, our aim is to establish nine MacRobert type integrals involving generalized hyper geometric functions. Several special cases have also been given.

**M-15**

# SOME VALUE DISTRIBUTION RESULTS OF MEROMORPHIC AND ENTIRE FUNCTIONS

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The core objective of this article is to investigate zero distribution for q-shift linear difeerential- difeerence polynomials, monomials of entire(meromorphic) functions. The finding of entire(meromorphic) functions is either zero of finite order which may be viewed as the analogues of Hayman Conjecture. These results generalise and improve the results due to Luo L. and Xu J. and Dhar R.S.

KEYWORDS: Entire function, meromorphic function, monomial, difference polynomial, q-shift, zero order.

**M-16**

# GENERALIZATION ON VALUE DISTRIBUTION OF L-FUNCTIONS

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In this article we mainly study the value distributions of L-functions in investigate with the uniqueness of certain type of difference polynomials and obtain some results which improve and extend.

**M-17**

# NEW CRITERIA ON OSCILLATION OF LINEAR DELAY DIFFERENTIAL EQUATIONS

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In this article, we shall particularly deal with oscillation criteria for the linear delay differential equation. We discuss the oscillation criteria for the equation of the type* $\chi^{l}(\nu) = \chi(\nu) + p(\nu)\chi(\nu - \tau) = 0, \nu \geq \nu 0$ where the function $\tau \in C([\nu 0, \infty], (0, \infty))$. We provide modern adequate status carry out oscillation of the solution for this kind equation.

**M-18**

# APPROXIMATIONSINARINGUSINGANEQUIVALENCERELATIONWITHREFERENCEPOINT

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In this paper, we introduce an equivalence relation with a reference point using an ideal of a ring. We find rough set approximations of a nonempty subset of a ring usingthisequivalencerelation.Weobtainpropertiesoftheroughsetapproximations.

**M-19**

# FAINTLY G*ωα-CONTINUOUS FUNCTIONS

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In this paper a new class of continuous functions called faintly g*ωα-continuous functions and relationship among faintly g*ωα-continuous functions with other functions have been discussed. Several properties of these spaces have been discussed here.

KEYWORDS: g*ωα -closed sets, g*ωα -continuous functions, g*ωα -compact spaces and faintly g*ωα -continuous functions

# *PHYSICS*

**P-01**

# $Fe^{3+}$DOPEDTRIGLYCINESULPHATESINGLECRYSTALS-ELECTRICAL, DIELECTRIC, STRUCTURAL AND OPTICAL PROPERTIES

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In this paper we have investigated electrical, optical and dielectric properties of pure Triglycine sulphate $(NH_2CH_2COOH)_3 \cdot H_2SO_4$ (TGS) and $Fe^{3+}$ doped TGS. A good optical quality single crystal of TGS and $Fe^{3+}$ doped TGS have been grown with the slow evaporation method. The crystalline phase purity and change in the unit cell parameters are investigated using powder X-ray diffraction method. The functional groups were confirmed by FTIR technique. UV visible spectral studies showed good optical transmittance window in the visible region of the electromagnetic spectrum. The dielectric constant is found to decreases with doping. The decrease in dielectric constant in the case of $Fe^{3+}$ doped TGS has an application in pyroelectric infrared detectors as thermal sensors. High melting point (233℃) of Triglycine sulphate (TGS) crystals makes it as suitable in many scientific applications. Since the amino acids are the major constituent of TGS, it is soluble in water.

KEYWORDS: Triglycine sulphate, Functional groups, Optical Transmittance, Pyroelectric effect

**P-02**

# DENSITY FUNCTIONAL THEORY COMPUTATION AND THIRD ORDER NONLINEAR OPTICAL STUDIES ON BENZODIAZEPINE DERIVATIVE: AN OPTICAL LIMITER

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The present work discusses the nonlinear optical properties of a benzodiazepine derivative and the quantum chemical computation on geometry optimization using Gaussian ’09 program at B3LYP level with 6-311++G (d, p) basis set. The second-order hyper polarizability , third-order susceptibility , nonlinear refractive index , nonlinear absorption coefficient have been investigated using the Z-scan technique. The Z-scan results confirm that the compound exhibits positive nonlinear absorption and a positive nonlinear refractive index. The optical limiting property of the material is due to its positive absorptive nonlinearity via reverse saturable absorption and the optical limiting threshold was measured. The obtained results reveal that the compound is a promising material for laser assisted applications.

KEYWORDS: Polarisability, nonlinear, optical property.

**P-03**

# CHARACTERIZATION OF COPPER INCORPORATION OF ZnS THIN FILMS BY SOL GEL DERIVED SPIN COATING TECHNIQUE

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Nanomaterial shall show significant development in the research field.Among the nanomaterials, the thin films have shown vast progress in the fabrication of the optoelectronic devices. The copper doped zinc sulphide (CuZnS) thin films were deposited by sol gel derived spin coating technique. The effects of doping concentration of the films have been investigated. The XRD patterns of the CuZnS films were showed cubic crystal structure. The structural properties of the films were improved with doping concentration. The absorbance of the films was found to be ultra violet region. The slightly deviation was found in the bandgap of the films. All the deposited films have showed p-type conductivity and conductivity was improved with copper doping.

KEYWORDS: Thin film, optoelectronic devices, sol gel, spin coating, copper doping.

**P-04**

# REVERSE SATURABLE ABSORPTION BEHAVIOUR IN Mn-SUBSTITUTED NICKEL-ZINC FERRITES

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Non-linear optical phenomena have significant applications in light modulators, frequency converters, light absorbers etc. In the present investigation, manganese substituted nickel-zinc ferrite of the stoichiometry $Ni_{0.5}Zn_{0.25}Mn_{0.25}Fe_2O_4$ was synthesized by chemical co-precipitation method and its non-linear optical response were characterized by z scan technique using Nd -YAG laser of wavelength 532 nm. The prepared ferrite system has cubic spinel structure; confirmed from XRD analysis with an average crystallite size of 29 nm. Elemental confirmation was found was done by EDX analysis, band gap to be 1.8 eV. The open aperture z scan curve shows reverse saturable absorption behavior with an absorption coefficient of the order $10^{-11}$ m/W and from the closed aperture, the self-defocusing nature of the material was revealed. The sample shows significant optical limiting due to the reverse saturable absorption behavior.

KEYWORDS: Reverse saturable absorption, cubic spinel structure, optical limiting.

**P-05**

# EFFECT OF PREPARATION TIME ON CHEMICAL BATH DEPOSITED ZNO THIN FILMS FOROPTOELECTRONICDEVICES

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The thin films have exhibit essential applications over the decades. In the II-VI semiconductor thin films, Zinc oxide (ZnO) thin films have shown superior characteristics in the device applications. In the present work, ZnO thin films were synthesized by low-cost chemical bath deposition(CBD) method. The deposited films have showed hexagonal phase for different deposition time in the XRD studies. The crystallite size was improved with deposition time. The absorbance of the films enhanced with deposition time which have observed in the near UV region. The bandgap of the film was found to be 3.1eV. The conductivity of the film was found to be increased with deposition time of ZnO films.

KEYWORDS: ZnO films, deposition time.

**P-06**

# INVESTIGATION OF PHYSICO-CHEMICAL PROPERTIES OF METAL SULFIDE NANOPARTICLES

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In the current work, cobalt sulfide nanoparticles were synthesized using chemical co-precipitation method. Two different sources of sulfur sources were used for the preparation of cobalt sulphide nanoparticles such as thiourea ($CH_4N_2S$) and Sodium sulfide ($Na_2S$) to check their influence on properties of end product. The samples prepared were annealed at two different temperatures such as 300 °C and 500 °C, respectively. X-Ray diffraction (XRD) and Raman spectroscopy were conducted to study the structural properties of the particle. From the Scherrer method the crystallite size of the particles was calculated. It was also seen from the peaks in XRD pattern that two different phases of the particles were obtained. Due to the volatile nature of cobalt at higher temperature oxide formation was prominent ($Co_3O_4$). Raman spectroscopy was conducted further to confirm the different phases obtained from the peaks seen in XRD. Optical property of the particle was analyzed using Photoluminescence (PL) spectroscopy. A strong emission in the region 436.63 nm which is in the visible region was observed. To further examine the morphology of the particles prepared Field Emission Scanning Electron Microscopy (FESEM) was conducted to examine the shape and size of the particles. It was found that the size varied 90 nm to 100 nm which was calculated using Image J software. From this study we inferred that prepared cobalt sulphide nanoparticles can be used in several applications like photonic applications.

KEYWORDS: Nanoparticles, chemical co-precipitation, Cobalt Sulfide, Cobalt Oxide

**P-07**

# THE STUDY OF THIRD-ORDER NONLINEAR OPTICAL PROPERTIES OF REDUCED GRAPHENE OXIDE ZnO HYBRID SYNTHESIZED USING TWO DIFFERENT METHODS.

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Graphene oxide (GO) is a highly oxygenated single layer of carbon atoms with oxygen-containing functional groups in which hydroxyl and epoxy groups are attached to the basal plane and carboxyl and carbonyl groups are attached to the sheet edges. These covalently attached oxygen functional groups lead to strong structural defects which modify the thermal and mechanical properties. Reduced graphene oxide (rGO) is formed by the partial removal of oxygen-containing functional groups through chemical reduction. This helps in restoring the π conjugated system which in turn increases the electrical conductivity. The addition of metaloxide nanoparticles is expected to further extend the conjugation of the nanostructure network thereby increasing the nonlinear optical properties. GO was synthesized using the modified Hummers method, in which graphite powder was used as the main precursor and $KMnO_4$ as the oxidizing agent. The solvo thermal method was used for the synthesis of crystalline ZnO nanoparticles. Ultrasonication and chemical reduction methods were used for the synthesis of rGO-ZnO nanocomposites. In the chemical reduction process, hydrazine hydrate was used as the reducing agent.

The synthesized samples were characterized using XRD and morphological details were studied using FESEM.The spectroscopic characterization was performed using UV, IR, and FT-Raman analysis. The surface area of the synthesized samples was analyzed using BET. The nonlinear optical properties of the samples are determined using the open and closed aperture z-scan technique.

The laser beam interacts with the sample as it is moved along the z-direction which experiences different in tensities at different z positions. From the open aperture z – scan studies the nonlinear absorption coefficient(β) of the samples was obtained. The samples possess high β values which specify their higher absorption property. The positive β value extends their applicationas optical limiters. The optical limiting behavior helps in the protection of various optically sensitive devices and the humane ye from highly intense optical beams.

KEYWORDS: ZnO, rGO – ZnO, hydrazine hydrate, NLO, open aperture z - scan, closed aperture z-scan, nonlinear absorption coefficient(β), nonlinear refractive index($n_2$) optical limiting.

**P-08**

# INTEGRATING MOLECULAR DYNAMICS AND MOLECULAR DOCKING SIMULATION STUDIES TO INVESTIGATE LIGAND PROTEIN INTER ACTIONS IN STIGMASTEROL AGAINST MYCOBACTERIUM TUBERCULOSIS PANK(4BFS)

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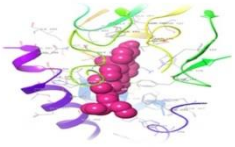
Stigmasterol is a steroid, isolated by column chromatography of the hexane extract of the stem bark of*Garcinia imberti*., containing a rigid tetracyclic(6-6-6-5) backbone with one secondary hydroxyl group at one end and one C10 branched hydrocarbon chain at the other end. These are sterol lipids with a structure based on the stigmastane skeleton, which consists of a cholestane moiety bearing an ethyl group at the C24 atom. In-order to understand the biological activity of the ligand with the proteins (1DQY, 2IXC, 2Q1X, 4BFS, 4FDO, 6W63, 6W6Y, 6W01, 6VYB, 6M71) molecular docking analysis was carried out. Thedocking results shows that the compound has anti-tuberculosis activity with a glide score of-6.151kcal/mol against 4BFS. The Ramachandran plot was used to check the stereochemistry of the protein structure (4BFS). The docked complex has also been subjected to molecular dynamic simulations in order to visualize better binding sites and the effect of ligand on 4BFS conformation. From molecular dynamic simulations root mean square deviation, root mean square fluctuation, radius of gyration etc. were calculated. The binding free energy of the receptor protein complex was computed to revalidate the inhibitor affinity for the receptor protein complex predicted by docking and molecular dynamic simulation studies. Besides, investigations of absorption, distribution, metabolism, excretion and toxicity have predicted that the compound has a promising drug-like character.



**P-09**

# EFFECT OF ELECTRON BEAM IRRADIATION ON THE STRUCTURAL AND OPTICAL PROPERTIES OF POLYMER ELECTROLYTE FILMS

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The effect of 8 MeV Electron beam (EB) irradiation on the optical properties of cadmium chloride ($CdCl_2$) doped polyethylene oxide (PEO) has studied. The doped films are exposed to a beam of 8MeV electron at 25, 50, 75, 100 kGy doses. The films are characterized using Fourier Transform Infra red (FTIR) in the KBr medium. The FTIR results of films after electron beam irradiation shows appearance of new peaks and shifts in the position of peak proved the formation of hydrogen bonding. The micro structural arrangement was investigated by Scanning Electronic Microscopy (SEM) and the images reveal that there is a substantial improvement in the surface morphology in irradiated films. The X-ray Diffractometry (XRD) result shows that reduction in the crystallinity and increase the amorphous. The optical absorption study was carried out with help of the Ultra violet–visible (UV-vis.) absorption spectroscopy. The optical absorption edges shifts towards higher frequency upon EB irradiation, which indicates a lowering of the energy gap, it can be evidenced by formation of carbonaceous clusters. The number of carbon atoms in clusters is estimated according to modified Tauc's equation. The optical parameters like absorption co-efficient, optical direct and indirect band gaps (Eg), band edges, and optical activation energy (Ea) are determined for different EB doses. These results reveal that the electron beam irradiation is a powerful tool to modify the structural and optical properties of polymer electrolyte.

KEY WORDS: Electron beam (EB) irradiation, polyethylene oxide, polymer electrolytes, optical band gap, activation energy, carbon cluster.

**P-10**

# SYNTHESIS AND OPTICAL PROPERTIES OF CADMIUM CHLORIDE DOPED POLYANILINE COMPOSITES

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This paper reports cadmium chloride ($CdCl_2$) doped polyaniline (PANI) have been synthesized at different dopant weight percentage by chemical synthesis. Optical absorption studies were performed using ultra violet (UV)-visible spectrometer in the wavelength range from 190–800nm for pure and $CdCl_2$ doped Polyaniline. The chemical interaction, structural and morphology analysis of pure and doped PANI carried out by Fourier Transform Infra red (FTIR) spectroscopic and Scanning Electronic Microscopy (SEM). The UV–vis absorption data's were recorded by Shimadzu 2550 (UV 1800 ENG 240V) UV-Visible Spectrophotometer and spectra show λmax at about 350 nm and 635 nm due to dopant. Using UV-Visible absorption spectra the optical parameters like optical energy direct and indirect band gap were determined from Tauc's plots. The optical band gap energy is found to be 2.35 eV for as-doped film and it decreases with increase of dopant concentration. Following modified Tauc's equation, the carbonaceous cluster size is estimated and it increases with increase in dopant concentration. Doped PANI results show a shift in the FTIR peaks at 2923cm−1 and 1226cm−1. The SEM result shows a systematic change in the surface morphology of the PANI with dopant.

KEYWORDS: Polyaniline, Optical absorption, surface morphology, carbonaceous cluster, optical band gap.

**P-11**

# STRUCTURAL, ELECTRICAL AND ELECTROCHEMICAL PARAMETERS OF PEO – $Li_2SO_4$ COMPOSITE FOR BATTERY APPLICATIONS

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Polymer electrolyte system based on polyethylene oxide (PEO) complexed with $Li_2SO_4$ was prepared using solution cast technique at different weight percentages as a polymer electrolyte for battery application. The prepared composites were characterized by various tools like XRD, FTIR and Ultraviolet-visible (UV-Vis.) Spectroscopy techniques. The dc electrical conductivity measurement was made by using two-probe technique at different temperatures. The fabrication of electrochemical cell in the configuration based on anode/polymer, electrolyte/cathode and cell parameters was carried out using the Wagner polarization technique. The X-ray diffraction analysis shows the complexation of polymer with salt and existence of both crystalline and amorphous phases. An FTIR spectra shows the significant change in the intensities as well as frequencies of spectra and the appearance of new peaks confirms the better complexation of PEO– $Li_2SO_4$ composites. The UV–Vis. spectra reveal that the absorption bands positioned at different absorption intensities with addition of dopant. The optical band gaps was evaluated using Tauc's expression and band gap found decreases from 5.42 to 2.41eV (direct) and 4.79 to 4.20eV (indirect). The changes in the dipole strength, transition dipole moment, oscillator strength, and Urbach energy have been investigated with dopant concentration. The electrical conductivity was found increases with increasing of dopant concentration and estimated the electrochemical cell parameters OCV (open circuit voltage) is 1.62V and (Current) SSC is 273μA. These obtained results suggest that these polymer systems are potentially suitable candidature for solid state battery, optoelectronics display and electro chromic devises etc.

KEYWORDS: Optical band gap, optical constants, FTIR, dc conductivity, activation energy, electrochemical parameters.

**P-12**

# IMPACT OF $Sr^{2+}$ ON STRUCTURAL, OPTICAL AND PHOTOCATALYTIC PROPERTIES OF ZnO NANOPARTICLES

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Pure ZnO and Sr doped ZnO nanoparticles are synthesized by precipitation method using Zinc nitrate and KOH in aqueous solution.The prepared samples are based on different composition(0.2 -1 mol%).The influence of Sr dopant contents on absorption, emission, morphology and photocatalytic activity are investigated systematically. Synthesized samples were investigated by X-ray diffraction (XRD), field emission Scanning Electron Microscopy (FE-SEM), Energy dispersive spectroscopy (EDS), UV-visible, and Photoluminescence (PL) spectroscopy. The phase purity and crystalline size were characterized using X-Ray diffraction and Scanning electron microscopy. No characteristic peaks of of any other impurities are detected in XRD patterns which indicates that samples are of high purity. The average particle size of pure ZnO nanoparticles was about 40nm.Reduction in crystalline size upon increasing the amount of Strontium was confined by peak broadening. By using Scherrer equation the average crystalline size is decreased from 40nm to 20nm.SEM images clearly indicate that added Sr concentration is expected to influence the morphology of ZnO. The presence of strontium in the lattice was confirmed by EDS.UV-Vis spectra of doped and undoped ZnO nanoparticles were studied. The spectrum shows maximum absorption peak at 365nm. Photocatalytic activity of ZnO and Sr doped ZnO nanoparticles were studied. The results show that the Photocatalytic activity of $Sr^{2+}$ doped ZnO was much higher than that of pure ZnO. It shows maximum absorbance for pure ZnO and decrease in absorbance as the doping concentration increases. Also the maximum absorbance peak shifts towards lower wavelength side as the doping increases.

KEYWORDS: nano particles, X-ray diffraction, FE-SEM

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