GONZAGA COLLEGE
OF ARTS AND SCIENCE FOR WOMEN

Affiliated to Periyar University, Salem - 636 011
Accredited by NAAC with 'B' Grade
Kathampallam, Elathagiri - 635 108, Krishnagiri District

National Conference on Recent Advances in Materials (NCRAM – 2023)

21 & 22 September 2023

Organized by

PG & Research Department of Physics
PG Department of Chemistry
& Department of Biochemistry

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(NCRAM – 2023)

CONVENER

Dr. R. DHINESH KUMAR

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SECRETARY MESSAGE

Dear All,

I am delighted to congratulate the PG & Research Department of Physics, PG Department of Chemistry and Department of Biochemistry, Gonzaga College for bringing out the compilation of the deliberation of "**National Conference on Recent Advances in Materials (NCRAM – 2023)**" which was held on 21 & 22 September 2023. I am given to understand that the Conference has motivated the students and participants to enkindle their 'Scientific temper' in the discipline. I hope this compilation will become an instrument to initiate further fruitful and professional discussions and create passion for research on the said subject.

Let me take this opportunity to congratulate the Principal, Vice-Principal, Convener, Coordinators, Organizing Secretaries, Committee Members of the Conference and wish them all the best in the efforts to deepen the academic excellence and intellectual quest of the students and the college as well.

Rev. Mother C. Noel Rani, FSAG
Secretary

PRINCIPAL MESSAGE

Dear Reader,

With immense joy, pride and satisfaction, the editorial team has brought out the proceeding of National Conference on Recent Advances in Materials (NCRAM - 2023). This conference is a collaborative effort taken by the Department of Physics, Chemistry and Biochemistry. These three departments have made tremendous progress in all areas especially in research and publications. The faculty are extra-ordinarily compassionate and committed towards students for their academic and carrier growth.

This proceeding is a collection of research writing of young and aspiring innovators who have brought out their talents in experiments and expertise in research as a footprint to look forward to. I congratulate the Editorial Board of this proceeding for shaping through efficient coordination. I express my deep sense of appreciation to the faculty who guided and encouraged the students and researchers in accomplishing this pleasant task. It is indeed a great pleasure for me to recognise the involvement shown by the convener, staff coordinators and faculty members in organizing a National Conference on Recent Advances in Materials (NCRAM - 2023) which is a remarkable event in the annals of their departments. I am sure that this conference will create an eco system to young researchers to understand the ever-changing economy, innovation in technology, development in all departments and culture due to the advances of materials. I wish to acknowledge all the students and staff members for their creative contributions. I offer my prayers for its grand success.

With Best Wishes

Rev. Dr. E. Glitta Sumangali, FSAG

Principal

VICE - PRINCIPAL MESSAGE

Dear All,

Science and technology are two sides of a coin and they are inseparable. Recent advances in materials have brought a trending change in an individual's critical thinking. Advances in technology have led people to become smarter. God created humans so great and powerful that before etching history on his head, He asked Human: Tell me, what is the history that you have decided to create? The human brain is beyond a mere myth or dream; you are here dealing with what is deeply human and truly scientific. Today's globe is experiencing an exponential growth of a wide range of technology, creating the new prospect that is completely a novel world where everyone will have access to plenty.

Yet the scarcity mentality dominates the mind and body of the majority of people. The soldiers in the jungle discovered the enemy: "It is us". Abundance for all is actually within our grasp. The National Conference on Recent Advances in Materials is an interdisciplinary field for research and discovered new materials that we are enjoying right now is the achievement of science. Yet more amusing technology needs to be invented by the young scientist like you. Many things that we thought clearly impossible have now become possible, even within a short span of a few decades. The dream that is not possible for us is possible for someone, which is happening in reality.

The human brain is such an extraordinary capacity with lots of miracles that lead you into search! If you have a real thirst, you will definitely quench your thirst for knowledge, power, whatever it may be. The Alma matter, hidden the riddles in each one's life to chase those dreams. The righty chosen title on Recent Advances in Materials will definitely pave the ways and means to search your dream. I greatly appreciate the convener of the conference Dr. R. Dhinesh Kumar, Department of Physics, Ms. K. Devi, Ms. V. Karthika, Ms. J. Sumathi, Head of Physics, Chemistry and Biochemistry, organizing secretaries and committee members of various departments for choosing the right title for the national conference towards the wellbeing of the students. I wish you all once again. Thank you.

Rev. Dr. A. John Dayana, FSAG

Vice-Principal

CONVENER MESSAGE

Dear All,

I am extremely happy to inform that in the history of Gonzaga College we organize a first ever National Conference on Recent Advances in Materials (NCRAM - 2023) during 21 & 22 September 2023 jointly by PG & Research Department of Physics, PG Department of Chemistry & Department of Biochemistry. This year, we made tremendous efforts to raise the standard of the National Conference.

Initially we have been thinking about organizing a National Conference for quite some time and the first aspect which we had to discuss was that would we be able to make it meaningful and fulfill the expectations of the participants and the aspirants. This took us some months to think over the issues to be floated, the format, the key participants, their orientation, and so on. I am sure that you will gain from this event.

The present requirement of our society is to develop the abilities to address different challenges of individuals with a scientific temperament. Material science is an interdisciplinary field at the forefront of science and engineering in the 21st century.

The conference aims to provide a platform for national relationships among the researchers involved in the field of material science. The overwhelming response of various participants from across the country has been phenomenal and I thank all of them for sharing their work in the conference. I expect this conference will prove a memorable and productive discourse.

I wish all the best.

Dr. R. DHINESH KUMAR
Convener, NCRAM - 2023

ORAGANISING COMMITTEE

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Department of Biochemistry

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Department of Biochemistry
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Dr. N. Chitra Asst. Professor, Dept. of Bio-Chemistry
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Department of Bio-Chemistry
Ms. S. Saiechana A/P
Ms. T. Valli A/P
Department of Chemistry
Ms. P. Jaishree A/P
Ms. S. Ajithakumari A/P
Ms. L. M. Manimegalai A/P
Ms. A. Immaculate Jayanthi A/P
Mr. R. Sakthivel A/P
Resource Persons
Day 1
Dr. MARILYN D'MELLO
SERB - National Post Doctoral Fellow
Centre for Nano and Soft Matter Sciences
(Autonomous Institute under the Dept. of Science and Technology, Govt. of India)
Bangalore, Karnataka, India
Dr. SRINIVASAN KRISHNAN
Assistant Professor
Department of Chemistry
Thiruvalluvar University
Serkadu, Vellore – 632 115
Tamil Nadu, India
Dr. G. DEVANAND VENKATASUBBU
Associate Professor
Department of Nanotechnology
SRM Institute of Science and Technology, Kattankulathur – 603 203
Tamil Nadu, India
Day 2
Dr. E. K. GIRIJA
Assistant Professor
Department of Physics
Periyar University, Salem – 636 011
Tamil Nadu, India
Dr. R. THANGAPPAN
Assistant Professor
Department of Energy Science and Technology
Periyar University, Salem – 636 011
Tamil Nadu, India

About the College

Gonzaga College of Arts and Science for Women is managed by the Congregation of the Franciscan Sisters of St. Aloysious Gonzaga, Puducherry, a registered charitable entity commited to the cause of Education and social upliftment of the less privileged humanity and women in particular. The Congregation was founded by Servant of God Michael Ansaldo in the year 1775 at Puducherry. The College was established in the year 2009. It is affiliated to Periyar University, Salem. We have 13 UG, 8 PG and one M.Phil Departments catering to the needs of over 1200 girl students. True to its Motto, "Educate to Empower", the institution works with commitment to create a just and humane society, upholding national integration and religious harmony, with special emphasis on the enrichment of the poor, marginalized and downtrodden women in society. As recognition of its endeavours and achievements in the academic, cultural and social realms, NAAC had accredited the college with B Grade in 2016, with a CGPA of 2.55. The modern amenities and the student friendly faculty pedagogy facilitate the intellectual formation of the young minds to become wisely resourceful for making our nation an artisan well of brain power.

About the Conference

National Conference on Recent Advances in Materials (NCRAM – 2023) is organised by PG & Research Department of Physics, PG Department of Chemistry & Department of Bio-Chemistry. The main objective of the conference is to bring together the scientist/scholar and students to provide a common platform for sharing their scientific thoughts and ideas. This conference is expected to give the participants exposure to some of the latest developments in recent advances in materials. The conference is expected to be an excellent opportunity to enhance knowledge, generate new ideas and promote advancements and modifications in academic research.

National Advisory Committee

- Prof. R. Jayavel, Dean AC Tech, Anna University, Chennai
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- Dr. S. A. Martin Britto Dhas, Sacred Heart College, Tirupattur
- Dr. V. Collins Arun Prakash, Sacred Heart College, Tirupattur

Topic to be Covered

- Crystal Growth and Characterization
- Nanomaterials
- Energy Materials and Storage
- Green Chemistry
- Electrochemistry
- Bio-Nanomaterials
- Composite Materials
- Spectroscopy
- Thin Films
- Magnetic Materials

Call For Abstracts

The abstract of research papers should be submitted to physicsdept@gonzagacollege.edu.in through e-mail attachment in MS-Word (Times New Roman; Line Spacing 1.5; Title: 14 Points; Author Name & Affiliation 10 points; Other Font-size: Content, Keywords & E-mail ID – 12 points). The abstract should not exceed 300 words. The selected abstracts will be allowed for oral/poster presentations. Award will be given for the best presentation.

REGISTRATION FEES

Research Scholars and Students	– Rs 200/-
Faculty Members	– Rs 300/-
Industrial People & Others	– Rs 500/-

- The fees cover the Conference Kit, Lunch & Refreshment
- Certificate will be given to all the registered participants

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Registration Link: https://forms.gle/b9uxJXyuVUztGxBR7

Important Dates

Abstract Submission Opens	: 28-08-2023
Last date of Abstract Submission	: 19-09-2023
Intimation of acceptance (by Mail)	: 20-09-2023
Last Date for Registration	: 20-09-2023

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Kathampallam, Elathagiri – 635 108, Krishnagiri District, Tamilnadu, India

Programme Schedule

Date: 21-09-2023 (Day 1) **Venue: Auditorium** **Time: 10.00 a.m.**

10.00 -10.10 a.m.	Invocation
Welcome Address	Dr. R. Dhinesh Kumar Asst. Professor of Physics, Gonzaga College of Arts and Science for Women, Krishnagiri
10.10 -10.30 a.m.	Inauguration
Inagural Address	Rev. Mother C. Noel Rani, FSAG, Secretary
Presidential Address	Rev. Dr. E. Glitta Sumangali, FSAG, Principal
Felicitation	Rev. Dr. A. John Dayana , FSAG, Vice-Principal
Keynote Address	Dr. Marilyn DMello SERB – NPDF, Centre for Nano and Soft Matter Sciences, Bangalore
Chief Guest Introduction	Mrs. L. M. Manimegalai Asst. Professor of Chemistry, Gonzaga College of Arts and Science for Women, Krishnagiri
10.30 –11.30 a.m.	Dr. Marilyn DMello
Session - 1	SERB – Nation Post Doctoral Fellow, Centre f or Nano and Soft Matter Sciences, Bangalore, Karnataka, India Topic : Metal-Organic Frameworks: From design to promising gas sensing materials
Chief Guest Introduction	Dr. G. Anbarasu Asst. Professor of Chemistry, Gonzaga College of Arts and Science for Women, Krishnagiri
11.30 – 12.30 p.m.	Dr. Srinivasan Krishnan
Session – 2	Assistant Professor, Department of Chemistry, Thiruvalluvar Univeristy, Vellore, Tamil Nadu India Topic : Metal Complexes of Hydrazide-Hydrazones - Study on Structural Diversities and Application as Single Source Molecular Precursors for low temperature synthesis of Metal/Metal Oxide Nanoparticles
12.30 – 01.30 p.m.	Lunch Break
Chief Guest Introduction	Dr. N. Chitra Asst. Professor of Biochemistry, Gonzaga College of Arts and Science for Women, Krishnagiri
01.30 – 02.30 p.m.	Dr. Devanand Venkatasubbu
Session – 3	Associate Professor, Department of Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India Topic : NanoHeal: Advancing Wound Care with Nanomaterial-Based Patches

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Programme Schedule

Date: 22-09-2023 (Day 2) Venue: Auditorium Time: 10.00 a.m.

Chief Guest Introduction 10.00 –11.00 a.m. Session - 4	Dr. M. Manivannan Asst. Professor of Physics, Gonzaga College of Arts and Science for Women, Krishnagiri Dr. E. K. Girija Asst. Professor, Department of Physics, Periyar University, Salem, Tamil Nadu, India Topic : Smart Materials for Advanced Biomedical Applications
Chief Guest Introduction 11.00 – 12.00 p.m. Session - 5	Ms. R. Thanal Asst. Professor of Physics, Gonzaga College of Arts and Science for Women, Krishnagiri Dr. R. Thangappan Asst. Professor, Department of Energy Science and Technology, Periyar University, Salem, Tamil Nadu, India Topic : Advanced Electrode Materials for Electrochemical Supercapacitors
12.00 – 12.30 p.m.	Valedictory
Valedictory Address	Dr. R. Robert Associate Professor, PG & Research Department of Physics, Government Arts College for Men, Krishnagiri, Tamil Nadu
Vote of thanks	Mrs. V. Karthika Asst. Professor & Head Dept. of Chemistry, Gonzaga College of Arts and Science for Women, Krishnagiri

All are Invited Cordially

CONTENT

IT - 01

METAL-ORGANIC FRAMEWORKS: FROM DESIGN TO PROMISING GAS SENSING MATERIALS

Dr. Marilyn Esclance DMello

Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru – 562162
Email: marilyn.dmello@cens.res.in

Abstract:

Gas sensors provide a real time feedback to our surrounding containing different amount of gases that are hazardous to human health. Chemiresistive sensing (a combination of chemical interaction to cause a modification in the electrical resistance of the overall material) is one of the simplest and most affordable one. The principle is simply based on the change in electrical resistance on contact with the target analyte/ gas. The nature of the sensing material and the target gas property decides the change in resistance (increase/decrease).[1] Developing sensors that are selective, sensitive and fast are highly desirable in any place starting from our homes, outdoor/indoor parking lots, hospitals, industries, etc.

Several nanomaterials have been explored as active sensing materials for chemiresistive gas sensing technology. Among those, metal oxides semiconductor (MOS) such as SnO_2 is one of the pioneers in the gas sensing area of research. Herein, the gas interaction (oxidizing/ reducing nature of gas) followed by the modification in the resistance of the MOS is subjected to the characteristics on the n-type or p-type MOS nature and the chemisorbed oxygen species.[2] However, their sensing mechanism is operative only at high temperatures (> 200 °C). Sometimes, these MOS suffer from long response/ recovery times as well as poor selectivity to a mixture of gases. Therefore, search is on for new class of materials that deliver ideal gas sensing characteristics namely greater selectivity, quick response and recovery times, reproducibility, low operating temperature, etc.

Metal-Organic Frameworks (MOFs) based materials are in spotlight as potential candidates for chemiresistive gas sensing application. MOFs are architecturally assorted materials made up of organic and inorganic components. MOFs show the potentiality for chemiresistive gas sensing due to tailorable pores/surface and this underlines the need of the presence of strong/moderate interaction sites (for analyte) to achieve good sensing characteristics (response %, response and recovery times). Some of the attractive features of MOFs over conventional gas sensors are: **i)** High pore volume and surface area, **ii)**

Adsorption reversibility, **iii)** Grafting of MOF's pore channel/ aperture, **iv)** Crystallinity and **v)** Stability. Here the key is to use the tailorable pore surfaces of MOFs for advantage and install apt functionality onto the framework surface depending on the target gas.[3] The challenge is to achieve good sensing characteristics by tuning the active sites on the surface.

This talk will focus on chemiresistive gas sensing technology and nurturing the inherent properties of MOFs in sensing of greenhouse gases like CO_2, flammable H_2 and toxic SO_2 and NO_2 gases.[4] All these have vital importance in safety and industrial processes. Also, insights into the structure-properties correlation for MOF-based sensors through various characterization tools will be described in brief. Overall, the talk will describe on the potentiality of MOFs in a rarely explored area i.e. chemiresistive gas sensing.

References:

1) a) S. M. Majhi, A. Mirzaei, H. W. Kim, S. S. Kim, T. W. Kim, Nano Energy. **2021**, 79, 105369. b) P. Srinivasan, M. Ezhilan, A. J. Kulandaisamy, K. J. Babu, J. B. B. Rayappan, J. Mater. Sci.: Mater. Electron. **2019**, 30, 15825-15847.
2) a) S. Das, S. Mojumder, D. Saha, M. Pal, Sens. Actuators B Chem. **2022**, 352, 131066. b) S. Das, V. Jayaraman, Prog. Mater. Sci. **2014**, 66, 112-255.
3) W. T. Koo, J. S. Jang, I. D. Kim, Chem. **2019**, 5, 1938–1963.
4) a) M. E. DMello, N. G. Sundaram, A. Singh, A. K. Singh, S. B. Kalidindi, Chem. Commun. **2019**, 55, 349-352. b) K. Jayaramulu, M. E. DMello, K. Kesavan, A. Schneemann, M. Otyepka, S. Kment, C. Narayana, S. B. Kalidindi, R. S. Varma, R. Zboril, R. A. Fischer, J. Mater. Chem. A. **2021**, 9, 17434-17441. c) M. E. DMello, N. G. Sundaram, S. B. Kalidindi, Chem. Eur. J. **2018**, 24, 9220-9223. d) M. E. DMello, R. C. Sahoo, R. Raghunathan, H. R. Matte, P. Yadav, G. V. Shanbhag, S. B. Kalidindi, Int. J. Hydrog. Energy. **2022**, 47, 9477-9483. and e) M. E. DMello, S. Vishwanathan, V. R. Bakuru, G. V. Shanbhag, S. B. Kalidindi, ACS Appl. Nano Mater., **2022** (6), 238-247.

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IT – 02

METAL COMPLEXES OF HYDRAZIDE-HYDRAZONES - STUDY ON STRUCTURAL DIVERSITIES AND APPLICATION AS SINGLE SOURCE MOLECULAR PRECURSORS FOR LOW TEMPERATURE SYNTHESIS OF METAL / METAL OXIDE NANOPARTICLES

Dr. SRINIVASAN KRISHNAN

Department of Chemistry, Thiruvalluvar University, Serkkadu, Vellore – 632 115
Tamil Nadu, India

Abstract:

This presentation, in addition to some basics of coordination chemistry, will discuss about the effect of metal ions, anions and pendant group on molecular and crystal structure of the metal complexes of hydrazide-hydrazones ligands. This talk will also describe the applications of these complexes as single source molecular (SSMP) precursors for the low temperature synthesis of various metal/metal oxide nano particles

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IT – 03

NANOHEAL: ADVANCING WOUND CARE WITH NANOMATERIAL-BASED PATCHES

Dr. G. Devanand Venkatasubbu

Department of Nanotechnology, SRM Institute of Science and Technology,
Kaatankulathur, Tamil Nadu

Abstract:

Wound healing is a complex biological process essential for the restoration of tissue integrity and function. In recent years, the integration of nanotechnology into the field of wound care has led to significant advancements in the development of innovative therapeutic approaches. Nanomaterials, characterized by their unique physicochemical properties, have demonstrated remarkable potential in enhancing wound healing processes. This abstract explores the design, fabrication, and application of nanomaterial-based wound healing patches. Nanomaterials offer distinct advantages, including high surface area-to-volume ratios, tunable mechanical properties, and the ability to deliver therapeutic agents in a controlled manner. These attributes have paved the way for the creation of

wound healing patches that not only provide physical protection to wounds but also actively promote tissue regeneration. Incorporating nanofibers, nanoparticles, and nanocomposites into patch structures has resulted in improved cell adhesion, proliferation, and migration, while also modulating inflammation and angiogenesis. Furthermore, the integration of growth factors, antimicrobial agents, and other bioactive molecules into nanomaterial-based patches has enabled the localized and sustained release of these factors, fostering an optimal wound healing environment. The controlled release kinetics offered by nanomaterials mitigate the challenges associated with rapid degradation and premature release often encountered with conventional wound dressings. The utilization of nanomaterials in wound healing patches represents a promising avenue for advancing wound care strategies. The ability to tailor patch composition, structure, and bioactivity at the nanoscale offers unprecedented control over wound microenvironments, leading to accelerated and more efficient wound healing processes. As research in this field continues, nanomaterial-based wound healing patches are poised to revolutionize the way we approach wound care, addressing both acute and chronic wounds with enhanced efficacy and precision.

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IT - 04

SMART MATERIALS FOR ADVANCED BIOMEDICAL APPLICATIONS

Dr. E.K. Girija

Department of Physics, Periyar University, Salem – 11.

Abstract:

Biomaterials may be natural or synthetic which are used to support, enhance, or replace damaged tissue or a biological function and these materials enable the improvement of quality of human life. The potential of biomaterials is demonstrated in diverse areas and every organ in human bodies have benefited from them in one or another form. As the need for biomaterials increases there is a huge market for them. Biomaterials can be labelled with four levels of smartness as inert, active, responsive, and autonomous depending on the degree of their interactions with the body.

Conventional treatment particularly for bone defect repair involves natural biomaterials such as autograft, isograft, allograft and xenograft. Although all these graft materials have strong osteogenic properties which are essential for bone repair and remodelling, they also have few disadvantages such as limited supply, immune rejection,

trauma, possible disease transmission, and high cost. Synthetic hydroxyapatite (HA) being structurally and chemically similar to the mammalian bone mineral it possess excellent inherent properties such as biocompatibility, osteoconductivity, and bioactivity the ability to chemically bond with the host tissues. Hence, synthetic HA is widely used as a bone defect filler, metal implant coating, bone cement, tissue engineering scaffold, etc. Moreover, nano scale HA particles have a large surface area which determines its unique physicochemical and biological properties which makes HA nanoparticles an attractive candidate for local drug delivery.

The use of waste as a resource for producing value added products is growing rapidly. Eggshell is one of the bio wastes generated in large quantity from the food processing industries and hatcheries. Conversion of eggshell into nano HA using microwave synthesis in a lab and pilot scale and its application as a bone regenerative material will be discussed. Further functionalization of nano HA as a local drug delivery agent for osteomyelitis and bone cancer and as a drug repurposing agent will be discussed. Additionally, development of multifunctional magnetic nanoparticle based bone implant for bone cancer treatment and functionalization of nano HA as a optical bio imaging agent will be discussed.

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IT - 05

ADVANCED ELECTRODE MATERIALS FORELECTROCHEMICAL SUPERCAPACITORS

Dr. R. Thangappan

*Department of Energy Science & Technology, Periyar University, Salem-636011, Tamil Nadu

Email: *rm.thangappan@gmail.com

Abstract:

Among different energy storage devices, super capacitors have garnered the attention due to their higher charge storage capacity, superior charging-discharging performance, higher power density, and long cycle life. Subsequently, introducing low-cost and highly-efficient super capacitors is a hot topic in the industrial and scientific realms. Carbon and metal based materials are considered as the most suitable electrode materials due to their intrinsic properties, economic attractiveness, environmental friendliness, and abundant availability. From this perspective, carbon-based materials are

widely explored as the active electrode materials for super capacitors (SC) by taking advantages of hierarchical porous structure, excellent chemical stability, multistage pore structure, high surface area, and excellent conductivity. Various studies have explored many methods to utilize carbon-based electrodes. The functionalization of nanomaterials with carbonaceous substances like graphene and CNTs are most the adaptable approach for improving the energy storage properties of electrode materials. Another growing and novel approach is phyto synthesis and/or biogenic synthesis of nanomaterials, in which C carbon-containing phyto compounds are introduced as stabilizing and functionalizing agents into the synthesized materials. Innovative methods of developing efficient energy storage electrodes are being offered via chemical and physical processes, such as micro fabrication of inter digital patterns based on SC, micro SC, and flexible electrodes. The scientific community is currently conducting extensive research to find efficient electrode materials for energy storage. Due to the ongoing discovery and development of novel, environmentally benign processes for the synthesis of materials, the variety and efficacy of SCs electrodes would also increase. The development of charge storage mechanisms, functional groups, and electrical conductivity are all essential in providing the appropriate electrochemical performance for real-world applications.

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PA - 01

SYNTHESIS, SPECTRAL CHARACTERIZATIONS AND MOLECULAR DOCKING STUDIES OF MONTELUKAST METHYL KETONE, LACOSAMIDE DERIVATIVES AS PROMISING ANTIBACTERIAL AGENTS AND ANTIVIRAL ACTIVITY TOWARDS NEWCASTLE DISEASE VIRUS (NDV) USING EMBRYONATED CHICKEN EGGS ASSAY (ECEA)

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Abstract:

In the present study, we report the synthesis of montelukast methyl ketone, lacosamide derivatives. The LCM retention rate and effectiveness of response were analyzed at three, twelve and twenty-four months. Lacosamide is a new generation antiepileptic drug that affects the slow inactivation of voltage-gated sodium channels. Newcastle disease is highly infectious viral disease causing huge economic losses worldwide. In this study the effect of from montelukast methyl ketone are investigated against Newcastle disease virus by an in-vivo assay. Seven groups of nine-day-old embryo chicken eggs were inoculated with various treatments of different concentration. All the groups except uninoculated negative control group were inoculated with velogenic NDV strain; five groups received different concentrations. Daily observe the rate of embryo survival. Allantoic fluid from treated eggs was collected for hemagglutination test. Results showed that embryo survival rate was higher 300µg/ml treated antiviral activity. The synthesized compounds were evaluated for their in vitro antibacterial activity against pathogenic strains of both gram negative and gram positive bacteria. The 3a derivative displayed superior antibacterial activity against E. coli, Pseudomonas aeruginosa in comparison to the reference drug. The 3b derivatives were antiviral activity towards NCD Virus. Molecular docking studies were used for design of the compound and understand the mode of binding between the compound and target enzyme. All the products were thoroughly characterized by 1 H-NMR, 13 C-NMR, FT-IR, Mass spectral and CHN analysis.

Keywords: Montelukast, THF, Antibacterial Activity, Antiviral Activity, Molecular docking studies and Spectral Characterization.

PA - 02

CU-PYROMELLITIC ACID (PMA) METAL-ORGANIC FRAMEWORK (MOF) INCORPORATED WITH SULFONATED POLY (ETHER ETHER KETONE) (SPEEK) MEMBRANE ENHANCED FUEL CELL PERFORMANCE IN POLYMER ELECTROLYTE MEMBRANE FUEL CELL

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Abstract:

The development of cost effective and stable Cu-Pyromellitic acid (PMA) Metal Organic Framework prepared via hydro-thermal method. As-synthesized Cu-PMA is used as an additive to form a nanohybrid composite with sulfonated poly (ether ether ketone) (sPEEK) for its application in polymer electrolyte membrane fuel cell (PEMFC). The optimum sPEEK/Cu-PMA nano-hybrid composite (0.5 wt. %) shows high proton conductivity (161.4 mS/cm), better ion exchange capacity (1.71 meq/g) and good water uptake (23.97 ± 0.016 %) in relation to sPEEK. The optimized sPEEK/Cu-PMA (0.5 wt %) nano-hybrid composite membrane exhibits higher PEMFC performance with current density of 800 mA at 0.6 V, which is 40 % greater than the 0.4 mA cm -2 for pristine sPEEK. Additionally, in a PEFC, the membrane electrode assembly (MEA) of the sPEEK/Cu–PMA-0.5 wt% composite membrane delivered an impressive current density of 960.14 mA= at an operating cell voltage of 0.6 V and a peak power density of 748 mW, which is B^2 times higher than that of the MEA prepared with sPEEK (a current density of 488.5 mA cm^2 at a cell voltage of 0.6 V, and a peak power density of 404.11 mW). Notably, the sPEEK/Cu–PMA-0.5 wt% hybrid composite membrane exhibited 86% retention of open circuit voltage (OCV) even after a stability test of 4100 h at 30% relative humidity and a cell temperature of 80°C, confirming its viability for energy conversion and storage devices.

Keywords: Cu-Pyromellitic acid (PMA), PEMFC, Nanocomposite membranes, durability, fuel cell performance, sPEEK, proton conductivity, Ion Exchange Capacity.

Reference:

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PA - 03

NOVEL SYNTHESIS OF STURDY AND DURABLE SUPERHYDROPHOBIC/SUPEROLEOPHILIC VISCOSE FABRIC SURFACES FOR OIL-WATER SEPARATION

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Abstract:

At present, Super hydrophobic surfaces, characterized by a high-water contact angle (>150°), have attracted worldwide attention for their potential applications and water treatment. The superhydrophobic viscose fabric have attracted significant attention in the areas of science and industry because of their unique water repellency, oil separation efficiency, excellent thermal and chemical stability as well as the potential for practical applications in functional coatings and fabric finishing. In this present work, Superhydrophobic viscose fabric material have been synthesized by chemical refluxation using saturated fatty acids (such as., Palmitic acid and Lauric acid) with 3-Glycidoxypropyl trimethoxy Silane. The synthesized viscose fabric has the advantages of high separation efficiency, stable recyclability, excellent durability and exhibiting the strong potential for industrial applications. The oil absorption capacity studies also demonstrated a high absorption volume of 13.94 g/g for PA-GPTMS-coated NWVF and 13.57 g/g for LA-GPTMS-coated NWVF materials. The surface-modified materials were investigated for sustainability and lifespan. Remarkably, the PA-GPTMS-coated NWVF material showed admirable results of superhydrophobic/superoleophilic behavior retained (WCA > 150°) in a harsh environment (70h at 120°C) and oil-water separation over 30 recycles. The above results suggested that the chemically modified nonwoven viscus fabrics would be a suitable potential candidate for the industrial-scale separation of immiscible oils/organic solvent contamination in water.

Keywords: Super hydrophobic Viscose Fabric, Oil/Water Separation, Recyclability, Durability, Oil Adsorption,

Reference:

1. Panneerselvam Vengatesh and Manickam Anbu Kulandainathan* ACS Appl. Mater. Interfaces -2015, 7, 1516−1526.

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PA - 04

SCREENING OF POTENTIAL PLANT-BASED LEAD COMPOUNDS DEMETHOXCURCUMIN FOR OLIVE KNOT DISEASE

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Abstract:

The current study strives to pick out potential targets of olive knot disease for hindrance from turmeric (Curcuma longa) compound Demethoxcurcumin. Olive knot disease is connected with rainfall and is prompted by the bacterium Pseudomonas savastanoi. The olive knot can be cured with the help of copper-containing bactericides. One of the proteins of Pseudomonas savastanoi is a siderophore. The protein siderophore is docked with many ligands such as demethoxycurcumin, camphor, caffeine, thymol, and cineole. These ligands are plant-based chemical compounds. The docking score is compared with control values of available drugs for Olive knot disease. Hence, the demethoxycurcumin chemical compound of turmeric has the highest docking score compared to cuprous oxide a copper-ions. The docking score for ligand demethoxycurcumin is -7.785 Kcal/mol, the glide score is -8.156Kcal/mol, and has three H-bond. The docking score for ligand cuprous oxide is -4.440 Kcal/mol, and the glide score is -4.440 Kcal/mol and has no H-bonds. The final compounds are taken for ADMET prognostications. Based on the docking score and glide score, the turmeric compound acted against pseudomonas savastanoi. The five compounds were calculated for ADMET parameters, and Lipinski Rule of 5 Violation, and the results were produced without any constraints. This study could recognize the Demethoxcurcumin of turmeric compound against olive knot disease.

Keywords: Plant Based, Demethoxcurcumin, Docking, siderophore, Knot disease.

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PA - 05

GREEN SYNTHESIS OF COPPER OXIDE NANOPARTICLES FOR ANTIMICROBIAL APPLICATIONS

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Abstract:

Nanoparticles, with their minute scale, have revolutionized various scientific fields, especially in medicine, offering unexplored opportunities for research. One intriguing avenue is the synthesis of nanoparticles using plant extracts, a method demonstrating significant potential in combating pathogenic bacteria through antimicrobial properties. Copper oxide nanoparticles have gained considerable attention among the array of novel nanoparticles. Traditional chemical synthesis methods employ various toxic chemicals as reducing agents for copper oxide nanoparticles, raising environmental concerns. This has driven the development of green synthesis techniques utilizing biological molecules from plants, often in the form of extracts. This innovative approach supersedes chemical methods by harnessing nature's toolbox, prioritizing safety and sustainability. Plant-derived compounds are intricately assembled, making them suitable for metal nanoparticle synthesis. This precise method not only facilitates particle formation but also customizes their properties for specific applications. This review leverages the abundant plant diversity to establish rapid, eco-friendly protocols, surpassing conventional methodologies. By tapping into the wealth of plant-derived compounds, researchers aim to expedite synthesis processes while adhering to green principles. One significant outcome of this endeavor is the exploration of copper oxide nanoparticles' antimicrobial potential. A comprehensive survey of existing literature reveals their efficacy against pathogenic bacteria. This insight holds immense value, paving the way for innovative strategies in combating such bacteria, potentially transforming healthcare and addressing the escalating threat of antimicrobial resistance.

Fundamentally, the synthesis of nanoparticles from plant extracts epitomizes sustainable innovation. This review encapsulates the remarkable journey toward an environmentally conscious approach while emphasizing the promising antimicrobial

applications of copper oxide nanoparticles. It offers a glimpse into a future where scientific progress aligns seamlessly with ecological principles

Key Words: Nanoparticles, Green synthesis, Antimicrobial activity

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PA - 06

SYNTHESIS AND CHARACTERIZATION OF TRANSITION METAL IONS DOPED CdS/ZnS NANOPARTICLES BY PRECIPITATION METHOD

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Abstract

Cadmium oxide Nanomaterials have been synthesized by precipitation method method at room temperature. In this present study, we used cadmium acetate and Sodium hydroxide as a common starting material. The samples of pure Nanomaterials were calcined at 400°C for 2 hrs. Structural, morphological, textural, microstructural and optical properties of the prepared Synthesis and characterization of metal ions doped oxides nanoparticles by precipitation method Cadmium oxide nanoparticles (NPs) have been investigated by X-ray diffraction (XRD), scanning electron microscope (SEM), Fourier transform infrared (FTIR), UV-Vis spectroscopy and photoluminescence (PL) spectroscopy. Doping of oxide materials with transition metals such as Ba and Zr has been shown (each metal individually doped). Doped oxide nanoparticles, which have a smaller crystallite size, a larger surface area, and a lower band gap than conventional oxide nanomaterials, may have improved photocatalytic activity in visible light. Finally, photocatalytic degradation of methylene blue (MB), methyl orange (MO), and other possible dyes is obtained under the influence of visible light.

Keywords: Cadmium Oxide nanomaterials, Oxide-Based Metals ions, Photocatalytic Applications

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PA - 07

STRUCTURAL AND MAGNETIC PROPERTIES OF $ZnFe_2O_4$ NANOPARTICLE SYNTHESIS USING POLYOL METHOD

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Abstract:

In the present work, $ZnFe_2O_4$ nanoparticles were prepared by polyol method at 180˚C. The prepared nanoparticles were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Transmission electron microscopy (TEM), X-ray photoelectron microscopy (XPS) and Vibrating sample magnetometry. XRD reveals the polycrystalline nature with crystallite size of 23 ±2 nm and FESEM depicts the presence of quasi-spherical particles with wide size distribution. More insights on the particle morphology and size of the nanoparticles were determined using TEM analysis. Charge state of the Zn, Fe and O were found to be 2^+,3^+ and 2^-.VSM clearly depicted the ferromagnetic behavior of the samples with coercivity 123 Oe and saturation 38 emu/g.

Keywords: $ZnFe_2O_4$ nanoparticles, Oxide-Based Metals ions, ferromagnetic behaviour

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PA - 08

PHOTOCATALYTIC PERFORMANCE OF Mo DOPED NiO (MNO) NANOPARTICLES AND GAS SENSING APPLICATION

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Abstract:

Mo doped NiO (MNO) nanostructures were prepared by solvothermal method and triethylamine gas sensing, Rhodamine B photo degradation in the visible light was investigated in detail. XRD results explicitly revealed that, Mo doping concentration have strong influence on the structure of NiO. Particle size was observed to be 10-25 nm and TEM images shows the presence of tiny particles with agglomeration. FESEM images depicts formation of spherical structures and optical band gap energy was in the range 3.20

eV – 3.54 eV with increase in Mo concentration. Triethylamine gas sensing was done based on resistive gas sensing method for temperature range 200 ˚C to 300 ˚C. Maximum performance of about 6.25% at 260 ˚C was obtained to 1% MNO nanoparticles and 80% Rhodamine degradation was achieved.

Keywords: TEM, Solvothermal, Rhodamine, Nanostructure

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PA - 09

IDENTIFICATION OF POTENTIAL INHIBITORS FROM AVICENNIA ALBA AGAINST WDSV THROUGH COMPARATIVE STUDY: ADMET SCREENING AND MOLECULAR DOCKING STUDIES

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Abstract:

The present study shows the identification of a potential target of Walleye dermal sarcoma virus (WDSV) for a novel inhibitor from "Avicennia alba" which has the compound, rascinnamie (C35 alkaloid). The structure of the drug target was selected from the Protein Data Bank (PDB) and was subjected to molecular docking against a compound the poly gag protein which is taken from the affected fish. Walleye dermal sarcoma virus (WDSV) is a type of retrovirus. It is a tumor caused by a virus, that develops from the deep layer of fish's skin (skin dermis)., Infection occurs throughout the year but occurs higher rate in early spring, during the swapping season. The virus spreads from fish through physical contact or water transmission. It cannot be transmitted to Humans. Till now there no antiviral drug against it. WDSV genome contains in addition to gag, pol, and env. Here Rascinnamine (C35 alkaloid) is docked against gag poly protein and also it is compared with other three compounds Fluocinolone acetonide, terpenoid R5, and carbolic acid (phenol) docked against gag poly protein. The docking score for ligand rascinnamie is -5.786 Kcal/mol, the glide score is -5.829kcal/mol and its molecular weight is 130 Kcal/mol. The docking scores of the other three compounds fluocinolone acetonide, terpenoid R5, and carbolic acid are -4.677 kcal/mol, -3.967 Kcal/mol, and -3.3937kcal/mol, the glide score are -4.677kcal/mol, -3.967kcal/mol and -3.938kcal/mol and there is no formation of H-bond. The final compound was taken from the ADMET parameter. By comparing these two kinds of docking scores and glide scores. Thus, the

conclusion shows this study recognizes that rascinnamie (C35 alkaloid) compound can be more effective for the WDSV because it has high docking and glide score.

Keywords: Molecular Docking, Avicennia Alba, WDSV, Alkaloids, ADMET

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PA - 10

HYDROTHERMAL SYNTHESIS OF Zn-DOPED α-Fe_2O_3 (MFO) NANOSTRUCTURES; SPIN DISORDER MAGNETISM AND PHOTOCATALYTIC PROPERTIES

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Abstract:

Hierarchical nanostructures play an important role in environmental clean –up and sustainability application .The magnetic and photocatalytic characteristics of flower –like Zn-doped α-Fe_2O_3 nanostructures were prepared by using a polyol –assisted hydrothermal method .crystallite sizes are in the range of 38-26 nm and the existence of 3D hierarchical nanostructures was observed in FESEM pictures .The optical band gap energy varies between 2.08 and 2.16 eV, while XPS examination exposes the ions' charge states and validates Zn^{3+} inclusion in the Fe^{3+}lattice .At room temperature, the addition of Zn to α-Fe_2O_3 results in a spin disorder ferromagnetism and coercivity of about 600 eV was achieved. Methylene blue (MB) day solution degraded by 82% when2.5%Zn doped with α-Fe_2O_3 under visible conditions for 180 min irradiation time

Keywords: Zn-doped α-Fe_2O_3, Photocatalytic, Ferromagnetism, Surface disorder

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PA - 11

SOL-GEL PREPARATION OF CeO_2 NANOPARTICLES FOR PHOTOCATALYTIC APPLICATION

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Abstract:

Cerium Oxide (CeO_2) nanoparticles were synthesized by sol-gel method. X-ray diffraction analysis shows that nanoparticles exhibit good crystal structures of CeO_2. FT-IR result shows the functional group of the prepared nanoparticles. High resolution scanning electron microscopic results display the morphology of CeO_2 nanoparticles. Energy dispersive x-ray spectroscopy proves the presence of constituting elements in the prepared materials. The CeO_2 nanoparticles show a significant shift in the UV–Vis absorption spectrum in the visible region. The photocatalytic activity of the samples were tested for the degradation of methyl orange (MO) in aqueous solutions under visible light irradiations. The CeO_2 nanoparticles exhibits enhanced visible light photocatalytic behaviour.

Keywords: Sol-gel, Nanoparticles, Photocatalytic

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PA - 12

HYDROTHERMAL PREPARATION OF MnO_2 NANOPARTICLES FOR PHOTOCATALYTIC APPLICATION

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Abstract:

Manganese dioxide (MnO_2) nanoparticles were synthesized by sol-gel method. X-ray diffraction analysis shows that nanoparticles exhibit good crystal structures of MnO_2. FT-IR result shows the functional group of the prepared nanoparticles. High resolution scanning electron microscopic results display the morphology of MnO_2 nanoparticles. Energy dispersive x-ray spectroscopy proves the presence of constituting elements in the prepared materials. The MnO_2 nanoparticles show a significant shift in the UV–Vis

absorption spectrum in the visible region. The photocatalytic activity of the samples were tested for the degradation of methyl orange (MO) in aqueous solutions under visible light irradiations. The MnO_2 nanoparticles exhibits enhanced visible light photocatalytic behaviour.

Keywords: Hydrothermal, Nanoparticles, Photocatalytic

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PA - 13

SPECTROSCOPIC (FT-IR, FT-RAMAN, NMR AND UV) ADMET, MOLECULAR DOCKING AND DYNAMICS SIMULATION OF CORYLIFOLININ AS ANTI-TUBERCULOSIS AGENT

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Abstract:

The spectroscopic characteristics, molecular structure, and biological characteristics of the Corylifolinin (Isobavachalcone-IBC) structure have been studied using computational techniques utilizing the standard B3LYP/6-311++G (d,p) basis set. Potential energy distribution (PED) was used throughout the process of assigning the fundamental wavenumbers of the IBC compound. In this work, we have reported the correlation between experimental and computed examination of the molecular structure, FT-IR/Raman, UV-Vis absorption, and NMR spectra of the title compound. The potential energy scan (PES) analysis of IBC was optimized in the ground state by the DFT/B3LYP technique with the 6-311++G (d,p) basis set. The Frontier Molecular Orbitals (FMO), Molecular Electrostatic Potential (MEP), local reactivity and quantum chemical descriptors were also analyzed. Furthermore, drug-likeness and ADMET predictions of the present ligand show good pharmacological activity. A docking simulation performed with the 2FUM receptor using the Auto Dock software showed that the IBC compound has inhibitory activity against Mycobacterium tuberculosis disease. All our results suggest that the IBC molecule could have a great effect in the treatment of tuberculosis disease. MD simulations were carried out for 100 ns to predict the RMSD, RMSF, and radius of gyration analyses.

Keywords: DFT; Spectroscopic profiles; ADMET; Drug-likeness; Molecular docking

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PA - 14

SYNTHESIS AND CHARACTERIZATION OF Nd_2O_3/MNO_2 BY HYDROTHERMAL METHOD FOR SUPER CAPACITOR APPLICATION

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Abstract:

Rare earth based compounds receives great interest towards supercapacitors for overcoming the limitation of lower energy density to high specific density and operating voltage. In the present work, the new and novel Nd_2O_3 /MnO_2Nanocomposites was prepared by Hydrothermal method and investigated as a working electrode for the supercapacitors application. The structural, morphological and optical properties of synthesized Nd_2O_3, MnO_2 and Nd_2O_3/MnO_2 were investigated using different characterizing techniques. The Nd_2O_3/MnO_2 hybrid was successfully coated on nickel foam as a working electrode in 2M Na_2SO_4 electrolyte solution. The Nd_2O_3/MnO_2 displays remarkable electrochemical performance exhibiting the specific capacitance of 180 Fg^{-1} at a current density of 1 Ag^{-1} in comparison with the pristine Nd_2O_3. The electrochemical stability of Nd_2O_3/MnO_2 is promising with charge retention of 97% cycling stability after 5000 cycles. The enhancement of specific capacitance of Nd_2O_3/MnO_2relative to Nd_2O_3 due to charge transfer at the interface between the MnO_2 and Nd_2O_3 is evident that Nd_2O_3/MnO_2 is a potential and promising candidate for designing efficient power source device with high energy and power density.

Keywords: Electrode materials, Cyclic stability, Specific capacitance, Composite, Interface.

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PA - 15

SCHIFF BASE METAL COMPLEXES SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY

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Abstract:

At Present the synthesis of Schiff Base ligand from 4-nitrobenzoic acid and thiosemicarbazide derivate with the metal ions Co (II), Co (II) have been successfully prepared in EtOH Solvent. The obtained complexes are further characterized by FTIR spectroscopy, UV–Vis spectroscopy, mass spectroscopy, ^{1}H & ^{13}C NMR, magnetic susceptibility and conductivity measurements. The Metal complexes show good activity towards Biological Applications.

Reference:

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2. G. Anbarasu, M. Malathy, P. Karthikeyan, R. Rajavel, Journal of Solid State Chemistry 253, 2017, 305-312.

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PA - 16

MICROWAVE ASSITED COMBUTION SYNTHESIS OF $Zn_{0.5}Cu_{0.25}Al_{0.25}Fe_2O_4$ NANOPARTICLES FOR OPTICAL AND MAGNETIC STUDIES

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Abstract:

$Zn_{0.5}Cu_{0.25}Al_{0.25}Fe_2O_4$ nanoparticles were synthesized employing L-arginine as fuel using MACT (microwave assisted combustion technique). The synthesized samples were characterized following methods such as XRD, FE-SEM, EDX, UV-DRS, FT-IR and VSM. The XRD confirmed the cubic spinel structure and the average crystallite size

observed lying in the range of 24 nm deduced using the Debye Scherrer's equation. The morphology of $Zn_{1-x-y}Cu_xAl_yFe_2O_4$ (x and y= 0.05) nanoparticles is observed using FE-SEM. EDX analysis is opted for the elemental mapping copper and aluminium doped zinc ferrite nanoparticles. Further band gap value was calculated using Kubelka Munk function, which was seen 1.80 eV. The strong absorption band at 459, 557 and 1121 cm^{-1} was associated with the vibrations of Zn-Fe-O and Cu-O-Al ferrite nanoparticles. The hysteresis loops exhibited conversion from ferromagnetic behaviour with increase in Cu and Al doping.

Keywords: copper and aluminium doped zinc ferrite; Structural analysis; Direct band gap, Vibrational analysis, Ferromagnetism.

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PA – 17

Cu (II) & Co (II) SYNTHESIS, CHARACTERIZATION AND CATALYTIC APPLICATIONS

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Abstract:

The Unsymmetrical Schiff base ligand interactions with Transition metals like Cu, Co complexes which have been synthesized and characterized by following spectroscopic methodology such as., elemental analysis, IR spectra, electronic spectra, ^{1}H-NMR. The catalytic activities of the as- synthesized complexes have been studied and found that the complexes exposed effective catalytic activity for oxidation of alcohols.

References:

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2. G. Anbarasu, M. Malathy& R. Rajavel., Journal of Porous Materials, 24, 1253–1261 (2017).

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PA – 18

EFFECTIVE ALKENES USING A HIGHLY ACTIVE AND REUSABLE IMMOBILISED CU COMPLEX ON $AlPO_4$

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Abstract:

The homogeneous Copper complex Cu (II) have been immobilised on amorphous $AlPO_4$ support through phosphamide bonds. The catalyst was characterised by UV–Vis and GC and its activity was compared to that of the homogeneous complex in the liquid phase hydrogenation of a range of alkenes. The heterogenized catalyst exhibited very good activities and excellent reusability.

References:

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PA – 19

SYNTHESIS AND CHARACTERIZATION AT $ZnFe_2O_4$ NANOPARTICLE BY MICROWAVE COMBUSTION METHOD

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Abstract:

Zinc ferrite nanoparticles were synthesized by microwave combustion method employing L-arginine as a fuel. The synthesized samples were characterized following methods such as XRD, FESEM, EDX, DRS-UV, FT-IR and VSM. The XRD confirmed the cubic spinel structure and the average crystallite size observed lying in the range of 16 nm deduced using the Debye Scherrer's equation. The morphology of the zinc ferrite

nanoparticles observed using FE-SEM. EDX analysis is opted for the elemental mapping of zinc ferrite nanoparticles. Further band gap value was calculated using Kubelka Munk function, which was seen 1.88 eV. The strong absorption band at 439 and 537 cm^{-1} was associated with the vibrations of Fe-O and Zn-O of $ZnFe_2O_4$ nanoparticles. The hysteresis loops exhibited conversion ferromagnetic behaviour.

Keywords: Structural analysis; Direct band gap, Vibrational analysis, Ferromagnetic.

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PA – 20

A SIMPLE MICROWAVE ASSISTED COMBUSTION SYNTHESIS OF $Zn_{0.7}Cu_{0.15}Al_{0.15}Fe_2O_4$: STRUCTURE, OPTICAL AND MAGNETIC STUDIES

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Abstract:

$Zn_{0.7}Cu_{0.15}Al_{0.15}Fe_2O_4$ nanoparticles were synthesized by combustion method employing L-arginine as a fuel. The synthesized samples were characterized following methods such as XRD, FESEM, EDX, DRS-UV, FT-IR and VSM. The XRD confirmed the cubic spinel structure and the average crystallite size observed lying in the range of 23 nm deduced using the Debye Scherrer's equation. The morphology of the $Zn_{1-x-y}Cu_xAl_yFe_2O_4$ (x & y = 0.15) nanoparticles observed using HR-SEM. EDX analysis is opted for the elemental mapping of copper and aluminium doped zinc ferrite nanoparticles. Further band gap value was calculated using Kubelka Munk function, which was seen 1.88 eV. The strong absorption bands at 445 and 557 cm^{-1} was associated with the vibrations of Zn-O, Fe-O and Cu-O-Al of Al and Cu doped $ZnFe_2O_4$ nanoparticles. The hysteresis loops exhibited conversion ferromagnetic behaviour.

Keywords: Structural analysis; direct band gap, Vibrational analysis, Ferromagnetic.

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PA – 21

A STUDY ON THE DIELECTRIC PROPERTIES OF PURE AND Mg-DOPED CADMIUMOXIDE NANOPARTICLES SYNTHESIZED BY CO-PRECIPITATION METHOD

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Abstract:

Cadmium Oxide (CdO) and Mg doped CdO nanoparticles have been synthesized by Co-precipitation method at room temperature. The synthesized nanoparticles were characterized by powder X-ray diffraction analysis (XRD), UV-Visible analysis, FTIR, SEM, TEM and Dielectric studies. The XRD analysis shows that the obtained sample has face centred cubic structure and the intensity of the peaks slightly decrease with Mg doping. The optical study shows that the doping ions lead to an increase in the absorption edge wavelength and a decrease in the band gap energy of CdO. FTIR spectra confirmed the presence of functional groups in the pure and Mg doped CdO nanoparticles. The SEM images clearly show spherical shaped nanoparticles and TEM photograph of both nanoparticles display spherical structure with agglomeration. The dielectric behaviour of the pure and Mg doped CdO was studied at room temperature at wide range of frequencies. Dielectric constant and loss were found to decrease with increase in frequency.

Key Words: Cadmium oxide, Co-Precipitation, XRD, FTIR, UV-Vis, SEM, TEM, Dielectric constant and Dielectric loss

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PA – 22

GROWTH AND CHARACTERIZATION OF NON-LINEAR OPTICAL CRYSTAL SODIUM LITHIUM TETRACHLORIDE (SLTC) SINGLE CRYSTAL

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Abstract:

Nonlinear optical crystal is recently attracted the research scientist due to its wide application in the field of optoelectronics and photonics. Inorganic nonlinear crystal

possess to good second harmonic generation efficiency. The SLTC single crystals were grown from aqueous solution by slow evaporation technique at room temperature. The grown crystal was subjected various physical characterizations. The Unit cell parameters of as the grown crystal (SLTC) was estimated by single crystal X-ray diffraction technique and it indicates that the crystal is Orthorhombic in structure. The grown crystal of SLTC has good crystalline nature which was observed from powder diffraction technique (XRD) study. The vibration frequencies of the functional groups are identified by FTIR spectroscopic study. The SLTC crystal having good optical transmission in the entire visible region and hence SLTC crystal may suitable candidate for optical device and fabrication. Nonlinear optical property of the crystal was confirmed by SHG test using Kurtz-perry powder technique. The photoconductivity studies have been carried out.

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PA – 23

BIO SYNTHESIS OF SILVER NANOPARTICLES FROM THE MARINE SEAWEED SARGASSUM WIGHTII AND THEIR ANTIBACTERIAL ACTIVITY AGAINST SOME HUMAN PATHOGENS

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Abstract:

In this paper we have reported biological synthesis of nano sized silver and its antibacterial activity against human pathogens. The nanoparticles of silver were formed by the reduction of silver nitrate into aqueous silver metal ions during exposure to the extract of marine seaweed Sargassum wightii. The optical properties of the obtained silver nanoarticles were characterized using UV-Visible absorption (UV-Vis) and room temperature Photoluminescence (PL). The X-Ray diffraction (XRD) results reveal that the synthesized silver nano particles are in the cubic phase. The existences of functional groups were identified using Fourier Transform Infrared Spectroscopy (FTIR). The morphology and size of the synthesized particles were studied with Atomic Force Microscope (AFM) and High Resolution Transmission Electron Microscope measurements (TEM). The synthesized nanoparticles have an effective antibacterial activity against S.aureus, K.Pneumonia, and S.typhi.

Keywords: Biosynthesized, AgNPs, antibacterial activity, AFM, TEM.

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PA – 24

INVESTIGATION ON STRUCTURAL OPTICAL AND DIELECTRIC PROPERTIES OF MgO NANOPARTICLES: SYNTHESIZED BY CO-PRECIPITATION TECHNIQUE

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Abstract:

Metal oxide nanomaterials are important and excellent materials, because of its special properties like chemical stability, high photo catalytic activity, high electric permittivity, non-toxic nature. So it is used in various applications like optical, electrical, electronic, antiseptic, antibacterial, environmental, semi conductors and catalytic devices. Magnesium oxide nanoparticles with different morphologies, including sphere, flower-like, sheet, rod like and plate shapes have been synthesized in different solvents and surfactants. Present work focused on to synthesis of Magnesium oxide (MgO) Nanoparticles and its applications. These nanoparticles are prepared by simple suitable chemical method like Chemical Co-precipitation using Magnesium chloride as core precursor. The synthesized Metal oxide nanoparticles have been characterized by X-ray Diffractometer (XRD) to confirm its structure; the optical properties like Absorption, reflection, band gab, refractive index of the prepared NPs were studied by UV-Vis Spectrometer. The electrical conductivity of the material was investigated by Impedance analysis.

Keywords: MgO nanoparticles, Co-precipitation, XRD, UV- Vis, Impedance Analysis.

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PA – 25

A STUDY ON THE DIELECTRIC PROPERTIES OF SHOCK TREATED SiO_2-NANOPARTICLES FROM RICE HUSK ASH BY SIMPLE THERMO-CHEMICAL TREATMENTS

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Abstract:

In the form of nanoparticles, silica is a significant inorganic component of rice husk. As a result, high purity amorphous silica nanoparticles can be synthesized by conventional thermo-chemical procedures. Hence, in this study, an eco-friendly chemical treatment method was used to try and synthesize amorphous silica nanoparticles from rice husk ash. Using a variety of material characterization techniques, the obtained nanoparticles' characteristics were confirmed by comparison with amorphous silica nanoparticles of commercial standard. For both silica samples, X-ray diffraction investigation demonstrates amorphous behaviour, whereas Fourier-transform infrared spectroscopy spectra mainly revealed siloxane and silanol groups. As a result, this silica nanoparticle can be used in the fields of nano-additives, sensors, and microelectronics.

Keywords: Silica nanoparticle, Rice husk ash, amorphous silica, Characterization

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PA – 26

EFFECT OF HYDROPHOBICITY AND SIZE OF THE LIGANDS ON THE INTERCALATIVE BINDING INTERACTIONS OF SOME METALLO-SURFACTANTS CONTAINING II-CONJUGATED SYSTEMS WITH YEAST tRNA

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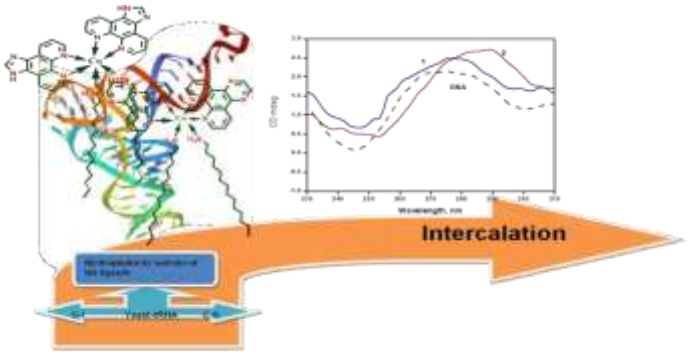
Abstract:

The intercalative yeast t-RNA binding behavior of some metallo-surfactant complexes, $Co(ip)_2(TA)_2](ClO_4)_3$ **(1)** and $[Co(dpq)_2(TA)_2](ClO_4)_3$ **(2)** where TA = Tetradecylamine (Myristylamine), ip = imidazo [4,5-f][1,10] phenanthroline and dpq =

dipyrido[3,2-d:2'-3'-f]quinoxaline containing π-conjugated systems (both below and above critical micelle concentration) have been investigated by means of absorption spectral titration, competitive binding, circular dichroism, cyclic voltammetry, and viscometry measurements. Absorption spectral titration results implicates yeast tRNA has significant effects on the binding behaviors of two surfactant complexes via intercalative mode showed significant absorption band of hypochromicity with red shift. The intrinsic binding constant values below and above CMC were determined as $K_b = 6.12\times10^5$ M^{-1}, 2.31×10^6 M^{-1}, for complex (1) and 7.23×10^5 M^{-1}, 3.57×10^6 M^{-1}, for complex (2). In both sets of complexes (1) and (2), the complexes bind more strongly to yeast tRNA in above critical micelle concentration can be hydrophobic and confirm intercalation. Competitive displacement studies confirmed that complexes bind to yeast tRNA via intercalative mode. Cyclic voltammetry studies suggest the increasing amounts of yeast tRNA, the cathodic potential E_{pc} for the two complexes shows a positive shift in peak potential indicated the process of binding via intercalation. These observations were further validated by CD, and hydrodynamic measurements. All these studies suggesting that a surfactant complex binds to yeast tRNA appear to be mainly intercalative because of hydrophobicity due to extending aromaticity of the π system of the ligand and planarity of the complex has a significant effect on tRNA binding affinity increasing in the order of complexes containing ligands ip < dpq.



GRAPHICALABSTRACT

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PA – 27

RARE EARTH-DOPED NIZN SPINEL FERRITES: ENHANCING MAGNETIC PROPERTIES FOR ADVANCED APPLICATIONS

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Abstract:

Rare earth-doped nickel-zinc (NiZn) spinel ferrites have emerged as a fascinating class of magnetic materials due to their exceptional magnetic and electrical properties. This abstract provides an overview of the key findings and implications of recent research in this field. The incorporation of rare earth elements, such as cerium (Ce), lanthanum (La), and gadolinium (Gd), into NiZn spinel ferrites has been extensively explored to tailor their magnetic behavior. These dopants introduce remarkable improvements in various aspects of these ferrites, including saturation magnetization, coercivity, and magnetic permeability. Such enhancements are particularly promising for applications in high-frequency transformers, inductors, and microwave devices. Moreover, rare earth doping influences the microstructural and crystalline characteristics of NiZn spinel ferrites. Researchers have identified the critical role of sintering techniques and sintering temperatures in achieving optimal magnetic properties. The microstructure and grain size also play vital roles in determining the overall performance of these materials. This paper highlights the growing importance of rare earth-doped NiZn spinel ferrites in modern electronics and telecommunications. The ability to fine-tune their magnetic properties makes them indispensable in the development of advanced components for power conversion, signal processing, and electromagnetic shielding. Rare earth-doped NiZn spinel ferrites represent a compelling avenue of research and development in the field of magnetic materials. Continued investigations into their synthesis techniques, microstructure, and applications will undoubtedly contribute to the advancement of cutting-edge technologies in various industries.

Keywords: Rare-earth, Spinel ferrites, Ni-Zn, Magnetic material

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PA – 28

SPECTRAL, STRUCTURAL AND COMPUTATIONAL ANALYSIS OF PIPERAZINE HEXANEDIOIC ACID

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Abstract:

Piperazine hexanedioicacid (PH) is an odourless white crystalline organic compound which is used as an anthelmintic agent and in the manufacture of pesticides. The full geometrical optimization of the structure was carried out at density functional theory (DFT) methods using Gaussian'09 program package with B3LYP/6-311++G(d,p) basis set to calculate the optimized bond length, bond angle and dihedral angle of the molecule and to construct the molecular orbitals. HOMO and LUMO energy gap explain the charge transfer interactions taking place within the molecule. Molecular orbitals and their properties used by the frontier electron density predict the most reactive position in electron systems and explain several types of reaction in conjugated system. The Atomic charge analysis illustrates the distribution of charge in the molecule. The atomic natural charges have been calculated by NBO method. The interaction behaviour was studied by Electron Localization Function and Localized Orbital Locator.

Fig. Optimized Structure of PH

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PA – 29

SYNTHESIS AND CHARACTERIZATION OF $CE_{1-X}CD_XO_2$ / PAA NANOCOMPOSITES AND ITS NLO APPLICATION

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Abstract:

CeO_2/PAA and Cd^{2+} substituted CeO_2/PAA nanocomposites have been prepared using in-situ chemical method. For all of the nanocomposites, XRD studies confirm the cubic structure of CeO_2. The SEM micrograph shows that the CeO_2 nanoparticles are spherical in shape and aggregate less with increasing Cd^{2+} ion concentration. The formation of nanocomposites containing Cd^{2+} substituted CeO_2 nanoparticles and PAA polymer is confirmed by FTIR spectra. On the absorbance edge, optical absorption spectra show the blue shifted phenomenon. The two emission bands attributed to near band edge emission and blue emission are visible in photoluminescence spectra. The Z-scan technique was used to conduct nonlinear optical studies on CeO_2/PAA and Cd^{2+} substituted CeO_2/PAA nanocomposites. The Z-scan plots show that all of the nanocomposites have negative nonlinear refraction and saturable absorption. The third order nonlinear optical susceptibility and figure of merit of CeO_2/PAA nanocomposites increase with increasing Cd^{2+} substitution concentration and are found. The current findings suggest that Cd^{2+} substituted CeO_2/PAA nanocomposite is a viable candidate for the fabrication of future nonlinear optical devices.

Keywords: CeO_2 nanoparticles, Poly (acrylic acid), nanocomposites, XRD, SEM, third-order nonlinear optical susceptibility.

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PA – 30

GREEN SYNTHESIS CHARACTERIZATION OF ANTIBACTERIAL AND ANTIMICROBIAL STUDIES OF ZNO NANOPARTICLES FROM SENNA OCCIDENTALIS

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[2] Professor Department of Chemical Engineering, KEC, Perunduari.

Abstract:

The green synthesis of the nanoparticles is fascinating field of modern science .The present study states a green approach for synthesis of pure ZnO nanoparticles and ZnO doped with CuO. Nanoparticles employing leaf extract of Senna Occidentalis. Leaf extract was used as biological reducing agent for synthesizing pure ZnO nanoparticles from zinc acetate and doping of CuO nanoparticles from copper acetate. The resultant nanoparticles were characterized using various analytical techniques, such as UV-Visible Spectroscopy, Fourier Transform Infrared Spectroscopy, X-Ray Diffraction, Scanning Electron Microscope Analysis and Energy Dispersion X-Ray Analysis. The nanoparticle was stored in dried condition. The X-Ray Diffraction studies confirmed the crystalline nature of nanoparticles indicating particle size within the range provided by electron microscopy. Both nanoparticles were tested for their antimicrobial and antibacterial potential and the pure ZnO nanoparticles has good active against bacterial infection comparing to doping CuO. Hence, an easy and effective green approach for syntheses of pure ZnO nanoparticles have efficient antibacterial potential is reported in this study.

Keywords: Senna Occidentalis, Green synthesis, ZnO nanoparticles, Antimicrobial activity, antibacterial activity

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PA – 31

EXTRACTION PURIFICATION AND ANALYSIS OF BROMELAIN FROM PINEAPPLE PEEL & ITS APPLICATIONS IN INVITRO

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Abstract:

Bromelain is a major proteinase proteolytic enzyme, isolate from the pineapple (Amanascomosus) in the plant bromelainis accumulated in the entire plant to different extent and properties depending on its sources. The objective of the present study was to compare the amount and activity of bromelain present in stem, core, fruit, and peel of the plant. Bromelain was isolated from the peel of the adult adult pineapple plants by buffered extraction through membrane filteration method. Purification of enzyme is done by centrifugation, salt precipitation technique and dialysis. Bromelain was assayed for its activity by meat tendirization, gelatin hydrolysis, cottage cheese production. The homogenity of bromelain was confirmed by SDS-PAGE (sodium dodecylsulphate polyacrylamide gel electrophoresis) analysis. It was found that the peel bromelain had a better activity than fruit, stem and core bromelain. The product exhibited better proteolytic than crude extract.

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PA – 32

2D-BCNO AS A NEW PHOTOCATALYST FOR REMOVAL OF ORGANIC POLLUTANTS

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Abstract:

2D- BCNO will be introduced as a new visible light active photocatalyst for the removal of organic pollutants. By varying the composition, the bandgap of 2D-BCNOcan be fine-tuned to absorb the entire visible region. Followed by the synthesis and characterization, the degradation efficiency of such 2D-BCNO will be evaluated using MB (Methylene blue) as an organic pollutant. The effect of photocatalysis using the new

catalyst will be observed similar to the earlier reports on the traditional catalysts like ZnO and TiO2 [1, 2].

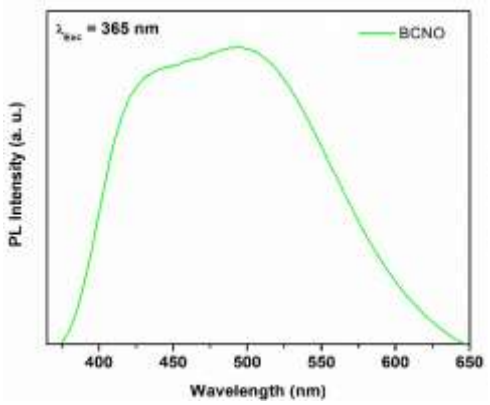

Fig. Photoluminescence spectra of 2D-BCNO excited using 365nm.

References:

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2. S. G. Anju, S. Yesodharan, E. P. Yesodharan, Zinc oxide mediated sonophotocatalytic degradation of phenol in water, Chem. Eng. J. 189– 190 (2012) 84–93

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PA – 33

INVITRO PHYTOCHEMICAL AND ANTIBACTERIAL ACTIVITY OF PAPAVER SOMNIFERUM LEAF EXTRACT

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Abstract:

Opium poppy (Papaver somniferum) is one of the earliest medicinal plants known to mankind. It produces some of the most widely used medicinal alkaloids like morphine, codeine, thebain and porphyroxine which are the most important component of this plant. It is one of the best-known relieving pains. Opium Poppy (Papaver somniferum L) is considered as one of the earliest medicinal plants known to mankind. Derived from the Greek name “opos” meaning juice, referring to its psychotropic latex, the plant was known and extensively used since Antiquity during religious rituals and for medical purposes, mainly as hypnotic and pain reliever agent. In Cretan folkmedicine it was recommended along with other poppies until the early 20th century to induce children sedation, by the name: “Hypnos” meaning sleep. The Hypnos (meaning sleep inGreek) remedy of the

Cretan traditional medicine is related to the folk use of the poppy plantto induce sleep in infants and children. This extracts have traditionally been used to relax smooth muscle tone, making them potentially useful in the treatment of diarrhoea and abdominal cramping. The extract has been used as a sedative analgesic and antitussive. The uses of opium poppyis described to be the major therapeutic (for treating dysentery, diarrhoea, spasms, pain etc.) component. The present paper is an attempt to provide recent update on phytochemical and antimicrobial activity along with the medicinal uses of Papaver somniferum. The phytochemical analysis of the plant is commercially and has great use in pharmaceutical companies for the production of new drugs.

Key words: Opium poppy, Medicinal uses, Phytochemicals and Antimicrobials.

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PA – 34

SYNTHESIZING La_2O_3 NANOPARTICLES FOR PHOTOCATALYSIS

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Abstract:

This study details the successful production of lanthanum oxide (La_2O_3) nanoparticles via the sonication method and delves their photocatalytic characteristics. The structural, optical, and morphological attributes of the La_2O_3nanoparticles were comprehensively investigated using a range of techniques, including X-Ray Diffraction (XRD), UV–Visible Spectroscopy (UV–Vis), Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray Analysis (EDAX), and Fourier Transform Infrared Spectroscopy (FTIR). The XRD patterns unmistakably illustrate an improvement in crystallinity as the sample is calcinated. UV–Visible spectroscopic analysis reveals an augmentation in the material's bandgap with calcination. SEM images uncover reduced agglomeration on calcinating, while FTIR peaks confirm the presence of metal-oxygen bonds. Concerning photocatalytic efficacy, the calcinated La_2O_3sample demonstrated an impressive 85% degradation efficiency when subjected to halogen light for 180 minutes, effectively decomposing Methylene blue dye in the test solution.

Keywords: La_2O_3, Sonication method, and photocatalytic efficiency.

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PA – 35

TUNNING THE PHASE TRANSITION AND BAND GAP OF INDIUM SELENIDE UNDER DYNAMIC SHOCKED CONDITIONS

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Abstract:

Indium selenide is a semiconducting material that has a layer-by-layer crystal structure. In the present work Indium selenide is treated with dynamic shock wave using a Semi-automatic Reddy tube as 100, 200, 300, and 400 shock pulses. In_4Se_3 was switched from orthorhombic to rhombohedral (α- In_2Se_3) phase at 100 shock pulses and remains the same phase up to 400 shock pulses by applying 2.0 MPa of pressure and a temperature of 864 K. The crystal structure orthorhombic to rhombohedral was examined using Powder X-ray diffraction, and Raman analysis. Morphology and optical properties of the material are investigated using Scanning Electron Microscope, and UV-DRS. The results from XRD and Raman confirm the phase transition by the formation and disappearance of the peak. The morphology analysis forms a layered shape while increasing the shocks and from the optical analysis, the band gap of the material was changed from semi-conducting material to an insulator.

Key Words: Indium selenide, Dynamic shock wave, UV-DRS.

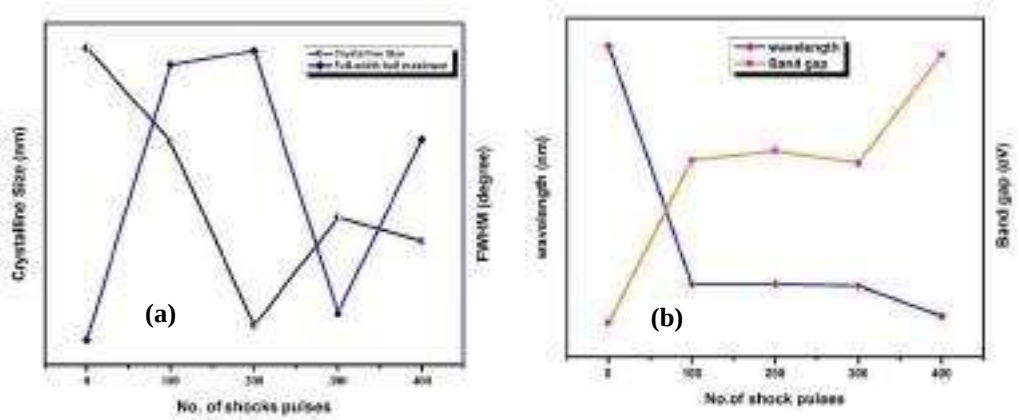

Fig.1 a) No. of shock pulses Vs Crystalline Size b) No. Shock pulses Vs Wavelength Vs Band gap.

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PA – 36

SCREENING FOR EXPRESSION OF stx1 GENE IN ESCHERICHIA COLI FOR SHIGA TOXIN ISOLATED FROM URINARY TRACT INFECTED SAMPLES

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Abstract:

Few microorganisms are as versatile as Escherichia coli. An important member of the normal intestinal microflora of human and other mammals. E. coli has also been widely exploited as a cloning host in recombinant DNA technology. But E. coli is more than just a laboratory workhorse or harmless intestinal inhabitant; it can also be a highly versatile, and frequently deadly, pathogen. Several different E. coli strains cause diverse intestinal and extra intestinal diseases by means of virulence factors that affect a wide range of cellular processes. The main aim of the study is to isolate the shiga toxin(stx1) gene from the urinary tract infected samples. We collect 45 urine samples randomly selected 5 samples, to isolate the Escherichia coli green coloured colonies. Then we isolate the pure DNA on those green coloured colonies from the Escherichia coli. And then we target the stx1gene from the urinary infected samples by using an Agarose gel electrophoresis and PCR (polymerase chain reaction).

Key words: shiga toxin, versatile, virulence, Rcombinant DNA

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PA – 37

CHEMICAL COMPOSITION ANALYSIS OF PLECTRANTHUS AMBOINICUS

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Abstract:

Plants are produced before the beginning of human evolution. The plants are obtain their energy through photosynthesis via this process the carbon dioxides are utilized and releases oxygen for human consumption. Plants are used for food, medicine, non food products, aesthetic uses and etc. The drugs are used for treating the diseases and infections. These drugs are mostly derived from plants and their extracts. In ancient times

the peoples are use plant alone treat diseases they called as ayurvedic medicine. In recent also it available. The plants are found throughout the world. In some countries like America, Russia, India are spending the more many to identify the new plant and their medicinal property. And they transport the medicinal plant for other countries for money. Herbal medicines are safe to eat since it as less toxic and minimum side effects alone and low cost when compare to other medicine. Plants have medicinal values because it contains Phytochemicals which are the chemical compounds present in all the plants. It contains primary metabolites (carbohydrates, proteins and lipids) and secondary metabolites such as, phenols, steroids, glycosides, quinones/ anthroquinone, cyanogenic glycosides, alkaloids, flavonoids, leucocyanidines, tannins, anthocyanin, volatile oils and terpenoids. Because the presence of phytocompounds it is used in the treat many diseases. The phytochemicals which is found in the plants have antimicrobial activities such as antibacterial activity, antifungal activity, antiviral activity, antiprotozoal activity. Plectranthus amboinicus is widely used as a traditional medicine mainly for respiratory tract infections. Because due to the presence of phytochemical on the plant. It contain the carbohydrates, proteins, phenols, steroids, glycosides, quinones/ anthroquinone, cyanogenic glycosides, alkaloids, flavonoids, leucocyanidines, tannins, anthocyanin, volatile oils, and terpenoids. So the project work concluded that the essential oils has highly recommended to eradicate newly emerging infections.

Keywords: Phytochemicals, Plectranthus amboinicus, Plants, Metabolites & Ayurvedic medicine

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PA – 38

HYDROTHERMAL PREPARATION OF La_2O_3/Mn_2O_3 NANOCOMPOSITES FOR OPTICAL APPLICATIONS

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Abstract:

In this work pure La_2O_3, Mn_2O_3 nanoparticles and La_2O_3/Mn_2O_3 nanocomposites were synthesized by simple hydrothermal technique. X-ray diffraction analysis was used to analyses the crystal structure and phase purity of the developed La_2O_3 and Mn_2O_3

nanoparticles as well as La_2O_3/Mn_2O_3 nanocomposites. Formation of distinct phases for both Mn_2O_3 and La_2O_3 in the La_2O_3/Mn_2O_3 was reveals the preparation of crystalline nanocomposite. Average Crystallite size of Mn_2O_3, La_2O_3 and La_2O_3/Mn_2O_3 nano composite was about 18, 15 and 14nm respectively. UV-Visible absorption spectroscopy shows good optical absorption behavior hence the prepared samples can be used in optical applications. The stretching and bending vibration of the prepared samples were investigated by FT-IR analysis. The SEM analysis enumerates that the La_2O_3/Mn_2O_3 nanocomposites has nanosphere along with nanorods morphology with high agglomeration.

Keywords: Nanocomposites, X-ray Diffraction, FT-IR, Nanosphere etc.,

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PA – 39

HYDROTHERMAL SYNTHESIS OF PURE AND LANTHANUM DOPED CERIA NANOPARTICLES

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Abstract:

Optical and structure properties of pure and La doped Cerium Oxide (CeO_2) nanoparticles were studied and reported. Crystalline ceria (CeO_2) nanoparticles have been successfully synthesized by fast hydrothermal method at 180°C for 5 hours. As-synthesized CeO_2 and La doped cerium oxide powders were calcinated at 500°C for 5 hours. The structure and optical of the synthesized nanoparticles were characterized through XRD and UV techniques. The functional behavior of the Pure and Lanthanum doped Cerium Oxide nanoparticles were investigated by FTIR and X-ray diffraction pattern of the samples shows the formation of single phase cubic structured CeO_2 nanoparticles without any secondary impurities. This result was supported by Fourier transform infrared spectroscopy analysis. Bandgap energy of the CeO_2 NPs were increased from 3.66 eV to 3.8 eV on increased the dopant of Lanthanum. The FTIR spectrum of the ceria exhibits strong broad band below 600 cm^{-1} which is due to the (Ce–O–C) mode.

Keywords: Nanoparticles, Hydrothermal, XRD etc.

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PA – 40

EFFECT OF NiO NANOPARTICLES AND ITS INVESTIGATION OF STRUCTURAL, OPTICAL, MAGNETIC, AND ANTIBACTERIAL ANALYSIS

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Abstract:

The present work is focused on the stability of the shockwave –exposed using Nickel Oxide (NiO) by green synthesis method using prunus dulcis (Almond gum). The NiO are synthesis by sol-gel methods, and exposed to 300 shock pulse having mach 2.2. Interestingly, most of the materials are discovered to have undergone phase transition at shocked conditions, or different changes in stability and efficiency have been found. The Pure and shock given NiO nanopowders were subjected to various characterization techniques such as XRD, FTIR, VSM, UV-vis, SEM, EDAX, PL and antimicrobial applications. The XRD analysis revealed that the intensity of the peak gradually increased under shock conditions. The observed peak at 583cm^{-1}, 573cm^{-1}, 570cm^{-1} in all shock given FTIR spectrum shows the metal oxygen stretching frequency of NiO also it confirms the stability and efficiency of NiO under shock waves loaded condition and there are no chances in the control and impact of the shock wave. So its confirms the NiO also have higher stability molecular against the impact of the shock waves. SEM images established in the shock loaded NiO nanoparticles have good stability and good structural. There is no change in the morphology even in the control and shock wave loaded conditions in the NiO. The UV-vis absorbance spectra the NiO nanoparticles is strongly affected due to the shock waves owing to the impact of blue shift exist in the material as a result, the bandgap increase in the shock waves loaded conditions. The vsm analysis, in shock loaded conditions the hysteresis loop is reduced as the shock pluses are increased. The anti-microbial effect on the green synthesis of NiO nanoparticles and identify the gram positive and gram-negative bacteria the test was carried out. This gives a positive result in the gram stain.

Keywords: Shock wave measurements; Electron microscopy, Vibrational sample magnetometer, antimicrobial activities.

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PA – 41

STRUCTURAL AND OPTICAL PROPERTIES OF CADMIUM DOPED BISMUTH SULFIDE NANOPARTICLES BY SOLVOTHERMAL METHOD

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Abstract:

Cd doped Bismuth Sulfide nanoparticles were synthesized through Solvothermal method. The nanoparticle having different elemental compositions was prepared by varying Cd weight percentage. Studied on structural, morphology, optical properties and functional group analysis of these nanoparticles were carried using powder X-ray diffraction, SEM analysis, UV–Visible absorption and FTIR analysis. The X-ray diffraction pattern of the as prepared samples revealed that it possesses orthorhombic structure. SEM image exhibits the flower like structure nanoparticles. The UV- vis spectrum showed the absorption peak at 260nm and the band gap energy of prepared sample was calculated and is found to be 4.77 eV. The decrease in the absorption coefficient due to cadmium doping percentage was observed in FTIR spectra and the strong absorption peaks could be attributed to Bi-S stretching modes.

Keywords: Solvothermal method; Bismuth Sulfide: Morphologies; orthorhombic

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PA – 42

SYNTHESIS, CHARACTERIZATION AND APPLICATION OF IRON OXIDE NANOPARTICLES PREPARED VIA SONICATION METHOD

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Abstract:

The present research demonstrates the synthesis of Iron Oxide nanoparticles through sonication method.XRD (X-Ray Diffraction Analysis), FTIR (Fourier Transform - Infrared spectroscopy), UV-Vis (Ultraviolet - Visible spectroscopy) and SEM (Scanning Electron Microscopy) were used to analyse the structural, vibrational, optical and morphological properties of the prepared samples. From the XRD, it can be seen that as

the sonication time is increased, the crystallinity of the prepared samples seems to improve. The results obtained from UV-Visible spectroscopy are utilized to calculate the band gap of the prepared samples. It was observed that the bandgap of the prepared material increases with increase in sonication time. The metal oxygen bond present in the FTIR spectra confirms that the formation of the iron oxide nanoparticles. From the morphological analysis it is evident that the prepared iron oxide samples show rice- like morphology. The optimised rice-like samples were subjected to Photocatalytic performance and the results have been discussed.

Keywords: Iron Oxide Nanoparticles; Sonication Method; Photocatalytic, Rice-like morphology.

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PA – 43

THE IMPACT OF SHOCK WAVES ON Bi_2Te_3 NANOPARTICLES LEADS TO A CAPTIVATING METAMORPHOSIS, RESULTING IN A MIXED-PHASE COMPOSITION PROMINENTLY FEATURING Bi_4Te_5.

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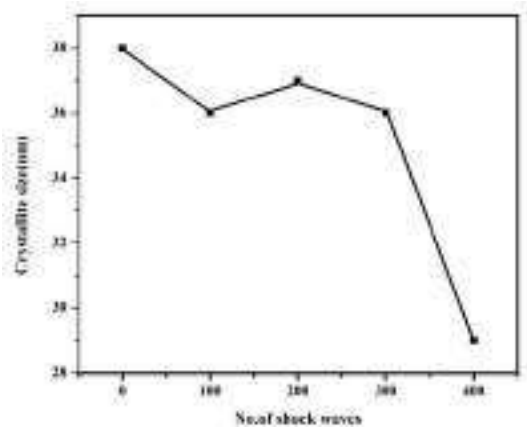
Abstract:

Bismuth Telluride (Bi_2Te_3) is an interesting semiconducting material for optoelectronics technology. The stability of the material in harsh conditions is not available in the literature, especially in dynamic shock-wave-loaded conditions. To explore it, commercially available Bismuth Telluride was purchased and investigated using a Semi-automatic Reddy tube. The samples were subjected to different series of shock waves like 100,200,300 and 400 which had 2MPa transient pressure and an 864K temperature with a 2.2 Mach number. XRD, RAMAN, UV-DRS, and SEM were characterized before and after shock-loaded conditions. The crystallinity of the Bismuth Telluride Bi_2Te_3 has been analyzed by X-ray diffraction which confirms the formation of rhombohedral $Bi_2Te_3$with space group R-3m.The Raman spectrum reveals the vibrational modes of the control Bi_2Te_3 and shock-loaded Bi_2Te_3. The band gap of $Bi_2Te_3$was determined using UV-DRS. Using SEM, the morphology of Bismuth Telluride was studied which obtained irregular morphology, and the particle size was calculated. Due to the

impact of the shock wave, the secondary phase Bi_4Te_5 is observed in XRD and Raman at 300 shock waves Also there are changes in crystallite size and slight changes in band gap are also observed.SEM analysis results in the morphology and there is a change in particle size due to the impact of shock waves. The secondary phase Bi_4Te_5 is observed thus the Bismuth Telluride is unstable under dynamic pressure. The process detailing how the secondary phase is initiated by shock waves is explained.

Keywords: Bismuth Telluride, Impact of Shock waves.



Variation of crystallite size of Bismuth Telluride (Bi_2Te_3) against several shock pulses

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PA – 44

STUDY OF STRUCTURAL, OPTICAL AND ELECTRICAL PROPERTIES OF Fe DOPED ZnS NANOPARTICLES PREPARED BY SOLID-STATE REACTION

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Abstract:

Zinc Sulfide (ZnS) is one of the leading semiconductors for optoelectronic device applications. Here, we focused on producing the transitional semiconducting material of undoped and Fe-doped ZnS nanoparticles by the method of solid-state reaction for such applications. The prepared nanoparticles were studied for structural, morphological, elemental, optical, and electrical properties by XRD, FE-SEM, EDS, UV-visible spectroscopy, PL, and Keysight B2900 source meter, respectively. XRD revealed that the

prepared nanoparticles have a cubical structure with a strong preferred orientation along (1 1 1) plane. The EDAX spectrum verifies that the synthesized nanoparticles include the host (Zn & S) and dopant (Fe) elements. The formation of spherical-shaped clusters was confirmed by FE-SEM images. Using absorption spectra energy band gaps were investigated. Novel luminescence features i.e., blue, green, and orange-red emission peaks were observed in the photoluminescence spectra.

Keywords: Nanoparticles, Solid-state reaction, Crystal structure, Semiconductor, Photoluminescence.

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PA – 45

INVESTIGATING THE TEMPERATURE AND FREQUENCY DEPENDENT DIELECTRIC PROPERTIES OF La^{3+} DOPED CCTO CERAMICS: TUNING THE SINTERING DURATION

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Abstract:

In this study, the influence of sintering duration on the dielectric properties of La doped CCTO ceramics synthesized using the sol-gel method. The structural characterization via XRD has unveiled the presence of an Im3 space group and a body-centered cubic structure. Additionally, we utilized XPS to confirm the electronic states of the prepared material.SEM analysis reveals the notable variations in grain size observed in the range of 1–2µm.The dielectric constant of all the ceramic samples were greater than 10^3 to 10^4 at lower frequencies and at higher temperatures. The Nyquist plot showed non-Debye type relaxation behavior.

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PA – 46

INVESTIGATION OF FREQUENCY AND TEMPERATURE DEPENDENT IMPEDANCE, MODULUS AND CONDUCTIVITY PROPERTIES OF $MgO@SiO_2$ CSN

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Abstract:

Herein, MgO and $MgO@SiO_2$ core-shell nanocomposits (CSN) were prepared using co-precipitation cum stober method chemical synthesis route. Powder XRD analysis, FTIR studies reveal the crystalline nature, surface functionality, and molecular structure of the title material. TEM and XPS studies envisage the formation, cationic distribution and electronic states of $MgO@SiO_2$ CSN. The impedance properties of MgO and $MgO@SiO_2$ CSN were examined with respect to frequency (1Hz–1MHz) at selected temperatures (323 K- 673 K). The complex impedance plot is utilized to delineate the contribution of grain and grain boundary resistances. The analysis of Nyquist plots of impedance and modulus indicates negative temperature coefficient of resistance behavior and suggest a non-Debye type of relaxation. Eventually, the conductivity spectra were analyzed using the universal Jonscher power law $\sigma_{ac} = \sigma_{dc} + A\omega^n$, and the activation energy were found to be 0.34eV from Arrhenius plot.

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PA – 47

INVESTIGATION OF FREQUENCY AND TEMPERATURE DEPENDENT DIELECTRIC BEHAVIOR OF PARAMAGNETIC α-$Mn_2O_3@SiO_2$ CORE SHELL NANOCOMPOSITES

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Abstract:

This article investigates the dielectric response of α-$Mn_2O_3@SiO_2$ core shell nanocomposites in the frequency range 1Hz-1MHz at various temperatures (323K-673K).

The powder XRD analysis, FT-IR, TEM and VSM techniques were employed to confirm the structure, functional groups, crystallinity and magnetic properties respectively. The SAED patterns strongly support the XRD findings and reveal the formation of α-Mn_2O_3@SiO_2 core shell nanocomposites. The value of ε_r and tanδ increases with increasing temperatures at lower frequencies though they decrease at high frequencies. The cole-cole plots reveal non-Debye type of relaxation and positive temperature coefficient of resistance type behavior. Further, the analysis of dielectric data indicates that the α-Mn_2O_3@SiO_2 displays positive temperature coefficient of resistance type behavior and the frequency dependent ac conductivity obeys the well-known Jonscher's power law.

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PA – 48

STRUCTURAL AND OPTICAL PROPERTIES OF CADMIUM OXIDE (CdO) AT SHOCK LOADED CONDITIONS

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Abstract:

In our present work, we have synthesized CdO nanoparticles by chemical co-precipitation method which has promising applications in solar cells, photodiodes, phototransistors, catalysts etc., The structural characterisation of the as-synthesised sample was analysed by XRD technique. The XRD pattern shows that the synthesized sample has face-centered cubic structure with crystallite size of 58.1nm. The optical properties of CdO was analysed using UV-Vis absorption spectrum. This Spectrum revealed the bandgap of CdO is eV and this shows the prominent blue shift in the bandgap with respect to the bulk bandgap of 2.9eV. In order to study the effect of shockwaves on nanocrystallite sample, the as-synthesised nano CdO was subjected to shock waves in the series of 50,100,150,200 with a Mach no. of 2.2 so as to investigate the after effect of shock. The XRD pattern of shock loaded nano CdO reveal that the average crystallite size decreases as the counting of shock pulses are increased. The crystallite size were computed to be 57.9nm, 56.91nm, 54.0nm, 53.9nm at 50,100,150,200 shocks respectively without any phase changes in the virgin vs shock loaded samples. The compositional & electrical properties of the samples under the application of shock waves are yet to be analysed.

Keywords: Chemical precipitation, XRD, UV-visible, shockwaves.

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PA – 49

REVIEW OF PHENYLHYDRAZONE, SEMICARBAZONES AND THIOSEMICARBAZONES USING THE APPROPRIATE CARBONYL COMPOUNDS AND THEIR BIOLOGICAL ACTIVITIES

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Abstract:

Phenylhydrazide , Semicarbazides and Thiosemicarbazide condense to form the chemicals Phenylhydrazone, semicarbazones and thiosemicarbazones. Using the appropriate carbonyl compounds .These are effective synthesis-related intermediates for they are widely employed in the field of medicinal chemistry since they are both pharmaceutical and bioactive compounds. One of the most important goals in medicinal and bioinorganic chemistry is the creation of novel, advantageous bioactive molecules with a variety of biological functions. Antibacterial, antifungal, antioxidant, antiviral, and other properties of Phenylhydrazone, Semicarbazones, Thiosemicarbazones, and their derivatives have been studied. The compound's IR and 1 H-NMR data have been used to characterize their structures. Studies have been done on substances with the formulae C=N-N , -N=N-, -NC=S. To organize the various biological activities of some synthesized Phenylhydrazone , Semicarbazone and Thiosemicarbazone derivatives with carbonyl compounds, the synthetic root of some of these derivatives and complexes are reviewed as for biological activities in accordance with this biological potential.

Keywords: Phenylhydrazide , Semicarbazides and Thiosemicarbazide, IR, 1 H-NMR

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PA –50

COMPUTATIONAL STUDIES ON DETOXIFYING AFLATOXIN B1(AFB1) IN PLANTS USING GREEN ALGAE: MOLECULAR DOCKING AND ADMET STUDIES

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Abstract:

Aflatoxin B1(AFB1) is the most toxic aflatoxin produced by a large number of Aspergillus species. AFB1 is associated with serious health consequences like lung cancer. For this reason, it is recognized as a human group 1 carcinogen by the international Agency of research on cancer. Our work investigates the detoxifying the content of aflatoxin b1 in plants by targeting a protein hypD of Aspergillus flavus and hypE of Aspergillus parasiticus which is responsible for producing the AFB1 toxins. Green algae are used as an inhibitor due to its antioxidant property. The understanding of the molecular mechanics involved in the toxic effects can be addressed by computational studies. Computational tool helps to visualize the structure and its orientation. The protein structure of hypD and hypE were downloaded from uniport (in PDB format) and subjected to protein preparation; to add hydrogens and to optimize the residues. Active sites of the modeled protein were identified using sitemap tool of Schrodinger package. The various ligands were downloaded from the CMNPD database and subjected to the ligand preparation. After that a structure based virtual screening by molecular docking were performed. Detailed analysis of the best scoring molecules was performed for Lipinski's rule for drug likeliness, and ADMET properties. Thus, we report three (CMNPD26463, CMNPD18937, CMNPD345) compounds with a docking Score -8.03, -7.969, -7.161 and having a human oral absorption of 93%.

Keywords: AFB1, hypD, hypE, molecular docking, ADMET.

Abbreviations: AFB1; Aflatoxin b1, PDB; Protein Database, CMNPD; Comprehensive Marine Natural Products Database, ADMET; Absorption Distribution Metabolism ExcretionToxicity.

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PA –51

REVIEW OF ELECTROCATALYSTS FOR PRODUCING HYDROGEN, OXYGEN, AND SYNTHETIC GAS

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Abstract:

The most effective way to produce high purity hydrogen and oxygen is by water electrolysis, and it can use renewable energy sources to provide the necessary power input. The hydrogen created in this way can be utilized as a fuel for IC engines or as a reducing agent in chemical reactions like the Fischer-Tropsch synthesis (FTS). Both low temperatures (usually below 100 °C) and high temperatures (between 500 to1000 °C) are capable of achieving water splitting, and various ionic agents can be electrochemically transported during the electrolysis process in both cases. In order to guarantee high electro catalytic activity and long-term stability, certain criteria apply to each of the electrolysis methods such as alkaline, polymer electrolyte membrane, and solid oxide electrolysis. The purpose of this article is to give a quick overview of how the catalyst-electrode materials & structure and nature affect the performance of the electrolyzer. The creation of effective anode and cathode materials suitable for large-scale water electrolysis is given, along with current developments in this area. For the various electrolytic water splitting technologies, the trends, barriers, and possibilities for future advances are outlined.

Keywords: Electrolysis, Polymer electrolyte membrane, Solid oxide electrolysis and Co-electrolysis electrode materials.

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PA –52

ROOM TEMPERATURE FERROMAGNETIC AND PHOTOLUMINESCENCE PROPERTIES OF PEROVSKITE NANOPARTICLES

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Abstract:

Perovskite nanoparticles ($BiFeO_3$) were synthesized using simple, low-cost sol-gel auto combustion method using Bismuth nitrate pent hydrate $Bi(NO_3)_3.5H_2O$, and iron nitrate nano hydrate $Fe(NO_3)_3.9H_2O$ as source materials. The final product was subjected to post annealing at 450^oC, 550^oC, 650^oC and 750^oC and studied the impact of annealing temperature on structural, surface, optical, magnetic and photoluminescence properties. From the different characterization techniques, it was found that the synthesized $BiFeO_3$ nanoparticles were conformed in rhombohedral structure with mean crystallite size of 40 nm. From the EDAX spectra, no new elements were found other than the source material. Using Tauc's relation the band gap was calculated and it varied from 1.9 eV to 2.02 eV. The photoluminescence studies revealed a clear, broad emission peak visible region (566 nm). The magnetic studies conformed the ferromagnetic nature of $BiFeO_3$ nanoparticles. The photo catalytic behaviour of the Bismuth ferrite (BFO) nanoparticles has been studied by the degradation of the Methylene blue (MB) dye. It is observed that BFO shows a good photo catalytic degradation of dye in the visible light irradiation.

Keywords: Ferrites, Photocatalytic, Band gap, Photoluminescence, nanoparticles:

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PA –53

CaO NANOPARTICLE DISPERSED WITH POLY ARYLENE ETHER RADICAL INITIATOR WITH 2-ACRYLAMIDO-2-METHYLPROPANE SULFONIC ACID (AMPS) IN PROTON EXCHANGE MEMBRANE FOR FUEL CELL APPLICATION

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Abstract:

The novel synthesized poly (arylene ether) (PAEs) polymer, and 2-Acrylamido-2-methylpropane sulfonic acid (AMPS) of the polymer through simple radical polymerization reaction, is confirmed by Fourier transform - infrared, proton NMR. The CaO nanoparticles are prepared raw material of the snail shell collected in grinding method. The materials were calcinated at 950 °C and analysis by using FE-SEM, and HR-TEM analysis. CaO nanoparticles dispersed with in dispersed PAEs-AMPS polymer prepared and confirmed by the Powder X-ray diffraction, SEM and thermogravimatric analyses. The various percentages of CaO nanoparticles 1, 2, 3, and 5% dispersed with PAE-AMPS polymer nanocomposites membrane were analyzed water uptake, swelling ratio, ion exchange capacity, oxidative stability and proton conductivity. It obtained the SEM image of the CaO nanoparticle displayed in spherical like structure. The 3% CaO nanoparticle dispersed PAEs-AMPS polymer nanocomposites membrane showed the IEC value 0.87 mmol/g -1 and high proton conductivity 1.59 x10 -3 S/cm -1 at 100 °C. The oxidative stability value displayed the of 13.4% degradation after being exposed to Fenton reagent at 70 °C for eight hours.

Key words: CaO Nanoparticle, proton exchange membrane fuel cell application.

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PA –54

MoS_2 DISPERSED POLY VINYL ALCOHOL (PVA) CROSS-LINKED WITH CARBOXYLATED - AMIDO-2-METHYL-1-PROPANESULFONIC ACID (C-AMPSA) IN MEDIUM TEMPERATURE PROTON EXCHANGE MEMBRANE FUEL CELL APPLICATION

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Abstract:

In this study, chemically poly (vinyl alcohol) (PVA) cross-linked with carboxylated - Amido-2-Methyl-1-Propanesulfonic Acid (C-AMPSA) were used to create a new series of polymer electrolyte membranes. Three distinct monomer mercaptosuccinic acid Amido-2-Methyl-1-Propanesulfonic Acid, were used in a typical polymerization procedure. The newly synthesized polymer was examined by the using FT-IR, SEM, and XRD, blend membranes among the developed PEM materials displayed greater ion-exchange capacity and water uptake values than the other membranes. Additionally, the proton conductivity of the PVA-cross linked C-AMPSA membrane is 0.0367 S cm $^{-1}$ at 30 C, whereas virgin PVA displays the conductivity of protons is 0.0259 S cm^{-1}. The PVA-C-AMPSA blend membranes are interesting candidates for fuel cell applications, according to the overall experimental findings. Finally, the displayed good OS (oxidative stability) with a value of 45.2 % degradation after being showing to Fenton reagent at 70 °C for 8 h.

Keywords: MoS_2nanosheet, PVA –cross linked membrane and proton conductivity.

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PA –55

ENHANCING THE PHOTOCATALYTIC ACTIVITY OF MgO DOPED rGO NANOMATERIAL FOR ENVIRONMENTAL APPLICATIONS

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Abstract:

Recent developments of material science envisioned to derive nanomaterials with unique characteristics having ample application potential in various fields. The present

study is employed to obtain hydrothermally synthesised pure and MgO doped rGO nanoparticles and to explore their properties. Characteristics of synthesized nanocomposite samples have been analysed using various investigation tools such as experiments are carried out with the aid of techniques such as X-ray diffraction (XRD). Ultraviolet-visible (UV-Vis.), photoluminescence (PL), and Fourier transform infrared (FTIR). etc., Spectroscopic tools are helpful enough to examine the optical properties of the present samples. In which, FTIR spectra reveals the existence of MgO and doped rGO nanoparticles by exposing relevant absorption bands against definite wavenumbers. Observed scanning electron microscopic (SEM) images of MgO doped rGO nanoparticles exhibit their morphological features. Dye decomposition ability of n-MgO composite has been examined under UV irradiation and it endorse their photocatalytic efficiency. Percentage of dye removal efficiency has been observed to be depends on the quantity of catalyst loaded in the sample.

Keywords: Magnesium Oxide, Nano Particles, Hydrothermal, X-Ray Diffraction, SEM with EDX, UV, FTIR, PL, Photocatalytic Degradation.

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PA –56

SHOCK INDUCED MODIFICATIONS IN THE STRUCTURAL, OPTICAL AND DIELECTRIC PROPERTIES OF GLYCINIUM MALEATE SINGLE CRYSTALS

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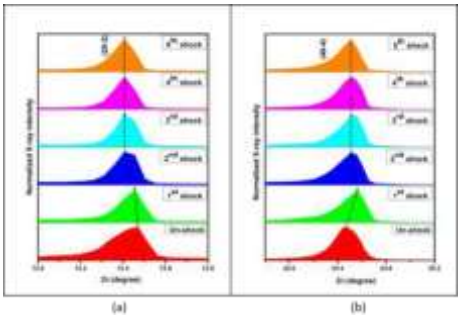
Abstract:

The slow evaporation method was used to grow the single crystal of glycinium maleate (GM), an amino acid-based molecular crystal. Dynamic shock waves of Mach 1.7, coupled with transient pressures of 1.048 MPa and transient temperatures of 644 K, were directed on to the crystal. X-ray diffractometry (XRD), UV-visible spectroscopy, and dielectric spectroscopy that serves as the probes to study structural, optical and dielectric properties of the crystal. Hydrogen bonds preserve the intermolecular connection between the glycine and maleate ions in the crystal structure of glycinium maleate. It is found that glycinium maleate shows high structural stability upto 5^{th} shock- recovered condition. The network of hydrogen bonds that may be responsible for the glycinium maleate's structural

stability during shock-recovered conditions. With a steady absorption edge, the optical transmission of the test crystal increased from 38% to 51%. Additionally, the crystal's resistivity decreases as capacitance increases due to the crystal's enhanced polarizability.

Keywords: molecular crystal, shock waves, structural stability, transmission, dielectric constant



Diffraction pattern of (a) (20-2) and (b) (40-4) diffraction peaks of un-shocked and shock recovered GM crystal

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PA –57

PREPARATION OF ANATASE/RUTILE MIXED PHASE TiO_2 NANOPARTICLES FOR PHOTOCATALYTIC DYE DEGRADATION

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Abstract:

Being a promising material with better properties and functionalities, Titanium dioxide (TiO_2) has captivated enormous applications in photocatalysis, energy and storage devices, self-cleaning, Dye-sensitized solar cells (DSSC's) pigments, and much more. In this paper, TiO_2 mixed phase (anatase/rutile) nanoparticles were synthesized to study their photocatalytic performance in degrading toxic dyes. By utilizing the hydrothermal method,TiO_2 nanoparticles were obtained. The structural parameters and the presence of the required phases are confirmed by the XRD analysis. Fourier transform infrared spectroscopy (FTIR) revealed different functional groups in the prepared sample. The optical behavior of the sample is analyzed using UV-DRS spectroscopy. The active energy modes of the nanoparticles are studied using the Raman analysis. The surface area of the prepared mixed phases was also measured using the Brunaeur- Emmett- Teller (BET) analysis.

PA –58

FACILE SYNTHESIS OF (Th_2O_3-NiO) MIXED OXIDE NANOCOMPOSITES LOADED CONJUGATED POLYMER AND POLYANILINE (PANI) BLENDED POLYVINYLIDENE FLUORIDE FOR EMI SHIELDING APPLICATION

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Abstract:

In this study, electrically conductive composites of ethylenedioxythiophene-based conjugated polymer(CNPR), polyvinylidene difluoride (PVDF), polyaniline (PANI) and (Th_2O_3-NiO) mixed oxide nanocomposites have been prepared by Facile precipitation technique followed and calcined treatment. A new conjugated CNPR polymer was synthesized and its chemical structure has been confirmed by Fourier transform infrared and 1H-NMR spectroscopy. The varying weight percentages of (1, 3 and 5%) (Th2O3-NiO) mixed oxide nanocomposites and 10 wt% CNPR dispersed PVDF nanocomposites were prepared and characterized using X-ray diffraction, thermo gravimetric analysis, scanning electron microscopy and energy-dispersive X-ray spectroscopy (EDX) analysis. The thermal studies indicated that the decomposition occurred at a temperature around 220^0C and 480^0C corresponds to the CNPR and CNPR/PVDF/ PANI / (Th_2O_3-NiO) (1, 3 and 5%), respectively. The EDX spectrum of neat CNPR polymer and their composites of CNPR/PVDF/PANI/ (Th_2O_3-NiO) (1, 3 and 5%). The CNPR/PVDF/PANI /5% (Th_2O_3-NiO) has a dielectric constant value of 3.9 at 1 MHz and the conductivity of this polymer composites value is found to be 5.8910–6 S cm–1 at 1 MHz, respectively. Results obtained from EMI shielding application the (Th_2O_3-NiO) and terpolymer-dispersed PVDF composites exhibit good interfacial adhesion as evidenced from conductive behaviors.

Key words: conjugated polymer**,** nanoparticles (Th_2O_3-NiO), pvdf, PANI,

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PA –59

GROWTH, CHARACTERIZATION AND THEORETICAL STUDIES OF TRIS (ALLYLTHIOUREA) – CADMIUM (II) CHLORIDE

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Abstract:

Single crystals of tris(allylthiourea)- cadmium(II) chloride (TATC) complexes was grown by conventional slow evaporation solution growth technique at room temperature. Lattice parameters are determined by single crystal XRD analysis. The structure and the crystallinity of the materials were confirmed by powder X-ray diffraction analysis. Optical properties of specimens are analyzed by UV-DRS spectroscopy and band gap energies are estimated. The modes of vibrations of functional groups present are identified by FT-IR studies. Surface morphology is examined by scanning electron microscopy. Thermogravimetric and differential thermal analysis reveal the purity of the sample and no decomposition is observed upto the melting point. Microhardness studies were also carried out to elucidate the mechanical behavior. Theoretical calculations were performed to derive the molecular geometry, first-order molecular hyperpolarizability (β), dipole moment (μ), polarizability (α), HOMO-LUMO energy, bond lengths and angles using B3LYP with LANL2DZ as basis set. The atomic charge distributions of the various atoms present are obtained by Mulliken charge population analysis. The second harmonic generation (SHG) efficiency of the as-grown specimens are estimated by Kurtz and Perry powder technique. The Hirshfeld surfaces, derived using single crystal X-ray diffraction data are analysed for the thiourea complexes using HF method with 3-21G as basis set and investigation of the intermolecular interactions and crystal packing reveal that close contacts are associated with strong interactions.

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PA –60

A STUDY ON THE PHYSICO-CHEMICAL ANALYSIS OF GROUND WATER QUALITY IN THE VILLAGES OF KADACHANALLUR, NAMAKKAL DISTRICT, TAMILNADU

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Abstract:

The present investigation focus on physio-chemical study of the ground water samples collected from the villages of Kadachanallur in Namakkal district, Tamilnadu. The physiochemical parameters of the ten samples (5 open well and 5 bore well samples) were analysed via appearance, colour, odour, taste, turbidity, electrical conductivity and total dissolved solids (TDS), pH, alkalinity and total hardness. Moreover the amount of salts present in the water samples such as calcium, magnesium, sodium, potassium, phosphate, nitrate, chloride, sulphate, fluoride, ammonia and iron were also estimated. The obtained results were compared with the standard desirable limit values of drinking water given by WHO and BIS. The present study shed light on the quality of ground water samples suitable for drinking purposes or not.

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PA –61

SYNTHESIS, SSPECTRAL INVESTIGATION, DFT, ANTIBACTERIAL, ANTIFUNGAL, AND MOLECULAR DOCKINGSTUDIES OF Ni(II), Zn(II), Cd(II) COMPLEXES OF TETRADENTATE SCHIFF-BASELIGAND

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Abstract:

By refluxing 4-nitro-o-phenylenediamine and 5-nitro salicylaldehyde, the Schiff base ligand wassynthesized. By reacting the appropriate precursor with the tetra-dentate Schiff base ligand, three nitro substituted nickel(II), zinc(II) and cadmium(II) complexes were synthesized. UV-Visible, FTIR, and ^{1}H-NMR Spectral investigations were used to characterize the ligand. Molar conductance, LCMS, UV-visible and FTIR spectrum analysis were used to characterize the produced complexes. The ligand and produced complexes were tested for antibacterial activity. DFT simulations were performed at the B3LYP/6-311G (d, p) and LanL2dz levels of theory were utilized tostudy the geometry of the ligand and the metal complexes it forms. In addition, the molecular orbital occupancy of HOMO and LUMO, as well as the molecular electrostatic potential (MEP), were computed. Docking experiments were conducted utilizing the active sites of the E. coli FabH-CoA complex (PDB ID: 1HNJ) receptor in order to detect the interactions between complexes and define their likely binding locations.

Keyword

Nickel (II) complex, Zinc (II) complex, Cadmium (II) complex, Tetra-dentate Schiff base ligand, Antimicrobial activity, DFT and Molecular docking

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PA –62

VIBRATIONAL SPECTROSCOPIC AND SOLVATOCHROMIC ANALYSES ON UNIDIRECTIONAL P-NITROANILINE SINGLE CRYSTAL

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Abstract:

Growing progress is being witnessed in terms of understanding and standardizing the various aspects of characteristic nature of existing NLO materials which have the potential to ignite the advancement of today's technology. On those counts, bulk single crystal of unidirectional P-Nitroaniline (PNA) was grown by sankaranarayanan - Ramasamy (SR) method. The crystal system has been confirmed from the single crystal X-ray diffraction and PXRD analyses. The Functional groups were identified by FTIR spectroscopy and Factor Group analysis was performed using theoretical calculations by taking into account of modes of vibrations which were obtained by Quantum computational method. Electronic Transition energy and Polarity scale were found from UV-visible absorption spectrum. The etching study was also carried out for the grown crystal using different solvents and time periods.

Fig.2 Photograph of as unidirectional grown crystal of PNA

Keywords: Organic Crystal; Paranitroaniline; Solvatochromic; Surface Properties.

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PA-63

FUNGAL MEDIATED BIO-SYNTHESIS OF SILVER AND THEIR ANTIMICROBIAL POTENTIAL AGAINST MTCC PATHOGENS

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Abstract:

In recent years, the synthesis of metal nanoparticles utilising fungus has received a great deal of attention and has been acknowledged as a safe and effective technique relevant in the biomedical field. In the current work, we isolated endophytic and phylloplane fungal species from Azadirachta indica, a therapeutic plant. Penicillium oxalicum, the most prevalent and prolific species of fungus, was tested for its ability to biosynthesize silver nanoparticles. The creation of nano-silver was verified based on the colour difference between the fungal extract and AgNO3 solution and as determined by UV-Vis Spectrophotometric measurement. The presence of silver nanoparticles was confirmed by the absorption peak at about 406 nm during UV-Vis spectroscopic analysis of the aforementioned material. According to the SEM findings, the synthesised silver nanoparticles were polygonal and elongated, with particle sizes falling between 70 and 100 nm. By using FTIR analysis, it was discovered that the bands at 3577.97 (alcohol O-H stretch), 2073.12 (alkyne C-C stretch), and 1637.28 (alkene C=C stretch) cm1 matched the strap vibrations of protein molecules. The greatest zones of inhibition at 25 l of AgNPs for the antimicrobial activity against the MTCC pathogens Candida albicans, S. aureus, and E. coli were 19 mm, 12 mm, and 13 mm, respectively. The tests conducted shown good effectiveness against the infections. It was discovered that using P. oxalicum, our current supply of fungal material, to make nanoparticles is affordable, environmentally friendly, and secure.

Key words: Silver nanoparticles, Penicillium oxalicum, Azadirachta indica A., Leaf surface fungi, antimicrobial activity, UV-Vis Spectrophotometer

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PA-64

PHYTOCHEMICAL ANALYSIS AND ANTIMICROBIAL ACTIVITY OF AN ENDOPHYTIC *FUSARIUM PROLIFERATUM* (ACQR8), ISOLATED FROM A FOLK MEDICINAL PLANT *CISSUS QUADRANGULARIS* L

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Abstract:

The endophytic fungi are an important source of bioactive natural products. This study includes evaluation of antimicrobial activity and phytochemical analysis of endophytic fungus ACQR8, recovered from the root tissues of a folk medicinal plant Cissus quadrangularis L., which was identified as Fusarium proliferatum by microscopic and molecular methods. The fungus showed broad spectrum antibacterial and antifungal activities against variety of important plant and human pathogens. To the best of our knowledge, this is the first study to record antifungal activity of any endophytic *Fusarium* sp. against phytopathogens *Rhizoctonia solani*, *Fusarium oxysporum* and the dermatophytes *Trichophyton mentagrophyte* and Microsporumgypseum. The minimum inhibitory concentration of the crude extract ranged from 40–120 µg/ml against pathogenic bacteria and 0.2–2.5 mg/ml against fungal pathogens. Besides, this study probably is also the first to document the phytochemical constituents of an endophytic Fusarium sp. Phytochemical testing and GC-MS (gas chromatography- mass spectrometry) analysis revealed the presence of fatty acids and its derivatives, phenolics, terpenoids and unsaturated alkenes in the crude extract which scientifically validates the highly promising antibacterial and antifungal activity exhibited by endophytic isolate ACQR8.

Keywords: Endophytic fungus, Fusarium proliferatum, Bioactive Compounds, Antimicrobial activity, GC-MS analysis

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PA-65

INVESTIGATION OF STRUCTURAL, DIELECTRIC, AND MAGNETIC PROPERTIES OF $ZnFe_2O_4$ PREPARED BY SINGLE-STEP CHEMICAL ROUTE METHOD

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Abstract:

In this study, we have successfully synthesized$ZnFe_2O_4$nanoparticles by one step chemical route method by dissolving 18.936 g/mol of [$Zn(NO_3)_2.6H_2O$] in water and 15.969g/mol of Fe-O in sulphuric acid. The structure of the sample was identified as a tetragonal phase by the X-ray diffraction (XRD) studies, grain dimension of the synthesized sample was calculated using Debye's Scherer's formula and the estimated particle size of 28nm.Scanning electron microscopy (SEM)analysis showed the uniform spherical distribution of the particles with the range of 20nmto 60nm. The formation of chemical bonding of Zn and Fe_2O_4 was confirmed from the absorption bands that occurred at531cm^{-1} and 497 cm^{-1} by Fourier transform infrared (FTIR) spectroscopy. The optical bandgap of the synthesized$ZnFe_2O_4$nanoparticles was estimated from the *Tauc plot* as 5.37eV based on the absorption spectrum resulted from UV-vis studies. Electrochemical performance including dielectric loss, dielectric constant, and permittivity, of the prepared Zinc ferrite nanoparticles was studied and the behavior of the sample at various temperatures was plotted and interpreted. The magnetic property of the synthesized $ZnFe_2O_4$nanoparticles was studied VSM analytical instrument at room temperature as shown in Fig. 10.From the result of the M-H hysteresis curve, it was observed that the width or the area of the curve is almost negligible, and it appeared as *S*-shaped coercivity which depicts the unique property of superparamagnetism, saturation magnetization (Ms), and coercivity (Hc)of the samples were calculated as 1.72 emu/g and 0.0004 emu/g, which is almost negligible

Keywords: Zinc ferrite, chemical route, dielectric measurement, Electron microscopy, magnetic behavior.

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PA-66

ENHANCED PHYSICOCHEMICAL PROPERTIES OF NONLINEAR OPTICAL MATERIAL:L-LYSINE MONOHYDROCHLORIDE NICKEL BROMIDE (LMNB)

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Abstract:

A good quality single crystal of L-lysine mono hydrochloride nickel bromide (LMNB) with an optimum size of 7 mm x 3 mm x 2 mm was obtained within 40 to 45 days. The unit cell dimensions and cell parameters of grown L-lysine monohydrochloride nickel bromide (LMNB) crystals were determined using single crystal X-ray diffraction studies. The crystalline nature of the grown crystal was determined using Powder X-Ray Diffraction (PXRD) studies. Infrared spectra are an important record because they reveal more about the structure of a compound. The optical transmission of a polished and suitable size LMNB crystal was investigated. This demonstrates that the LMNB crystal has a very low UV cut-off wavelength (230 nm) as well as a large transmission window across the entire visible region. Furthermore, the absence of absorption in the 237-1100 nm range indicates that the crystal has good optical transmission with few defects. The SHG efficiency of LMNB crystal was found to be approximately twice that of KDP. The Vickers hardness number of as grown LMNB crystal increases with applied load. Photoconductivity research looked into the nature of photoconductivity.

Keywords: LMNB crystal, PXRD, photoconductivity

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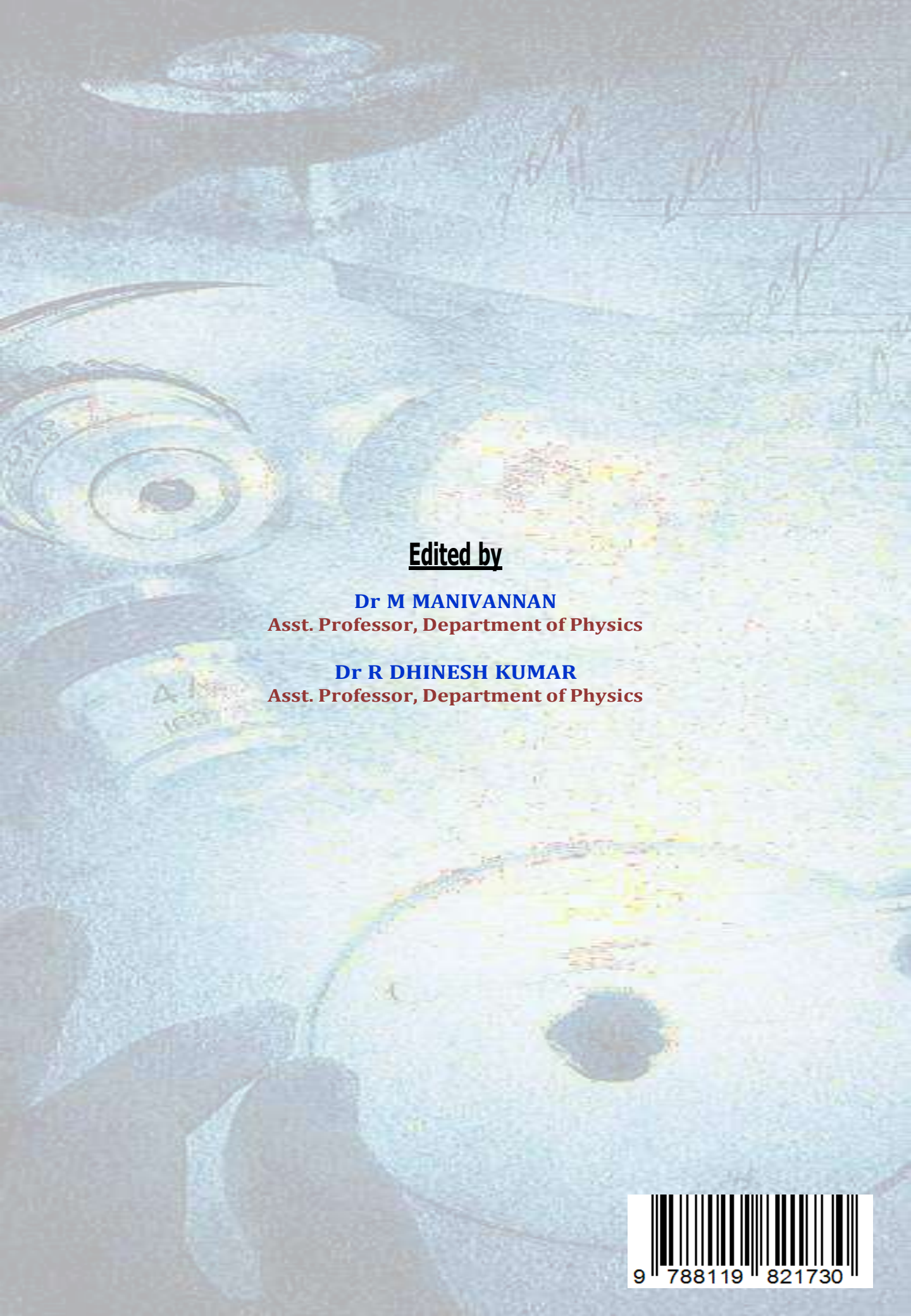

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