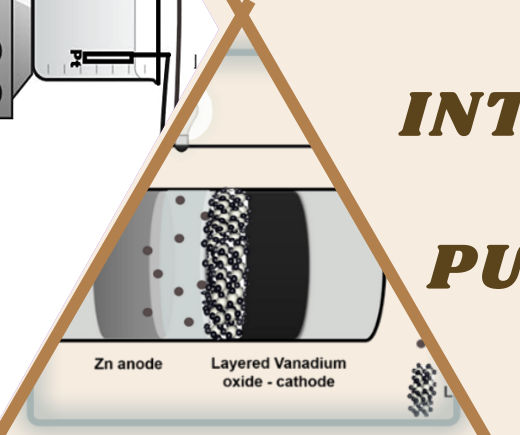
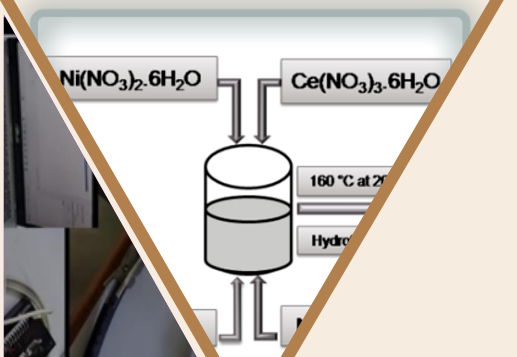


INTERNATIONAL CONFERENCE ON PURE AND APPLIED PHYSICS

23 & 24 MARCH 2023

ORGANIZED BY
DEPARTMENT OF PHYSICS
WOMEN'S CHRISTIAN COLLEGE
CHENNAI



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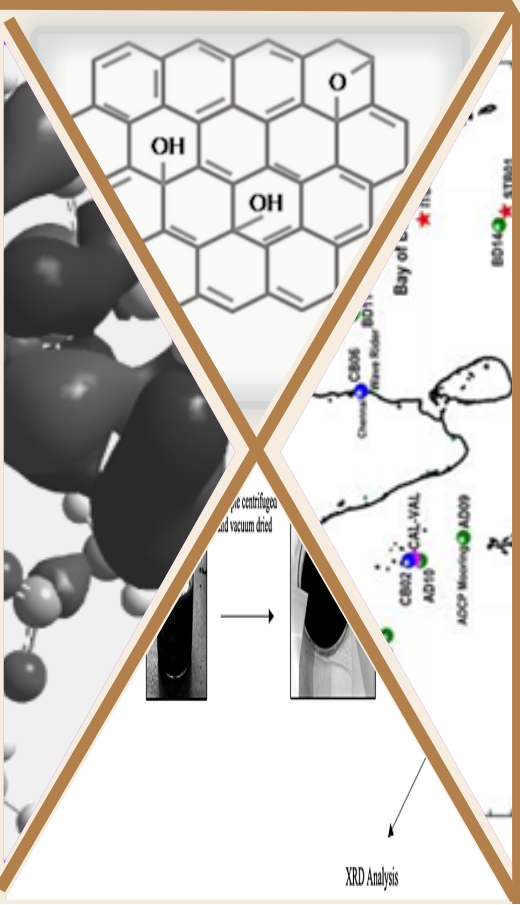

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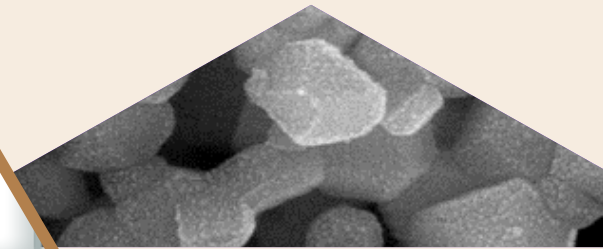

Book of Abstracts

International Conference on Pure and Applied Physics

23 & 24 March 2023

Organized by

Department of Physics
Women's Christian College
Chennai, India

Editors

Dr. A Christina Nancy

Dr. T S Renuga Devi

Dr. G Hannah Priya

Book of Abstracts: International Conference on 'Pure and Applied Physics'

First edition: 2023

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An Autonomous Institution affiliated to the University of Madras
Re-accredited by NAAC in 2019 with Grade A+
College with Potential for Excellence

Dr. Lilian I Jasper, M.A., M.Phil., Ph.D. principal@wcc.edu.in
Principal & Secretary

20th February 2023

Message

I would like to congratulate the Department of Physics on their Platinum Jubilee Year. It gives me immense pleasure to felicitate the Department of Physics on the occasion of their ***International Conference on Pure and Applied Physics****. The Department has been instrumental in training and moulding many young women who are now placed in eminent universities and research institutions across the globe. Conducting events like this in a sustainable manner over the years has paved the way for the Department to stay abreast of the latest developments in the field and maintain their enviable high standards.*

Wishing the Department of Physics the very best in all their endeavors.

Lilian Jasper
Principal

Women's Christian College

F.S. Mohan Eddy
President - WCC Association

23rd February 2022

Message

I am happy to know that the Department of Physics at WCC is organizing an international conference on 'Pure and Applied Physics' on the 23rd and 24th of March, on a hybrid mode at the College Campus.

This year 2023, marks a significant milestone for the Department at WCC – the conference commemorates the Platinum jubilee year of the start of B.Sc. degree program.

I am delighted that the program of the conference includes invited talks by a very impressive set of eight pioneering physicists who are all alumni of WCC.

On behalf of the WCC Association and my fellow Board Members, I wish the conference all success. The Board has been discussing ways to encourage research and innovation at WCC. There is a serious effort to upgrade the facilities and equipment at WCC. I hope the conference would help identify areas of interest where the students and faculty could initiate projects.

F. S. Mohan Eddy

Dr. R. Ravanan M.Sc., M.Phil., Ph.D., PSMS
Joint Director of Collegiate Education

O/o the Joint Director of Collegiate Education
Chennai Region, Chennai-600 015

Message

I am very happy to know that the Department of Physics of Women's Christian College is organizing a 'Two-day International Conference on 'Pure and Applied Physics' on 23rd & 24th March 2023. I understand that the Department is offering undergraduate physics course for 70 years in this reputed college, and has planned to celebrate it in a meaningful way by organizing this academic event. I congratulate the organizers for coming up with an inclusive topic so that the participants will be able to acquire knowledge in all interdisciplinary fields related to physics.

I hope this conference acts as a good platform for young minds to expand their understanding of scientific research. I appreciate all the efforts put in by the organizing committee members to make this conference see the light of the day. I wish the organizers and the delegates of the conference all the very best for a fruitful time during the conference.

15/3/2023

(**DR. R. RAVANAN**)

DR. R. SRINIVASAN
Member Secretary. **Tamil Nadu State Council for Science and Technology**
DOTE Campus, Chennai-600025

Date: 14.03.2023

I am happy to know that Women's Christian College Chennai, Tamil Nadu is commemorating the Platinum Jubilee Year of the Department of Physics. I appreciate the initiative taken by the management for the holistic development of downtrodden women students to improve their competency to meet the current requirement of the institutional and industries in global scale.

Physics is the most interesting subjects in innovative research in science worldwide. Young and brilliant researchers, industrial delegates and talented student communities are representing various countries, which have driven this event into the path of success.

I hope that the conference will be meaningful, purposive, relevant and credible worth remembrance and will be the best platform for dealing with recent problems related to the field. The organization of the conference will provide immense opportunities for interaction among the participants and the resource persons and detailed discussion in the conference will motivate the young, budding scientists, research scholars and faculty members. I convey my best wishes to the organizers and all those who are associated with this conference.

I wish the conference a grand success.

14/3/23

(**DR. R. SRINIVASAN**)

Science City

DEPARTMENT OF HIGHER EDUCATION, GOVERNMENT OF TAMILNADU

Periyar Science and Technology Centre Campus, Gandhimandapam Road, Chennai - 600 025.

24.02.2023

MESSAGE

An old adage says "Today's Classroom is Tomorrow's world for a child" as the Educational institutes provide the the required knowledge and skills to prepare them to face the challenges of the outside world. Despite several constraints educational institutions are producing skilled quality workforce doing exemplary service.

This kind of conferences act as a platform for the students and faculty to share their scientific knowledge and create an effective network paving way for a "knowledge society". I hope this conference promotes unity among physics scientists by strengthening cooperation within the physics community and fostering freedom of movement, association, expression and communication among students, faculty and the resource personnel, as well as sharing of data, information, and research infrastructures and materials.

I compliment the department of Physics, Women's Christian College for organising the two day International Conference on Pure and Applied Physics and hope the deliberations of the two day workshop enlighten the participants.

I wish the programme all success.

S. MALARVIZHI
Vice Chairperson
Science City

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Website : www.tntc.gov.in E-mail : tntc.science@gmail.com

Dr. S. Soundararajaperumal, M.Sc., Ph.D.,
Executive Director, I/C.

Message

I am very happy to know that the Department of Physics of Women's Christian College (WCC) is organizing the International Conference on Pure and Applied Physics during 23-24 March 2023

I came to know that the Conference aims to bring eminent Physicists and from across different parts of the world to deliver talks on current developments in the field.

The momentous WCC is the symbol of pride for the people of Chennai and it has produced numerous Scientists. Scientific innovations are not accidental or made overnight. They are made only after hard work, sincere efforts and sacrifice by the scientists. More than hard work, sharing of the ideas is the essential factor. This will result in a homogeneous development of the field. In this regard, I strongly hope that the International Conference on Pure and Applied Physics will be a great opportunity for the researchers to expose their hard work and to share their meritorious ideas.

This will also enable the students to meet and interact with the renowned Scientists. The efforts by the Physics Department of WCC to augment the knowledge of the students are always commendable and I offer my sincere appreciation to them.

My best wishes to all the delegates for stimulating and fruitful deliberations during the Conference and I extend my hearty good wishes to the organizers, the faculty and the students, for the successful conduct of the Conference.

S Soundararajaperumal
9.3.23
Executive Director I/C

Felicitation message

Dr. S. Balachandran
Head
Regional Meteorological Centre, Chennai

I am glad to know that that Women's Christian College, Chennai is celebrating the Platinum Jubilee of undergrad program in Physics. WCC, Chennai has been a pioneer in imparting higher education for women in Chennai and has contributed significantly towards women's education. Several alumni of this institution have had highly successful careers in various walks of life. It is quite heartening to note that alumni of Physics department are highly placed in prestigious scientific institutions in India as well as abroad and some of them would be attending the **International Conference on 'Pure and Applied Physics' [ICPAP 2023]** being organized by this department during 23rd & 24th March 2023 to serve as resource persons. This would be a great motivation for the present student community. I wish all the best for the grand success of the conference as well as for the institution to scale greater heights in the field of science education for women in the years to come. Looking forward to a grand centenary celebrations.

डॉ एस. बालचंद्रन/ Dr. S. Balachandran,
वैज्ञानिक एफ एंड हेड/ Scientist G & Head,
प्रादेशिक मौसम विज्ञान केंद्र/ Regional Meteorological Centre,
नंबर 6, कॉलेज रोड, चेन्नई -6/ No.6, College Road, Chennai-6.

Felicitation Message

I congratulate the staff and students of the Dept of Physics for organizing the two-day International Conference on "Pure and Applied Physics" [ICPAP 2023]. It's indeed great to note that the Alumnae of the Physics Department who are serving the Science Community as Researchers, Scientists and Administrators, will be back in campus to contribute to their Alma Mater.

An innovative and thought-provoking programme is wished for the Department in the name of our Lord.

S. Grace Nesamoney
President
WCC Alumnae Association

Greetings

I am happy that the department of Physics, Women's Christian College is organizing an international conference on **Pure and Applied Physics (ICPAP 2023).** Education is not only gaining information, but it is transformation. Through Education, College prepares young people for their livelihood and their lives. I congratulate the principal and faculty members of Physics department for their efforts and hard work in imparting sound learning and character-building in the past years. Women's Christian College has produced great people and leaders who contributed significantly to the nation's building and socio-economic development. United Board's vision is whole-person Education which promotes intellectual, ethical and spiritual growth. WCC also focuses on the same vision and facilitates students to develop high empathy, appreciate diversity, enhance communication skills, and build self-confidence. I am sure this conference will create a forum among the faculty, students and alumnae to discuss the practical challenges in the near future for sustainable development. On behalf of the United Board, I congratulate the principal, the head of the department of Physics and all the members of the organizing team for the hard work and efforts to organize this international conference. I wish you all the best for your conference and pray that you will move from Good to Great as you commemorate the Platinum jubilee of the start of B.Sc. degree program.

With Warm regards,

Maher Spurgeon
Consultant, Director
South Asia Programs, United Board.

Dr. A. Christina Nancy, M.Sc., M.Phil., Ph.D
Associate Professor and Head
Department of Physics
Women's Christian College
Chennai – 600006
Email: christinanancy@wcc.edu.in

Message

I am greatly excited and happy to write this message on the occasion of the International Conference on Pure and Applied Physics (ICPAP 2023) organized by the Department of Physics, Women's Christian College in hybrid mode on 23rd & 24th March 2023. In order to celebrate and commemorate 70 years of the B.Sc. Degree program in a unique and remarkable way, it was planned to invite distinguished alumnae of the department as resource persons for the conference. As a proud alumna of the department, I strongly believe that this event will be a great opportunity for the present students to meet pioneering physicists who graduated from our department, and are now serving the scientific community as distinguished researchers, scientists and administrators.

This conference aims to bring together experts in academia and industry from India and abroad to share their ideas and research findings in thrust areas of Pure & Applied Physics. Young scientists, students and faculty will have the opportunity to interact with their peers, assimilate knowledge on current developments in physics-related fields, and present their recent innovative research through oral and poster presentations.

I gratefully acknowledge the remarkable support extended by **our Principal, Dr. Lilian I Jasper**, without whose motivation the conference

would not have become a reality. I extend my thanks to all the **Advisory Committee members** for their willingness to help, suggestions given and wide publicity. A special thanks to all our **invited speakers** for accepting our invitation to address our delegates with lot of enthusiasm and passion. Their love for Physics and their alma mater is highly commendable. I also acknowledge the **delegates** of this conference who have shown an overwhelming response in participating from various states within India and abroad, and for their scientific contribution.

I would like to place on record my sincere thanks to the **faculty of the department** who devoted their time and energy in organizing this event, and worked as a committed team. I would also like to appreciate and thank **our students** for the perfect logistic support.

I wish to gratefully acknowledge and thank the **financial support** extended by our College Management, WCC Alumnae Association, the government agencies – TNSCST & TNSTC, and individual sponsors whose contribution helped in the smooth conduct of the conference.

Above all, I praise and thank God, the Almighty for His continuous presence, guidance and blessings during every step of this conference arrangement. We look back and say to the Lord, 'All that we have accomplished you have done for us' (Isaiah 26:12).

Dr. A. Christina Nancy
Convenor, ICPAP 2023

POSTER PRESENTATION

Invited Talks

IT1

Designing a quartz crystal microbalance tool - A route to study hydration of biomolecules

Water-Protein interaction has been a topic of research since many years. Water molecules around the hydrophilic and hydrophobic sites in a protein control its activity, folding and stability. A strong and highly directional network of hydrogen bonds in the solvated protein, polar hydration and the so called "hydrophobic effect" contribute to many of the above interactions. In spite of a wide body of knowledge, there still exist controversies over what happens in the interfacial zone of protein-water. The talk will deal with a new experimental tool using Quartz crystal microbalance (QCM) to study aqueous amino acids and peptide/protein in various solvent environments. By profiling solvation of such macromolecules across different solid-liquid boundaries, the work has explored how solutions and substrates conspire to create molecularly distinct, local environments. The lecture focuses on how localized (microscopic) changes in immediate aqueous protein systems change not just its bulk properties but also influence macroscopic phenomenon like wetting, spreading and adhesion.

Dr. Aruna Dhathathreyan *received her Ph.D. from the Department of Crystallography & Biophysics, University of Madras in 1984. She was a postdoctoral fellow and a scientist (1983-84,1986-1989) at the Max Planck Institute for Biophysical Chemistry, Gottingen, Germany. Briefly, she worked as a PDF at the Dept. of Biophysics, University of Groningen. After her return to India in 1989, she was a visiting Scientist at The Centre for Biotechnology, Anna University before starting her career as a scientist at the CSIR-CLRI in 1990 till June 2015 when she retired as Chief Scientist and Head, Biophysics Lab. Between 2018 and 2022, She was a Research Ambassador for the German Academic Research Program (DAAD). She was elected Fellow, Madras Science Foundation, 2011, was a visiting scientist under DAAD (2009) to Germany and later as INSA DFG visiting professor, 2010 (FRG).*

IT2

The photon, optical tomograms, and imaging the quantum state

The quantum-classical divide is a grey area, and some quantum (nonclassical effects) can be understood well using tools from classical physics. Quantum optics provides an ideal platform for assessing how well the rules of classical probability can reproduce results in quantum physics. We note that quantum mechanics is inherently probabilistic in nature. We will journey through important landmarks of relevance in the history of quantum physics. The main output from quantum optics experiments is the optical tomogram, which is similar to the medical scans that are commonly used, except that in this case it is the state of light that is imaged. We will familiarise ourselves with some colourful tomograms that obey the laws of classical probability, and identify nonclassical effects directly from these tomograms, without reconstructing the quantum state.

S. Lakshmi Bala *is a senior professor in the Department of Physios, IIT Madras, Chennai. Her doctorate work was in theoretical high energy physics, but later she has moved on to a variety of diverse research areas including dynamical systems and chaos, quantum dynamics, quantum optics and quantum information and computation. Although primarily a theoretical physicist, she has recently been working close to experiments, and analysing experimental data pertaining to the quantum state. She is a member of the Center of Excellence in Quantum information, Communication and Computing in IIT Madras. Her set of 41 video lectures under the NPTEL banner, also available on Youtube, on Quantum Mechanics, have been received well across the world. Recently she has been the primary author in a book titled `Nonclassical effects and dynamics of quantum observables' published as a SpringerBrief book, by Springer Nature.*

IT3

Living with the Sun

We live in the backyard of a star, the Sun. The Sun gives us energy and sustains life. However, the Sun emits enough radiation to cause harm, which in most cases, is prevented by the Earth's magnetic shield. However, extremely energetic emissions from the Sun can lead to geomagnetic storms that are detrimental to technology; the most well-known event being the magnetic storm of 1859 [1]. Another such storm in 1967 almost caused a nuclear war [2]. The Sun's effect on life and society is one of the major reasons that we study the Sun. Of course, there are purely intellectual reasons too — the Sun is the only star that can be studied in detail, and it helps us understand other stars.

In this talk I shall review what we know about the Sun as a star before talking about what we know of the cyclically increasing and decreasing emissions from the Sun. I shall then introduce the audience to the technique of helioseismology [3][4] — the study of the Sun using solar oscillations or sunquakes. This technique allows us to peer inside the Sun and determine the structure and dynamics of the layers of the Sun that are hidden to our eyes. I will then discuss results on what helioseismology has taught us about the internal variability of the Sun and how that is correlated with what we see at the surface.

Keywords: Sun: activity; Sun: variability; Sun: helioseismology; Sun: rotation

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***Sarbani Basu** is the William K. Lanman Jr. Professor of Astronomy at Yale University, USA. Prof. Basu was educated in India. She was a Physics major at the Women's Christian College and graduated from there with a B.Sc. in 1986. She obtained her Ph.D. in 1993 for work done at the Tata Institute of Fundamental Research. Subsequently, she was a post-doctoral fellow at the Queen Mary & Westfield College, London, and University of Aarhus, Denmark before moving to the US in 1997 to join the Institute for Advance Study, in Princeton. She joined Yale University in 2000. She Chaired the Department of Astronomy at Yale from 2016-2022.*

IT4

Topic: 'Novel Class of Unconventional Insulators'

Suchitra Sebastian *is Professor in Physics and EPSRC Established Career Fellow at the University of Cambridge. Her research seeks to discover exotic quantum phases of matter in complex materials. To this end, her group's experiments involve tuning the co-operative behaviour of electrons within these materials by subjecting them to extreme conditions including low temperature, high applied pressure, and intense magnetic field. Under these conditions, interactions between a trillion trillion electrons, as many as the stars in the observable universe, create surprising and unpredictable collective quantum phases akin to new materials 'universes'. Emergent quantum phenomena studied by Suchitra's research group include high-temperature superconductivity and a new unconventional insulating state of matter they recently discovered. Most recent awards Suchitra has received include the New Horizons in Physics Prize (2022) awarded by the Breakthrough Foundation and the Schmidt Science Polymath award (2022). Suchitra is founder director of the Cavendish Arts Science programme, and co-founder of Bread Theatre and Film Company. She participates in scientific research for non-imperialistic, non-militaristic purposes.*

IT5

Creating inclusive, and accessible Artificial Intelligence for health: Perspective from Quantitative Imaging study for head and neck cancer

Abstract

In recent years, there has been growing interest in developing inclusive and accessible artificial intelligence (AI) technologies in healthcare. The goal is to ensure that AI-powered healthcare systems and applications are designed to be accessible to everyone, and inclusive for patients from various characteristics and cultural backgrounds. AI systems also need to be designed with ethical considerations in mind, including issues such as privacy, security, and fairness.

In the perspective of Head and Neck cancers (HNC); it is officially classified as a rare (a.k.a "orphan") disease that does not receive anywhere near the same support socially and economically as lung, breast, or prostate cancers. However, these cancers are a biologically complex and epidemiologically heterogenous family of rare malignancies with the burden of HNC being intense in India. Around 200,000 new patients are diagnosed each year (about 20% of all cancer diagnoses) but often presenting in advanced stages of disease, with poor prognosis and short expected lifetime. One of the most challenging yet most important task following diagnosis is to know **which therapy is most likely to get a strong response from an individual tumour**. At present, this crucial decision is based only on doctor-derived observations such as age and extent of cancer, qualitative visual interpretation of radiological images and averaged statistics of randomized clinical trials. Cutting-edge advances in molecular biomarkers allow cancer treatment to be more personally tailored to the individual patient, using tests that reveal the activation of specific genetic pathways but are based on small selective samples extracted from the tumour. Non-invasive radiological images, derived by Computed Tomography (CT), Positron Emission Tomography (PET) and Magnetic Resonance (MR) imaging, remains

indispensable for diagnosis and decision-making because it allows analysis of a whole tumour in situ (in 3D and/or its evolution as a function of time). However, the disappointing clinical outcomes in HNC is testament that our state-of-the-art knowledge is simply not good enough.

Radiomics is a new and rapidly evolving field in oncology that uses artificial Intelligence-driven quantitative analysis of vast volumes of radiological imaging data. The basis of radiomics is high-throughput computer-assisted conversion of unstructured qualitative "pictures" into numerical quantifiable unique "features" that can be archived digitally and then mined at massive scale for clinical insight using machine learning and deep learning techniques. The radiomics hypothesis rests on the variability in clinical outcomes and/or responses to treatment being fundamentally grounded into differentiable phenotypes (observable physical properties) of the tumour, and hence computer vision-based analysis of phenotypes reveal prognostic signatures (i.e. combined sets of solitary features) that go much further than what unguided human eyes can perceive. Despite these early successes, there are barriers to clinical adoption and implementation of Radiomics in radiation Oncology.

In spite of such early successes, the barriers to clinical adoption and implementation of radiomics remains very high. Critics point out, with reasonable justification, that (a) radiomics ML and DL models are functional "black boxes" with virtually no transparency, explainability nor interpretability, hence it would not be ethical to use these in a clinical consultation setting because a medical expert could not "defend" the results of the model, (b) radiomics as a field of study is still too much in its infancy due to insufficient volumes of patient data for generating robust and widely generalizable models (i.e. excessive incorporation of biased and confounding factors), and finally (c) that there are still no prospectively randomized clinical trials proving that radiomics has any added value at all, either as a standalone or supplemental modality to existing diagnostic/prognostic disease stratification methods.

To address some of these limitations in this field our team from the Quantitative imaging research and Artificial Intelligence from Christian Medical College, Vellore, India, lab funded by Wellcome Trust, UK and Department of Biotechnology, India are building the tools, the team and the infrastructure for better understanding imaging biomarkers within our clinical workflow, primarily for head and neck cancer in our population. I will be sharing our experiences of running the largest prospective imaging trial for Head and neck cancer, multi-institutional radiomics studies and learning health systems.

***Hannah Mary Thomas T**, PhD (2016) is an Imaging Scientist in the Department of Radiation Oncology at the Christian Medical College, Vellore, India, supported by the DBT / Wellcome Trust India Alliance Early career fellowship. She co-founded the Quantitative Imaging and Artificial Intelligence (AI) research Lab and leads the Research team in building 1) Quantitative Imaging of Cancer and Normal Tissues, 2) Artificial Intelligence for health outcome prediction models and 3) Making AI accessible and inclusive. Dr Thomas has authored over 25 publications. She has been the recipient of many fellowships and awards in the last 15 years including the prestigious Fulbright-Nehru Doctoral and Professional Fellowship at the University of Washington, Seattle, USA and the Institute Advanced of Sciences External Academic Fellowship from University of Surrey, UK.*

IT6

Inference of syntax from vocal sequences and implications for neural mechanisms: Approaches in biophysics

Animal vocalisations, such as songbird songs, are a fascinating and complex learned behaviour that involves the generation and perception of sound. However, the neural and peripheral mechanisms underlying this behaviour are not yet fully understood. One of the approaches used in biophysics to gain insight into this behaviour involves the quantitative characterization of the structure of vocal sequences, also known as the syntax, based on statistical regularities. In this talk, I will discuss the inference of syntax models for animal vocalisations, using the example of songbird songs. These songs consist of variable sequences of acoustic units called syllables that follow probabilistic rules. The probability of producing a particular syllable in a song can depend on the syllables that came before it. Similar context dependencies are widely observed in animal behaviours, and the modelling techniques that I will describe are well-suited for uncovering such dependencies in other behavioural sequences as well. Using the example of Bengalese finch song, I will detail how context dependencies can be modelled using Partially Observable Markov Models (POMMs), which are a special case of Hidden Markov Models (HMMs) [1, 2]. POMMs consist of states and probabilistic transitions between them. Each state is associated with a syllable, and one syllable can be associated with multiple states. This multiplicity of syllable-to-states-association distinguishes a POMM from a simple Markov model and captures context dependencies. Previous studies have shown that disrupting auditory feedback by deafening adult Bengalese finches can cause changes in the structure and sequencing of syllables in their songs [3, 4, 5, 6]. This suggests that auditory feedback could play a role in shaping the context dependencies in songbird song syntax. A comparison of the song syntax of Bengalese finches before and shortly after deafening reveals that auditory feedback plays an important but not exclusive role in creating context dependencies, positing the need to investigate the role of intrinsic neural circuitry as well [7].

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Sumithra Surendralal *is an Assistant Professor at the Symbiosis School for Liberal Arts (SSLA), Pune, teaching undergraduate courses in physics and mathematics. Her research interests are broadly in the area of theoretical and computational biophysics. She also has a deep interest in science pedagogy. After completing a bachelor's degree in physics at Women's Christian College, Chennai, she studied in the Department of Theoretical Physics at the University of Madras for her master's degree. Working with Dezhe Jin, she received a PhD in physics from the Pennsylvania State University in 2016, where she worked on methods to infer syntax models of songbird songs.*

IT7

Spacetime foam

Abstract:

The search for gravitational waves spanned almost a century. This talk will discuss why it was so challenging to detect gravitational waves, even from the most powerful black hole merger. With the successful detection of gravitational waves in 2015, the focus is now on the finer variations in spacetime dynamics that might lead to a better understanding of the nature of the gravitational field. One important question is whether the gravitational field is a quantum field. Detecting the presence of a "foamy" spacetime can prove that the field is indeed quantum. This talk will address the following questions: (i) What is spacetime foam?, (ii) What are its origins? (iii) How can the possible presence of spacetime foam be detected?

Sharmila Balamurugan *did her Bachelor's in Physics (2009-2012) at Women's Christian College. She did both her Master's (2012-2014) and her doctoral research (2014-2020) at the Indian Institute of Technology Madras. Her doctoral research was on "Signatures of nonclassical effects in tomograms" under the guidance of Prof. S. Lakshmibala. She is currently a post-doc in the Quantum Information Science group of Prof. Animesh Datta at the University of Warwick, UK. She works on extracting signatures of quantum spacetime fluctuations from interferometric experiments. She was awarded the Alice Barnabas Physics prize for the best outgoing student of the B. Sc. Physics (Core) class, Chilukuri Ramasastri Memorial Prize for the best academic record in M.Sc. Physics, and Swati / Jayalakshmi Memorial Award for the girl securing the highest CGPA in the pre-final semester of her M.Sc. She also won the best poster award at 15th International Conference on Squeezed States and Uncertainty Relations 2017.*

IT8

The ATLAS New Small Wheel Upgrade and Physics at the LHC

About half a century ago, with tremendous collaborative efforts from both the theoretical and the experimental communities, a scientifically stunning piece of work known as the Standard Model (SM) was developed. The universe as we know it is governed by four forces namely gravity, strong force, weak force, and electromagnetic force. The Standard Model addresses all but gravity and their interactions with all the elementary particles discovered to date. The weak force is mediated by the W and the Z bosons, which are massive in nature, while the electromagnetic force is mediated by the photons, which are massless. One of the key predictions of the Standard Model is that the weak gauge bosons acquire their mass through the process of symmetry breaking and if so, a scalar particle must accompany the mechanism. The state-of-the-art technology facilitating the experimental reach of such energy scales to search for this particle is the Large Hadron Collider (LHC), located at the European Organization of Nuclear Research (CERN) in Geneva. Adorned as an engineering marvel, this hadron collider is the world's largest and most powerful accelerator machine that smashes hadrons, mainly protons, at extremely high energies, re-creating the early conditions of the universe. The proton beams are accelerated to nearly the speed of light and are then collided at a center of mass energy of 13.6 TeV, which is the largest ever reached in a laboratory. The energy released in these collisions materializes in the form of new particles like quarks, leptons, gluons, or even massive bosons. The LHC collides protons at four main points along its accelerator ring, where huge detectors are housed to detect the particles produced. The ATLAS and the CMS detectors are two such gigantic detectors that act like huge cameras capturing almost all the particles formed from the high energy collisions. In 2012, the LHC culminated the 40 year long search for the elusive scalar particle with the discovery of the Higgs boson (mH = 125 GeV) in both ATLAS and CMS. The discovery was momentous in the history of the LHC and confirmed the existence of the Higgs field in nature to which the

particles couple and acquire mass. With the last piece of the puzzle found, the Standard Model is deemed complete but leaves no explanations for some of the observed phenomena, as a result of which many models beyond the Standard Model have been hypothesized, often generally referred to as new physics. New physics at the LHC is explored by searching for new particles or by rigorously testing the Standard Model to investigate any deviations of the parameters from the SM predictions. A promising subject in understanding the origin of the Higgs particle and probing hints for new physics is the self-interactions of the electroweak gauge bosons, also known as vector boson scattering (VBS). At the LHC, VBS occurs when the incoming quarks in the colliding protons radiate the gauge bosons, which subsequently interact leaving distinct experimental signatures. The process is marked by two jets separated by large angles in the detector and is one of the rarest, occurring once in hundreds of trillions of proton collisions. With the discovery of the Higgs boson, VBS has garnered much attention from the 1 scientific community and is undoubtedly of paramount importance to unravel the mysteries of nature in the LHC era. In the first part of the talk, some of the recent results on VBS at the LHC will be presented. With the benchmark achievements and growing interest in the physics program at CERN, it becomes necessary to improve the performance of the LHC and churn out data at an even higher and astounding rate. The High-Luminosity Large Hadron Collider (HL-LHC), a project led by CERN, aims to deliver luminosity 7.5 times larger than the current design luminosity. The project is one of the top priorities of the European Strategy for Particle Physics and requires several technological innovations and upgrades. In order to cope with the extreme conditions of the HL-LHC environment, the experiments also require subsequent upgrades. The upgrades for the ATLAS experiment are performed in two phases. Phase I upgrade spanned over the years 2019 to 2022, and Phase II upgrades are scheduled along with the installation of HL-LHC between 2026 and 2028. During the Phase I upgrade, the innermost wheels at the end-cap region of the Muon Spectrometer were replaced by the New Small Wheels (NSW) to improve the triggering and tracking performances in a high particle rate environment. In the second part of the talk, the ATLAS NSW upgrade will be targeted.

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Oral Presentations

OP1

Green synthesis of NiO-CuO nanocomposite using Psidium guajava leaf extract and evaluation of its photocatalytic and third order NLO activity

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Recently, metal oxide semiconductors with larger surface area are widely used as catalysts for the degradation of toxic dyes because they possess an excellent combination of photochemical activity, thermal and mechanical stability. NiO-CuO nanocomposite was fabricated biologically using *Psidium guajava* leaf extract without adding additional chemical precipitating agents. The phytochemicals present in the *Psidium guajava* leaf extract acts as potential reducing agent to produce stable NiO-CuO nanocomposite. In this present work, FTIR, XRD, SEM, Photocatalytic activity and third order NLO properties of green synthesis nanocomposite were analyzed. The FT-IR spectrum and XRD studies confirm the presence of functional groups and the structure of NiO-CuO nanocomposite. The SEM images of the nanocomposite clearly confirmed the existence of nanoneedles. Z-scan studies confirmed that the title composite exhibited appreciable third order NLO properties. The nonlinear absorption coefficient (β) value is 2.48×10^{-4} cm^2/W for the nanocomposite. The high value of NLO susceptibility possessed makes the nanocomposite highly polarized. The occurrence of reverse saturable absorption (RSA) effect from the Z-scan studies confirmed that the composite is well suited for nonlinear optical and photonic devices. Photocatalytic tests confirmed that the green synthesized nanocomposite effectively degraded RhB dye under visible light. Under visible light illumination for about 90 min, the nanocomposite degraded 91.5% of rhodamine B dye. The obtained results confirmed that the nanocomposite

seems to be an effective non-toxic photocatalyst for degrading toxic dyes with better third order NLO properties.

Keywords: Nanocomposite; Green synthesis Leaf extract; SEM, Photocatalytic; Z-scan

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OP2

In silico Molecular Docking, ADMET and Quantum Studies of Trans-4-Trifluoromethyl Cinnamic Acid Exhibit HDAC8 Potent Inhibitory Activity

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The electronic absorption spectra of trans-4-trifluoromethyl cinnamic acid (4TFCA) have been recorded by using the TD/DFT procedure. Trans-4-trifluoromethyl cinnamic acid have a double bond -C=C- between the aromatic ring and the carboxyl group which disturbed the π-electron system of the molecule. The geometrical parameters of the ground state of the trans-4-trifluoromethyl cinnamic acid is calculated using the DFT/B3LYP/6-311G (d, p) method and an express molecular orbital analysis is achieved. Vibrational FTIR and FT-Raman assignments of trans-4-trifluoromethyl cinnamic acid were verified in the regions 4000-400 cm^{-1} and 4000-50 cm^{-1}. The observed vibrational

wavenumbers are in good matched with the computed wavenumbers. The HOMO-LUMO energy gaps have been computed. The stability of a molecule rising from hyper-conjugative $\pi \rightarrow \pi^*$ exchanges and charge delocalization has been calculated using natural bond orbital (NBO) analysis. The thermodynamic and charge responses have been studied. In addition, the molecular docking results exposed that trans-4-trifluoromethyl cinnamic acid has a highest binding (-6.10 kcal/mol) energy with HDAC8 and is utilized as a possible agent for Histone deacetylases action. ADMET analysis such as LD50 have also been studied for trans-4-trifluoromethyl cinnamic acid to evaluate its drug-images.

Keywords: DFT; Trans-4-trifluoromethyl cinnamic acid; Vibrational assignments; Docking; ADMET

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OP3

Quantum deleting machine

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In this work, we study the well-known Pati-Braunstein and our deleting machines. We analyze the retention fidelity and the distortion of the input qubit of the machines. We arrive at an interesting bound between the fidelity of retention and the distortion. It is observed that more we distort the qubit, less we retain the qubit in its original state. In other words, lower (higher) the distortion, higher (lower) the retention of the original qubit.

1. Introduction

Impossibility of perfect cloning [1] and impossibility of perfect deleting [2, 3] are two foundational theorems in the no-go theorems. This stems

from the fact that linearity principle of quantum physics prevents perfect cloning and deletion of unknown quantum states. While unknown states are impossible to predict accurately, the no-deleting principle argues that quantum information in a closed system cannot be destroyed, but it can be transferred from one position to another. Present work aims to find the connection between the copy qubit and the original qubit. This is possible by connecting retention fidelity - how efficiently the qubit is retained and the distortion - how much the original qubit is distorted in the process of retention. By finding the fidelities, we have observed an interesting bound. Significance of this observation is highlighted in the conclusion.

2. Pati - Braunstein deleting machine

If both inputs are the same, a second copy is deleted. If both inputs are different, the copy is allowed to pass through with no changes [2]. For the input state, $|\psi\rangle_{in} = \alpha|0\rangle + \beta|1\rangle$ with $\alpha^2 + \beta^2 = 1$ and the blank state be $|\Sigma\rangle = m_1|0\rangle + m_2|1\rangle$ with $m_1^2 + m_2^2 = 1$, deleting transformation for orthogonal qubit is given by

$$|0\rangle|0\rangle|A\rangle \rightarrow |0\rangle|\Sigma\rangle|A_0\rangle;\ |1\rangle|1\rangle|A\rangle \rightarrow |1\rangle|\Sigma\rangle|A_1\rangle;\ |0\rangle|1\rangle|A\rangle \rightarrow |0\rangle|1\rangle|A\rangle;\ |1\rangle|0\rangle|A\rangle \rightarrow |1\rangle|0\rangle|A\rangle \quad (1)$$

The output state is given by,

$$|\psi\rangle_{out}^{PB} = \alpha^2|0\rangle|\Sigma\rangle|A_0\rangle + \beta^2|1\rangle|\Sigma\rangle|A_1\rangle + \alpha\beta\,[|0\rangle|1\rangle|A\rangle + |1\rangle|0\rangle|\mathrm{A}\rangle] \quad (2)$$

where $|A\rangle, |A_0\rangle$ and $|A_1\rangle$ are orthogonal to each other. The reduced density matrix of input state:

$$\alpha^2|0\rangle\langle 0| + \beta^2|1\rangle\langle 1| + \alpha\beta[|0\rangle\langle 1| + |1\rangle\langle 0|] \quad (3)$$

Thus the fidelity of retention and distortion are found to be

$$F_R^{PB} = \langle\psi_{in}|\rho_1|\psi_{in}\rangle = 1 - 2\alpha^2\beta^2 \quad (4)$$

$$D_1^{PB} = Tr[(\rho_1 - \rho^{id})(\rho_1 - \rho^{id})^{\dagger}] = 2\alpha^2\beta^2 \quad (5)$$

As the deletion depends on input states, PB deleting machine is a state dependent machine.

3. Deleting machine (DM)

If both inputs are the same, the copy is allowed to pass through with no changes; if both inputs are different, a second copy is deleted [4, 5]. The deletion machine is defined for orthogonal qubits as

$$|0\rangle|0\rangle|A\rangle \rightarrow |0\rangle|0\rangle|A\rangle;\ |1\rangle|1\rangle|A\rangle \rightarrow |1\rangle|1\rangle|A\rangle;\ |0\rangle|1\rangle|A\rangle \rightarrow |0\rangle|\Sigma\rangle|A_0\rangle;\ |1\rangle|0\rangle|A\rangle \rightarrow |1\rangle|\Sigma\rangle|A_1\rangle \quad (6)$$

The output state is given by,

$$|\psi\rangle_{out}^{DM} = \alpha^2|0\rangle|0\rangle|A\rangle + \beta^2|1\rangle|1\rangle|A\rangle + \alpha\beta\,[|0\rangle|\Sigma\rangle|A_0\rangle + |1\rangle|\Sigma\rangle|A_1\rangle] \quad (7)$$

Thus, the fidelity of retention and distortion are calculated as

$$F_R^{DM} = \langle\psi_{in}|\rho_1|\psi_{in}\rangle = 1 - 2\alpha^2\beta^2 \quad (8)$$

$$D_1^{DM} = Tr[(\rho_1 - \rho^{id})(\rho_1 - \rho^{id})^{\dagger}] = 2\alpha^2\beta^2 \quad (9)$$

As the deletion depends on input states, deleting machine is a state dependent machine.

4. Bound nature

For the proposed deleting machines, the relation between the fidelity of retention and distortion exhibit the following bound: (i). $F_R^{PB} + D_1^{PB} = 1$ and (ii). $F_R^{DM} + D_1^{DM} = 1$. This bound between the fidelity of retention and distortion indicates that more we distort, less we retain the first qubit. Further, variation of retention fidelity (F_R) and distortion (D_1) with respect to the input state α is shown in the Fig.1. While retention fidelity increases (decreases), distortion decreases (increases) for the input state α. For $\alpha = \frac{1}{\sqrt{2}}$ corresponding to the superposition state $|\psi\rangle = \frac{1}{\sqrt{2}}\,[|0\rangle + |1\rangle], F_R = D_1 = 0.5$.

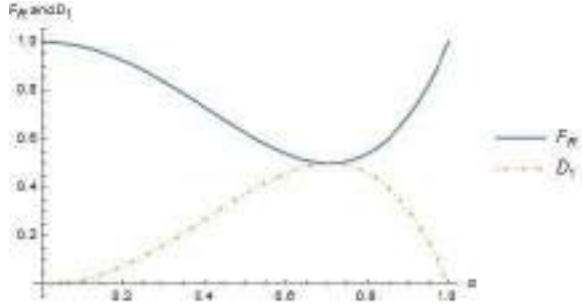

Fig. 1. Variation of F_R and D_1 with respect to input state α

Conclusion

We have analyzed the performance of Pati-Braunstein deleting machine and proposed deleting machine. Further, the sum of retention fidelity and distortion is always one. This implies that lower the distortion, higher the fidelity of retention of the input qubit. It will be interesting to see such a bound for other deleting and cloning machines.

Keywords: Distortion; Fidelity of retention; Deleting machine; Pati-Braunstein deleting machine

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OP4

Prediction for unknown energy levels of three times ionized krypton

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Three times ionized krypton (Kr-IV) is an As-like ion with ground configuration of $4s^24p^3$.In this work we have considered several previously reported levels of Kr-IV[1-3] and many new configurations have been added for the calculations. The theoretical prediction of energy levels of the even configurations $4s^24p^27s$,$4s^24p^26d$,and of odd configurations $4p^5$,$4s^24p^2(6p+7p)$,$4p^4(5p+6p)$,$4s^24p^24f$,$4s^24p4d5s$ are made using cowan's quasi-relativistic Hartree –Fock code [4] .These data

are important due its applications in collision physics, fusion diagnostics, astrophysics and as well as in the development of future tokamaks [5].

Keywords: Energy levels; Configuraton; Cowan code

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OP5

Optical and Magnetic Properties of Bi^{3+} doped $CaSnO_3$ Perovskite Nanostructures

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Undoped $CaSnO_3$ and Bi^{3+} (1, 3 and 5%) doped $CaSnO_3$ perovskite nanostructures were synthesized by chemical precipitation method. Structural measurements revealed orthorhombic perovskite structure. FT-IR studies demonstrated the metal oxide vibrations existing in the synthesized nanostructures. Raman measurements supported the crystal structures. A change in bandgap was witnessed from UV-Vis studies. Bi

doping in $CaSnO_3$ did not exhibit any significant change in the magnetization properties. The present investigation suggests that there is a possibility to tune the band gap of $CaSnO_3$ using Bi as a dopant.

Keywords: $CaSnO_3$, Chemical precipitation method, Bi doping, Bandgap

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OP6

Magnetic field induced structuration in ferrofluid for magneto-optical applications

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Ferrofluids are colloidal suspension of ferri/ferro magnetic materials, and these are contemporary materials for various applications like memory devices, MRI, optical sensor, EMI shielding, switches, magnetic fluid hyperthermia and targeted drug delivery. In this present study, we have followed a new approach to investigate the field-induced structuration i.e

magneto-optical and spin dynamics of such magnetic nanofluid at gradient magnetic field at room temperature. A series of $Zn_xFe_{3-x}O_4$ (x=0,0.1,0.2,0.3 &0.4) ferrofluid with different Zn^{2+} concentrations were synthesized by the wet chemical co-precipitation method and oleic acid was used as surfactant to prevent the agglomeration of MNPs. A static magnetic-optical experimental setup has been arranged to perceive the structuration process due to stoichiometry based dipolar interaction of dispersed magnetic nanoparticles under the influence of an external magnetic field. The diffraction fringes are observed in nanofluid when a green laser is passed from the diluted volume % nanofluid system. It is interesting to observe that the fringes width changes with varying the Zn^{2+} doping concentration due to change in the magnetic moment of the spins. Also, the variation of intensity of transmitted light has been corroborated with the forward scattering resulting from the Brownian motion of the MNPs. Further, a static magnetic measurement studies reveal the superparamagnetic characteristic is observed for all samples with the substitution of the Zn^{2+} ions has resulted in improvement in the saturation magnetization from 33.61 to 49.48 emu/g which has been corroborated by the super-exchange interaction between the magnetic ions through A and B sites. The room temperature microwave spins resonance studies exert the spin resonance drift with minimum doping concentration. In all samples a sharp resonance signal is observed, and enhancement of peak-to-peak line width is a indication of the strong super-exchange interaction between the magnetic ions through oxygen ions. Therefore, the experiment validates the chain formation in nanofluid, as MNPs are almost working as mesoscopic cylinders resulting in specified scattering patterns at different volume %. We believe that this approach can pave a new pathway for the development of a tuneable optical filters, optical limiters, and various photonics applications [1,2].

Keywords: MNPs, Polycrystalline, SEM, Ferrofluids, FTIR, EPR.

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OP7

Exploration of NiO-CeO_2 Nanoparticles and their nanocomposties as a superior electrode for supercapacitor application

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The current work annotates the synthesis of NiO-CeO_2 nanoparticles (NPs) and their carbaneous (rGO, g-C_3N_4) nanocomposites (NCs) in simple hydrothermal method by using urea and ammonium fluoride as stabilizing agent. X-ray diffraction pattern confirmed the face centered cubic structure of NiO-CeO_2 NPs and their NCs, no other phases were formed owing to the presence of rGO and g-C_3N_4. FTIR spectra confirm the presence of metallic oxide and functional groups present in the synthesized samples. Raman spectra reveal the modes of vibration and orderness/disorderness in the carbonaceous composite materials of synthesized. Furthermore, the synthesized samples were characterized to identify the electrochemical performance of synthesized electrodes such as EIS, CV and GCD. From the observed results, we found that the NiO-CeO_2/rGO NCs is an efficient electrode material for supercapacitors with remarkable specific capacitance at 10 mV/s in 2 M KOH and notable cyclic retention after 5000 cycles [1]. This work portrays a cost effective and comfortable synthesis of NiO-CeO_2 and their NCs electrodes which enhance specific capacitance for energy storage applications.

Keywords: NiO-CeO_2 NPs; rGO; g-C_3N_4; Supercapacitor

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OP8

Electro catalyst based visible- light active cerium doped cobalt oxide (Ce-Co_3O_4) nanoparticles for photocatalytic and photochemical activity

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Spinel Ce-doped cobalt oxide ($Ce_xCo_{3-x}O_4$) nanoparticles have piqued up the interest of researchers due to their exceptional combination of properties, particularly magnetic properties, and these properties are pushing boundaries to be a suitable candidate material in the field of electronics. $Ce_xCo_{3-x}O_4$ (x = 0.05, 0.1 & 0.3) powders had been synthesized using a scalable co-precipitation technique yielding

nanostructured spinel cobalt oxide particles. Eco-friendly techniques were used to fine-tune the morphology, particle size, and reaction rate of the nanoparticles (NPs). X-ray diffraction (XRD) showed the incorporation of Ce^{2+} ions inside Co_3O_4 host lattice, in settlement with FESEM analysis. FTIR found out a moderate extrude in major bands υ_1 and $\upsilon_2$withinside the frequency variety of 400 - 4000 cm^{-1}, because of stretching vibrations on the A and B-sites respectively. The optical band hole (E_g) from Tauc plots become observed with growing Ce^{2+} content material. VSM confirmed the transformation of magnetic behavior from paramagnetic to ferromagnetic because of Ce^{2+} ions doping. The supreme photodegradation rate was remarked to be ~93 percent with a period of 120 minutes, and this improved photocatalytic enforcement due to the effective evaluation of electron-hole recombination by the Co_3O_4 NPs. The stability is maintained over five reaction cycles without significant decrease in the absence of sacrificial agents. The photocurrent (I_{photo}) is higher than the dark current (I_{Dark}) for Ce-doped Co_3O_4, indicating the existence of more photogenerated carriers. The maximum photoconductive parameters such as photo-responsivity (R), external quantum efficiency (EQE), and detectivity (D*) were achieved for higher concentration of Ce-doped Co_3O_4 sample.

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OP9

Graphitic Carbon Nitrate Nanosheet anchored with Bi_2S_3 Nanorods Composite as an High-Performance electrode for Supercapacitor application

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Graphitic carbon nitrate nanosheets anchored with Bi_2S_3 nanorods composite by using a simple hydrothermal method. The prepared samples were characterized using XRD, FT-IR, SEM and EDS. Moreover, pure Bi_2S_3 nanorods, g-C_3N_4nanosheets and Bi_2S_3/g-C_3N_4 composite electrode material were tested in electrochemical studies. In compared to all electrodes, the Bi_2S_3/g-C_3N_4 composite obtained high specific capacitance of 631 Fg^{-1} at a current density of 1 Ag^{-1}, as well as an excellent capacitance retention of 94% retained after 5000 charging and discharging cycles in 1 M Na_2SO_4 electrolyte. The Bi_2S_3/g-C_3N_4 composite electrode exhibits superior electrochemical performance owing to the synergetic effect of Bi_2S_3 nanorods and g-C_3N_4 nanosheets. Also, the Bi_2S_3/g-C_3N_4 composite has been suggested as a promising electrode material for supercapacitor applications.

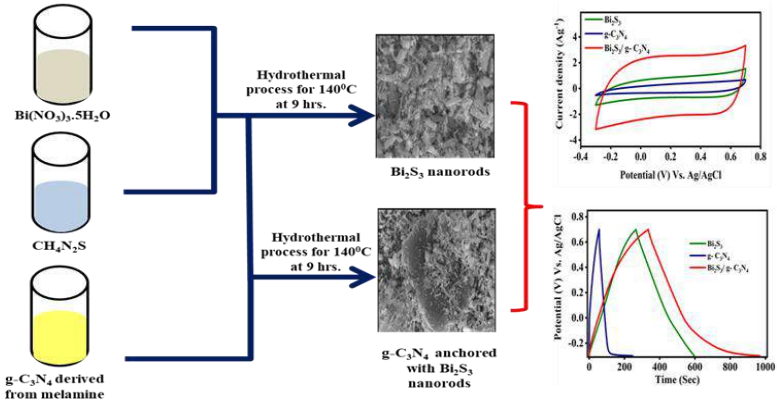

Fig.1. Preparation and electrochemical studies of Bi_2S_3/ g-C_3N_4 composite

Keywords: g-C_3N_4; Bi_2S_3 nanorods; Supercapacitors

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OP10

GC-MS, FT-IR, UV-Vis, Quantum Chemical, Investigation of 4, 25-Secoobscurinervan, 21-deoxy-16-methoxy-23-methyl

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In this paper, we have described the Green synthesis compounds from carbinol extract of hybanthusennea spermus plant. Therefore, the invention and progress of new drug material (4SDMM**)** for cancer activity by compared using theoretical method and experimental of FT-IR, UV-Vis has been performed. The FT-IR calculated vibrational frequency of each normal mode, UV-Vis spectral analysis excitation energies oscillator strengths and DFT calculation using B3LYP/6-311G(d, p) get optimized structure to predict bond angle, bond length, MEP, molecular atomic charges to find positive, negative charge, region that denoted electrophile and nucleophile attraction. Further, NBO analysis localized pair; lone pair and wave functions used Fock Matrix Perturbation Theory. The HOMO and LUMO analysis to accurate value of chemical stability and compound electrically operate.

Keywords: GC-MS, FT-IR, UV-Vis, DFT, NBO, MEP

1. Introduction

Currently, cancer is a significant national health issue,in india last year 2022 found 1,46,427 million cases, mostly affected lung, Breast cancer in male and female respectively. India has a third place in cancer; it would be increase 1.46 million at 2022 to 1.57 million at 2025 in future, the new natural drug material of title compound 3MIZPutilization in pharmaceutical against cancer activity. In literature review of some Authors, Phototherapy has proved to treat several health disorders such has urinary infections, inflammation and compounds present flavonoids, sugars, tannins, alkaloids, some psychopharmacological activities [1]. Anticancer activity showed powerful growth-inhibiting effects on the HEp-2 cell line [2]. Apricot pomace extract as a Green vapour phase corrosion inhibition effect of mild steel and investigate inhibitive action of the extract [3]. The existence of phytochemicals and their therapeutic effects are determined by the H. enneaspermus leaves [4]. The active

compounds isolated from H. eneaspermus, that to be exploited in drug development research [5].

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OP11

DFT Calculations of Ethyl 2-[1-(3-methyl butyl)-4-phenyl-1H-1,2,3-triazol-5-yl]-2-oxoacetate

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1,2,3-triazoles are important compounds having essential biological activities, including antibacterial, antifungal, antimalarial, antiviral, anticonvulsant, antidepressant, and anti-cancer properties. Efforts to investigate the molecular electronic structure to prove the molecule very stable and biologically active. The molecular structure has been optimized with the aid of a density functional theory (DFT) method

using B3LYP/6-311G** basis set. Furthermore, Natural Bond Orbital (NBO), Molecular Electrostatic Potential (MEP), Frontier Molecular Orbitals (FMOs), and Mulliken Population (MP) analysis were carried out. All of these analyses were done by using the gaussian 09 software package. Optimized geometrical parameters are in good agreement with the experimental data [1] except for some deflection owing to the molecular environment changes from the solid to the gaseous state. Selected optimized geometrical parameters are shown in Table 1. NBO result reveals the charge transfer from lone pair carbon atom [n2(C12)] toπ^*(C13-N14) with the high stabilization energy 240.94 kcal/mol, which is displayed in Table 2. In comparison with the blue and red region in the MEP map, it is displayed that the electrophilic and nucleophilic region lies within the range [-5.028e^{-2} (red in color) to 5.028e^{-2} (blue in color)], which confirms that the given compound is highly reactive. From FMO analysis, the HOMO-LUMO energy has been noticed to be (-6.8001eV and -2.5021eV) and it proves the hard nature of the compound. MP analysis using DFT, shows that electron density in the phenyl ring carbon atom changes on the molecule upon protonation, it has been shown in Fig 2. Prospectively, the presented optimization results based on the DFT method conclude that the molecule is very stable and biologically active be further used for future research related to biological activities.

Keywords: DFT; NBO; MEP; FMO's; MP

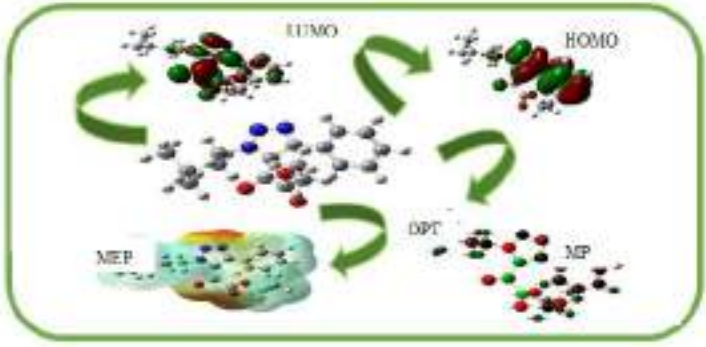

Fig. 1: Complete optimization structures using different methods

Table 1: Selected Optimized geometrical parameters compared with the experimental data

Bond Length	Calc.(Å)	Exp.(Å)	Parameter	Calc.(°)	Exp.(°)
C1-C12	1.469	1.4714	Bond Angle		
C13-C17	1.4642	1.4635	C2-C1-C12	118.9894	120.3515
N14-C29	1.4691	1.4681	C6-C1-C12	122.0128	120.5995
C17-O18	1.2159	1.2115	C12-C13-C17	134.0577	132.9037
C17-C19	1.5424	1.5298	N14-C13-C17	122.2614	122.8906
C19-O20	1.2013	1.1979	C13-N14-C29	130.8664	129.6748
C19-O21	1.3355	1.3209	N15-N14-C29	118.6478	119.4767
O21-C22	1.4575	1.4568	Dihedral Angle		
C22-C25	1.5132	1.4732	C2-C1-C12-N16	36.5251	43.5969
C29-C32	1.5316	1.5238	C6-C1-C12-C13	37.5804	39.6024
C32-C35	1.5399	1.5299	C1-C12-C13-C17	5.6354	10.9806
C35-C37	1.5351	1.5303	C17-C13-N14-C29	-3.9924	-11.9854
C35-C41	1.5361	1.5095	C29-N14-N15-N16	-178.678	-174.404

Table 2: Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Donor (i)	Acceptor (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
σ(C1-C12)	σ*(C5-C6)	2.22	1.25	0.047
σ(C13-C17)	σ*(C12-N16)	0.7	1.2	0.026
σ(N14-C29)	σ*(C12-C13)	1.23	1.31	0.036
σ(C17-C19)	σ*(C13-N14)	3.38	1.09	0.055
σ(C22-C25)	σ*(C19-O21)	2.41	1.02	0.045
σ(C29-C32)	σ*(C13-N14)	1	1.05	0.029
n1(C12)	π*(C13-N14)	240.94	0.06	0.119
n2(O18)	σ*(C17-C19)	21.94	0.62	0.104
n2(O20)	σ*(C19-O21)	30.38	0.65	0.128
n2(O21)	π*(C19-O20)	49.52	0.34	0.116
π*(C13-N14)	π*(C17-O18)	75.95	0.05	0.086

Table 3: Global chemical reactivity Descriptors

E_{LUMO}	-2.5021
E_{HOMO}	-6.8001
Energy gap (ΔE)	4.298
Ionization potential (I)	6.8001
Electron affinity (A)	2.5021
Hardness (η)	2.149
Softness (S)	0.4653
Chemical potential (μ)	-4.6511
Electronegativity (χ)	4.6511
Electrophilicity (ω)	23.2444
Charge transfer (ΔN_{max})	-2.1643

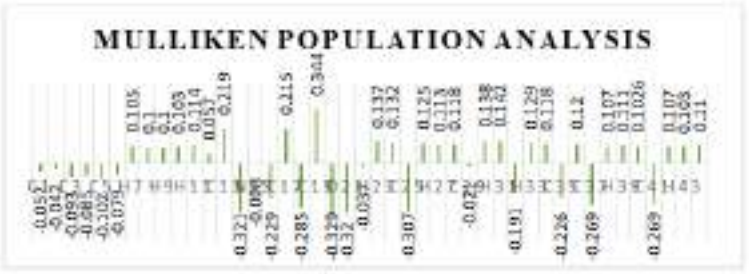

Fig. 2: Graph for Mulliken atomic charges

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OP12

Theoretical and structural investigation of Isopropyl 2- [2-(2,6-dichloroanilino)- phenyl]acetate an anti-rheumatic drug using

density functional theory with the aid of quantum computational methods

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The isopropyl 2-[2-(2,6-dichloroanilino)phenyl]acetate, an anti-rheumatic drug, which is a more potent, less ulcerogenic that replaces diclofenac [1]. The equilibrium geometry of the molecule shown in Fig.1, which is determined using the quantum chemical density functional method at the B3LYP6-31G** level. The calculated results are shown in Table 1. The decrease in $N_{12} - H_{13}$ (0.897Å) bond length states that the molecule has intramolecular hydrogen bonding between $N_{12} - H_{13} \cdots O_{28}$. Calculations were carried out in order to deduce the results of spectroscopic studies such as MEP, HOMO-LUMO and NBO analysis. The important aspects of NBO show that the interaction of $\pi^*(C_1 - C_6)$ and $\pi^*(C_4 - C_5)$ with $\pi^*(C_2 - C_3)$ leads to enormous stabilisation energies of 587.47 kJ/mol and 950.73 kJ/mol, respectively. The electrophilic and nucleophilic attacks have been carried out using MEP surfaces [2]; for IDPA, they are in the range $-4.548e^{-2}\ to\ 4.548\ e^{-2}$ shown in Fig.2. The HOMO-LUMO energy gap, shown in Fig.3, is high (5.0159 eV), leading to the conclusion that the molecule is kinetically stable [3].

Keywords: Diclofenac; Intramolecular; NBO; MEP

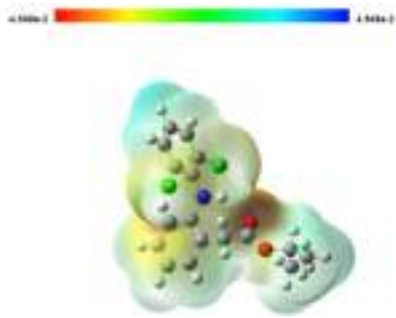

Table 1: Optimized geometrical parameters (DFT) of IDPA

Bond Length/ Å	Calc. Value	Exp. Value	Bond Angle/°	Calc. Value	Exp. Value	Dihedral Angle/°	Calc. Value	Exp. Value
C_1-C_2	1.392	1.381	$C_2-C_1-Cl_7$	118.246	118.09	$C_4-C_5-C_3-C_9$	-0.8842	-0.33
$N_{12}-H_{13}$	1.019	0.897	$C_2-C_3-C_4$	119.774	118.59	$C_8-C_4-N_{12}-H_{13}$	-151.897	-160.04
$C_{24}-C_{27}$	1.412	1.403	$C_4-N_{12}-H_{13}$	115.398	113.60	$C_9-C_8-N_{12}-C_{14}$	63.558	55.08
$C_{27}-O_{28}$	1.220	1.207	$H_{28}-N_{12}-C_{14}$	112.690	113.46	$C_{16}-C_{24}-C_{27}-O_{28}$	61.256	66.16
$C_{27}-O_{29}$	1.341	1.334	$C_{24}-C_{27}-O_{28}$	123.859	123.62	$C_{16}-C_{24}-C_{27}-O_{29}$	-118.857	-113.83

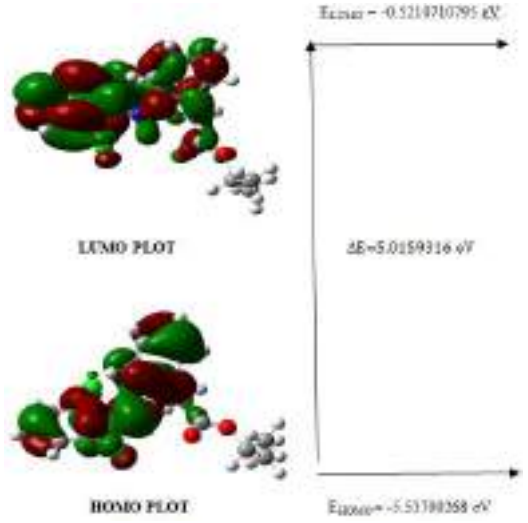

Figure 1. HOMO-LUMO Plot

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OP13

Exploring the influence of tin in micro-structural, magneto-optical and antimicrobial traits of nickel oxide nanoparticles

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Metal oxide nanostructures have gained enormous attention over the past few decades to the research commune due to their superior optical, electrochemical, magnetic, and thermal capabilities [1]. Specifically, semiconducting metal oxide nano-scaled structured binary oxides show intense physicochemical and biological functionalities in systemizing inquest for environmental remedies. Among them, magnetic nanoparticles often encounter novel features that differ significantly from the bulk magnets such as increased coercivity, super paramagnetism, lack of saturation magnetization at high fields, or transitions of the hysteresis loop [2-5].Transition metal oxide nanoparticles, especially nickel oxide (NiO) have profound interests to the scientific commune on account of their dimension-reliant attributes and peculiar progression in optical, electrochemical, and magnetic characteristics. Herein, the undoped and tin (Sn) doped nickel oxide nanoparticles of varied concentrations were synthesized by highly favourable citrate assisted sol-gel technique. An array of extensive investigations were discussed on the structural, optical,

and magnetic properties of synthesized nanoparticles. The crystallite size and strain of as-synthesized samples decreased with significant augmentation in dopant discrepancy which was confirmed by Scherrer and Williamson-Hall model. The optical energy band gap was evaluated from Ultra Violet-visible (UV-vis) spectroscopy analysis and a notable blue shift was observed over the wide absorption spectrum. Refractive index, Urbach energy, and other optical parameters anchored in opto-electrical applications were evaluated from optical studies [6]. Fourier Transform Infrared Spectroscopy (FTIR) analysis conducted at room temperature from spectral span of400-4000 cm^{-1} affirmed the cubic configuration and elucidated bond lengths of pure and tin-doped nanoparticles. Scanning electron microscopy studies portrayed surface morphological features and slight porous particles were observed. Transmission Electron Microscopy (TEM) analysis confirmed the spherical shape of nanoparticles and the grain size estimated is in accordance with the XRD results. The surface area and porosity of pure and doped samples were deeply investigated by Brunauer-Emmett-Teller (BET) analysis. Magnetic parameters such as saturation magnetization, coercivity, retentivity, magnetic moment were enumerated from Vibrating Sample Magnetometer (VSM) investigations and two critical magnetic parameters were extracted from the Law of Saturation to Approach model (LAS).The sample with 6% of Sn shows the highest coercivity of 147 Oe. Further, synthesized pure and doped traces of nickel oxide nanoparticles were deliberated for their competent application in the domain of antibiotics independent antimicrobial activity.

Keywords: NiO nanoparticles; Williamson Hall model; Urbach energy; Magnetic property; Antimicrobial activity

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OP14

Growth and Characterization of 5-Chloro Salicylaldehyde (5CSA) Covalent Molecular Crystals and Study the NLO, EIS Properties for Electrochemical Biosensor Applications

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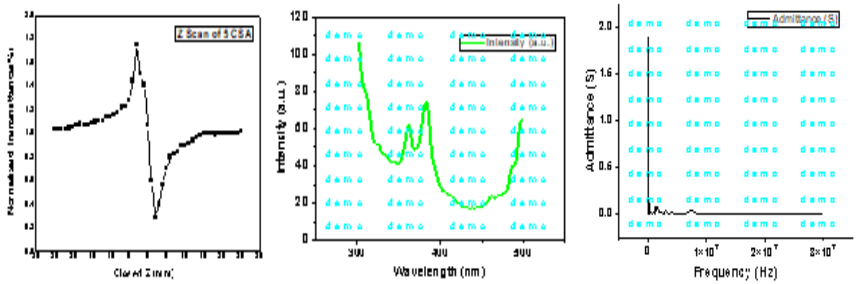
5-Chloro salicylaldehyde with aniline, synthesized and characterized to study the Non-linear optical properties and EIS for Electro chemical Bio sensing applications. The crystals grown by slow evaporation technique. The lattice parameters and crystallinity of the grown crystals estimated by PXRD and single crystal XRD. The optical absorption of the crystal recorded by UV-Vis spectra with lower cut-off wavelength of 563 nm. SHG studies showed emitted wavelength at 532 nm, and the photoluminescence studies showed a violet shift peaks at 384 nm and an energy band gap of 3.21 eV. The LDT analysis gives the observed energy value of E = 75 mJ and the power density for 5CSA crystal is around

12.5 GW/cm^2, which is higher thanurea, L-arginine phosphate, and barium borate. The IR spectral data of the compound reveal the formation of Schiff base ligand with -NH_2 Nitrogen and -OH oxygen atom. The third order nonlinear optical study done by Z scan technique Fig (a) reveals Nonlinear refractive Index n_2 ,3.84x10^{-8} (cm^2/W), absorption coefficient β = 2.11x10 $^{-4}$ (cm/W) and susceptibility (χ^3) = 4.07x10^{-6}esu.The EIS study reveals a high admittance and low impedance at very low frequency, this property leads to impedance biosensing applications.



Fig(a), (b) and (c) Z-Scan of 5CSA Crystal, PL of 5CSA Crystal and Admittance graph of 5CSA Crystal

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OP15

Biomineralization behavior of ternary mesoporous bioactive glasses stabilized through ethanol extraction process

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The development of bioactive implantable materials with multi-functional properties like tissue regeneration, tumor annihilation, anti-bacterial growth and angiogenesis advancement is of great importance. In this context, mesoporous bioactive glasses (MBGs) are gaining tremendous interest in designing the next generation of biomaterials for the bone defect treatment. In this work, ternary SiO_2-CaO-P_2O_5 MBGs have been synthesized by using the acid assisted sol-gel process. In contrast to the conventional process, we adopted an ethanol extraction process to remove surfactant, leading to superior textual properties and high silanol group density in resultant bioglass. Magic angle spinning nuclear magnetic resonance (MAS-NMR) technique has been used to elucidate the presence of different anionic species in the pristine glass samples and its variation with chemical compositions. The vibrational spectroscopy reveals the presence of high concentration of silanol group over the surface of pristine glass samples, which effectively accelerates the formation of hydroxyl carbonate apatite (HCA) layer. The MBG specimens show a good cell viability behavior without toxicity up to the concentration of 20 μg ml^{-1}. In the present results we observed that pore size along with surface area and silanol group density play an effective role in the growth of HCA layer.

Keywords: Mesoporous bioactive glass, Apatite phase, High surface area, Biomineralization

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OP16

Elastic Compliance of Myoglobin at Fluid/Solid Interface in the presence of Surfactants

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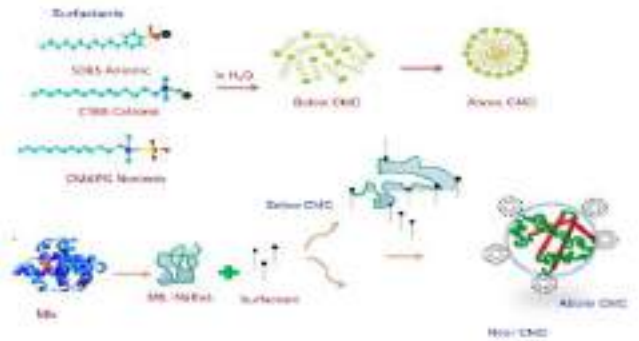
Many biological and chemical processes on earth deal with biomolecules and their interaction with water. The properties of water in biological systems have been studied for well over a century by a wide range of experimental tools, but there are still many hydrations related properties which have not been elucidated. Protein hydration - the perturbation of water structure and dynamics by the protein surface has been a particularly rich source of controversy and confusion [1]. Protein surface hydration is fundamental to its structural stability and flexibility and water plays a crucial role in its biological function. Protein – water interactions thus shape the free energy landscape that governs the folding, structure and stability of proteins. In general, water behaves differently near hydrophilic and hydrophobic groups on the protein surface [2]. X-ray, neutron diffraction, NMR, and femtosecond fluorescence measurements have been used to reveal the binding sites, structure, and dynamics of water near proteins [3]. Our research has been focussing on perturbation of the hydration of proteins using electrolytes, small molecules and surface-active agent (surfactants) [4-6].

In the present study, we analyse varying degrees of hydration of myoglobin (Mb) through its interaction with anionic, cationic and nonionic surfactants below and above their Critical micellar concentration (CMC) using elastic compliance as a tool. CMC an inherent property of the surfactant is used as concentration ballpark. We report a combined equilibrium – kinetic analysis of the interactions between Mb with three surfactants - anionic (sodium dodecylbenzene sulfonate-SDBS), cationic (cetyltrimethylammonium bromide-CTAB) and Nonionic (Dimethylmyristylammoniopropane sulfonate-DMAPS) using UV - Visible, Fluorescence and CD spectral studies. The kinetics of adsorption of Mb to solid surfaces in the presence of the surfactants and its mechanical properties have been studied using Quartz Crystal microbalance with dissipation (QCM-D).



Scheme1- Interaction of the surfactants below and above the CMC with the hydrated Myoglobin

QCM-D has been used to study the mechanical properties of protein and also the role of hydrodynamic water and the changes caused by the presence of surfactants. Depending on the type of surfactant- cationic, anionic and Non-ionic surfactant, the protein undergoes secondary structural changes with cationic surfactant like CTAB and non-ionic surfactant like DMAPS, however these changes are similar and not very dramatic compared to the pure protein. However, with anionic surfactant like SDBS the electrostatic repulsion between the positive surfactant and the negative protein seems to cause changes in the secondary structure as indicated by higher percentage of unordered structure particularly at highest concentration of SDBS (above CMC), 100% β-turn occur and these metastable states shift to unordered state over time. Overall, all properties studied indicate that in the environment of surfactant, its CMC, type of charge on polar head group play a role in determining the extent of hydration. Results from this work suggests that use of surfactants in application with protein, particularly in crystallization will have to take into account the optimal concentration required for crystallizing the biomolecule. This analysis, together with information on the hydration state of myoglobin can be used for designing surfaces of biomaterials.

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OP17

Improved electrochromic performance of potentiostatically electrodeposited nanogranular WO_3 thin films

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The main goal was to build electrochromic (EC) smart windows with large areas, low cost, durability, and multi-functionality to meet various technological challenges. EC nanostructured materials are promising for displays, rear-view mirrors, and smart windows owing to their long cycle life and chemical stability. In this scenario, the potentiostatically electrodeposited WO_3 thin films were used to fabricate an EC device to

eliminate the need for expensive heating or vacuum treatment. Different electrodeposited cycles were evaluated to optimize the structural, morphological, optical, and electrochromic properties. X-ray diffraction showed a small change in the hump intensity on all samples with identical diffraction orientations. Field emission scanning electron microscopy suggested that the deposited WO_3 thin film has a nanogranular morphology composed of many particles. Raman spectroscopy showed that tungsten oxide thin films undergo stretching and vibrational modes to form a pure WO_3 phase. The reversible insertion/extraction of Li^+ ions in WO_3 confirmed its transformation to Li_xWO_3. X-ray photoelectron spectroscopy and energy dispersive X-ray spectroscopy revealed the presence of W and O in the deposits. Moreover, cyclic voltammetry and in-situ transmittance measurements were performed to assess the electrochromic performance of electrodeposited WO_3 thin films using a 1 M $LiClO_4$+PC electrolyte. An electrochromic device, 4×3 cm^2 in size, was fabricated using nanogranular WO_3. The device showed the highest optical modulation (80%), better Li-ion diffusion coefficient (1.71×10^{-9} cm^2 s^{-1}), excellent reversibility (98 %), fast switching time of 3.5s and 6.0s for coloration and bleaching, respectively, and a remarkable CE (98.89 cm^2 C^{-1}).

Keywords: Tungsten oxide; Thin film; Electrodeposition; Nanogranules; Electrochromic Devices; Electrochromic properties

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OP18

Effect of prolonged exposure to traffic noise and elevated Hearing Threshold Level (HTL) - among auto rickshaw drivers in Chennai

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Objectives: The objective of the study is to investigate the risk for noise induced hearing loss in auto-rickshaw drivers and to observe the relation with duration of exposure and hearing threshold at audiometric frequencies.

Introduction: Exposure to excessive sound or noise pollution is a major problem in urban areas. Prolonged exposure to traffic noise leads to elevated hearing threshold among workers, typically affecting higher-frequency hearing which leads to irreversible hearing damage. Early identification and proper awareness of Noise Induced Hearing Loss (NIHL) are very essential to minimize the hearing damage and prevention in hearing health.

Method: We carried a cross-sectional study with total of 98 healthy professional auto-rickshaw drivers aged between 25 and 55 years. Study participants were categorized into three groups by the years of driving experience. Conventional pure tone audiometry (PTA) and extended high frequency audiometry (EHFA) testing were performed from 250 Hz to 16 KHz frequencies.

Results: There was an inclination in the average hearing threshold levels as the function of frequency and driving experience. The higher the driving experience, higher the hearing thresholds. The results indicated that hearing damage of drivers expected to occur sooner at 4 KHz to 8 KHz than damage at lower frequencies in conventional pure tone audiometry. However, the differences were more marked for EHFA especially in higher duration exposure group. Significantly higher threshold levels ($P<0.05$) were noticed for almost all the tested frequencies especially at extended high frequencies of 11.2, 12.5 and 14 KHz.

Conclusion: In this study, we noticed that auto-rickshaw drivers are at risk for the development of hearing loss especially after prolonged duration of noise exposure. This study recommends the need

for awareness, conducting periodic hearing tests, and educating drivers about the harmful effects of loud traffic noise in urban city areas.

Keywords: Noise induced Hearing Loss (NIHL); Duration of exposure; Hearing threshold; Frequencies; Hearing monitoring

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OP19

Wearable thermoelectric generators for Human body heat harvesting

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Wearable thermoelectric generators (TEGs) enable the conversion of human body heat into electricity, which can be utilized to run low power electronic devices in motion detection and healthcare monitoring. This paper presents a novel wearable TEG with 2 pairs of thermoelectric legs to harvest human body heat. The thermoelectric legs are made of P-type Bi_2Te_3 and N-type Co: ZnO coated cellulose fabrics, and are connected electrically in series. The flexible fabric is designed and used as substrate to enhance the flexibility of the TEG for wearable applications. The performances of the TEG, including the bulk thermoelectric legs, are characterized. The electrical conductivity and average Seebeck coefficient of Co: ZnO coated cellulose fabric was $4.80 Scm^{-1}$ and 390.5mV/K. TEG was worn on a human wrist to harvest body heat and

the results show output voltage oscillating from ~0.3mV to ~0.7mV with a different human body temperature varying from 308K to 309.4K. The analysis showed the output generated from the flexible device will be the more suitable for energy harvesting from the human body and can be used in powering electronics and/or sensors by Biomedical sensing applications.

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OP20

Layered Structures of Vanadium Oxide as a Hybrid Cathode Material for Long Cyclable Aqueous Zinc Ion Battery

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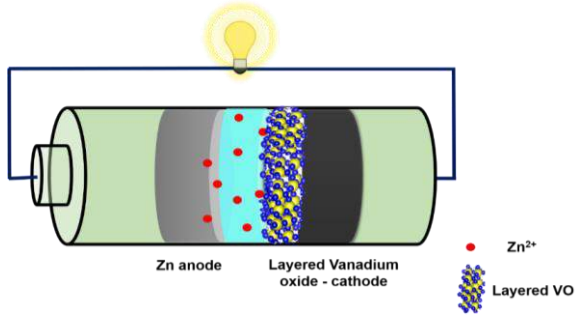
In recent years, aqueous zinc ion batteries (AZIBs) have garnered a lot of attraction due to their eco-friendly nature, low-cost and high safety. But still, there area lot of challenges in developing suitable cathode materials for effective usage in ZIBs. In this work, we have synthesised a layered-like vanadium oxide (V_6O_{13}) flaky structure that provided a large active surface area to the electrolyte and in addition to that the mixed (V^{4+}/V^{5+}) of valence states of V has significantly improved ionic diffusion of Zn^{2+} thereby improving the electrical conductivity of V_6O_{13}. As a result, the AZIBs based on a layered-like structured V_6O_{13} cathode with 1M $ZnSO_4$ electrolyte showed a very high specific capacity of 314 or 392 $mAhg^{-1}$ (0.1 Ag^{-1}) without the addition of any additives or electrode modification. The rate capability and cycle life are investigated at the current density of 2 Ag^{-1} for over 100 cycles and the capacity retention was around 88% and

a coulombic efficiency of 94% even after 100 cycles. Such material with high electrochemical performance can be used for portable electronic devices and electric vehicular applications.

Keywords: Vanadium Oxide; Zinc Batteries; Layered materials; Cathode; High stability.



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OP21

Non-enzymatic detection of uric acid by$CoFe_2O_4$@NF via electrochemical method

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Unhealthy lifestyle leads to a lot of diseases and one such condition is hyperuricemia caused by purine-rich diet [1]. An elevated uric acid (UA) level ≥ 7 mg/dL in blood is termed as hyperuricemia and this condition leads to other diseases such as gout, kidney disease and cardiovascular disease [2,3]. The current need is a diagnosis system which can detect UA so that early diagnosis of the disease can prevent mortality by decreasing the chances for further complications in the human body. Due to the complicated immobilization and the stabilization procedure of enzymatic sensors, non-enzymatic sensors are a better option for precise electrochemical sensing applications. Herein, we have fabricated a combustion derived $CoFe_2O_4$ modified Nickel Foam (NF) electrode for the detection of uric acid. The structure and morphology was analysed through X-ray diffraction (XRD) analysis Field Effective - Scanning electron microscope (FE-SEM) and High Resolution - Transmission Electron Microscope (HR-TEM) while their functional analysis revealed the presence of five Raman active modes of vibration confirming the successful synthesis of $CoFe_2O_4$ nanoparticles. The chemical kinetics of $CoFe_2O_4$@NF was studies by Electrochemical Impedance Spectroscopy (EIS) which was fitted with the equivalent circuit having a solution resistance of 0.076 Ω. Further, the fabricated $CoFe_2O_4$@NF biosensor was found to have an electrochemically active-surface area of 0.141 cm^2. Cyclic voltammetry (CV) for different concentrations of UA was carried out to study the redox mechanism occurring between the electrode and analyte with specific redox peaks. The number of electrons consumed during the anodic process was calculated using Laviron equation. The various electrode characteristics such as sensitivity, limit of detection and the limit of quantification was calculated from the amperometric studies for a wide linear range of detection of 20 μM to 3.6 mM. The oxidation peak arising because of the conversion of UA to allantoin was investigated through Differential Pulse Voltammetry (DPV). The selectivity of the modified electrode was further tested by amperometric method with the addition of common interference found in biological fluids such as glucose, oxalic acid and L-alanine and the results show that the $CoFe_2O_4$@NF electrode depicted good selectivity towards UA.

The results obtained by the currently developed method validate the application of $CoFe_2O_4$@NF electrode for real time application in clinical laboratories for early detection and prevention of diseases associated with hyperuricemia.

Keywords: Biosensors; Non-enzymatic; Uric acid; Hyperuricemia; Sensitivity

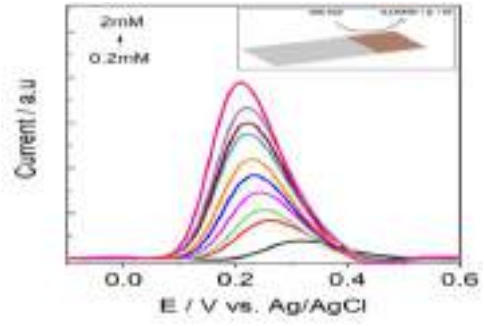

Figure1: UA sensing using $CoFe_2O_4$@NF

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OP22

An experimental Study of Ti_2MnSn Inverse Heusler alloy, inter metallic compound for promising Spintronic applications

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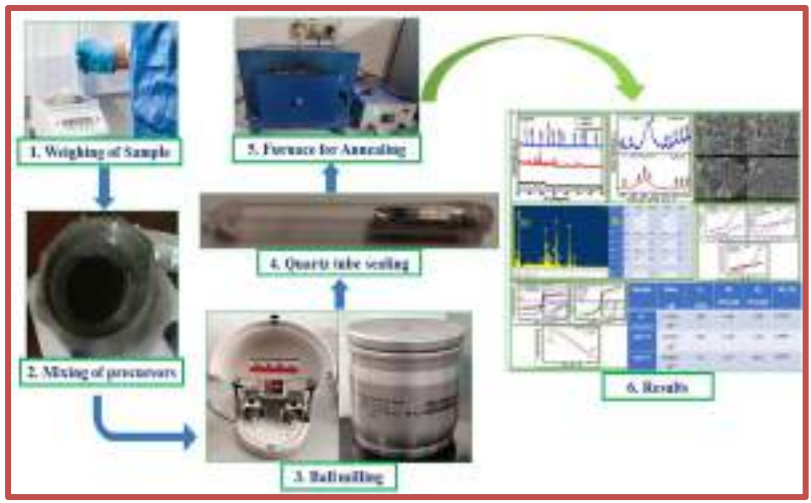
Heusler alloys are highly valued payable because of their relative abundance, mechanical and thermal stability, low toxicity, and potential for use in spintronic applications. Heusler compounds provide a platform for the investigation of innovative physical phenomena such as the thermoelectric effect, magneto-optical effect, magneto-caloric effect, unconventional superconductivity, half-metallicity, magnetic shape memory, significant exchange bias effect, large memory effect, magnetoresistance, and anomalous Hall effect. Herein, we established that Ti_2MnSn inverse Heusler alloy could be attained by automated ball milling synthesis of metal predecessors tracked by annealing. It is revealed that the prepared alloy exhibits the efficient structure (Hg_2CuTi – type Heusler phase) FCC with XA or Xα. The encouragement of dispensation parameters on structural, phase conformation, thermoelectric and magnetic assets of Ti_2MnSn are considered. XRD measurement reveals that the establishment of a face-centered cubic (FCC) super lattice structure with XA disorder was confirmed from the graph for the 1100 ˚C annealed sample.HR-SEM reveals the alloy development of accumulated morphology. The morphological study also absorbed that the particles were shaped by the arbitrary lapping of Ti_2MnSn Heusler alloy nanoparticles. A fundamental examination of the samples is accepted via EDAX spectra (energy dispersive x-ray analysis) which clearly shows that Ti_2MnSn is free from any overseas element. The thermoelectric properties responses as a temperature function show that the investigated alloy displays a high figure of the Seebeck coefficient. Moreover, electrical properties expose that the present alloy has a metal-like behavior. Magnetic properties endorse soft ferromagnetic properties with high saturation and low coercivity. The present study proposes that the Ti_2MnSn inverse Heusler alloy is a potential applicant for spintronics device applications.

Keywords: Ball milling; Annealing; thermoelectric; magnetic; Seebeck coefficient; spintronics



Graphical representation of Preparation of the Ti_2MnSn Inverse Heusler alloy

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Scholar, Department of Nuclear Physics for the useful discussion for Seeback measurements.

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OP23

Immunomodulation by Selenium ImpregnatedNano-Hydroxyapatite for cancer therapeutics

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Cancer, an uncontrollable, malignant disease is a threat to human beings causing millions of deaths worldwide every year. Cancer immunotherapy is an emerging, progressing and promising strategy that has gained popularity in recent decades as a viable therapeutic option for cancer patients with an impressive clinical outcome. A wide range of nanomaterials from synthetic to natural-biomaterial has been explored to improve anticancer immunity. However, concern with regard to potential systematic toxicity limit the extensive application of immunotherapy. Most studies stated that use of nanoparticles enhances the duration of immune response and reduce toxicity when compared to free immunotherapeutic agents. Despite, the adaptability, surface functionalization and tuneable physicochemical properties (size, shape and surface charge) have been successfully harnessed for immunotherapy against cancer. Selenium (Se) are considered as potential immunomodulatory agent as it has formed a great impact on macrophage programming due to the vital role of Se in immune system and successfully proved to induce M1 macrophage polarization which can promote anti-tumour activities of macrophages. Nano-hydroxyapatite (nHAP) with high biocompatibility, immuno-modulatory capacity and

anti-tumour ability could add synergistic therapeutic effect in mitigating cancer. In line with this, we aim to study the immune-modulatory behaviour of nHAP impregnated with Se and will be characterized by XRD, FTIR, SEM. Further, Biocompatibility of the prepared nano-composite was determined by standard haemolysis assay, cytotoxicity assay and protein adsorption by Bradford protein assay. Immunomodulatory studies of the characterised nano biomaterial will be carried out in the near future to optimise it for cancer immunotherapeutic strategies.

Keywords: Nano-hydroxyapatite; Selenium; Cancer immunotherapy; Macrophages; T cells

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OP24

Relaxation Effects on Photoionization Time delay in 2p subshell of Neon gas

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The photoionization of noble gas atoms, being of great importance for both basic research and many applications, has been reported extensively in literature [1-4]. Probing of atomic/ionic systems with an electromagnetic radiation and ejecting out a photoelectron is the process of photoionization. The ejected photoelectrons carry information about the parent atom/ion under study.

The present work reports the study of the effect of core relaxation on the photoionization of 2p subshells of the Ne noble gas atom. The essential dynamical quantity in the photoionization process is the dipole matrix element which is, in general, complex, i.e., a full categorization of the matrix element involves both the magnitude *and* the phase. Three different aspects of the photoionization process are investigated: the partial cross sections, which depend only on the magnitudes of the matrix elements [5]; the photoelectron angular distribution β parameters, which depend on both the magnitudes and the phases of the matrix elements [1], and the Wigner-Eisenbud-Smith (WES) time delays, which depend only on the phases of the matrix elements [6]. These quantities are calculated using the relativistic-random-phase approximation with relaxation (RRPA-R) [7]. In addition, to pinpoint the effects of relaxation in each case, (unrelaxed) relativistic-random-phase approximation (RRPA) [8] calculations are also performed for comparison. In the case of neon, we observe a delayed maximum in 2*p* subshell cross sections due to the presence of centrifugal barrier effects, i.e., shape resonances.

Time delay studies in photoionization processes [9- 10] have stimulated much interest among experimentalists and theoreticians in the last decade as the chronology of the event lies on an attosecond timescale. The study of time delay has major applications in satellite communications. More than a decade ago, the photoionization process was considered to be an instantaneous process without any time delay between absorption of photons and emission of photoelectrons. Schultze *et al.* [11] have determined the photoionization time delay to be 21 ± 5 at to seconds during the measurement of streaking traces from photoionization of neon

2s and 2p subshell [11]. The time taken in the interaction zone is different for electrons originating from different orbitals which are of the order of few attosecond [11]. The experimental time delay was verified theoretically by Schultze *et al.,* using multi-configuration Hartree-Fock method within an independent electron model.

The atomic time delay measured in these XUV/IR two-photon ionization experiments consists of two components: the Wigner-Eisenbud-Smith (WES) component τ_{WES}, and the Coulomb laser coupling component τ_{CLC}, also known as continuum-continuum (CC) coupling. The component τ_{WES} is associated with the XUV photon absorption, and is the focus of our attention in connection with time delay in the present study. Major factors which affect the time delay in photoionization include electron correlation and relativistic interactions, and these interactions influence τ_{WES} strongly in the region of the Cooper minimum, autoionizing resonances, etc. We report, in this work, the dipole photoionization cross section, photoelectron angular distribution parameter, β, and WES time delay for the $2p_{1/2}$ and $2p_{3/2}$ subshells of the noble gas neon using both RRPA and RRPA-R, and compare them to pinpoint the effects of relaxation. The WES photoionization time delay, τ_{WES}, for each dipole channel, is given by $\hbar$ times the energy derivative of phase, δ (E) of the complex dipole matrix element, $\tau_{WES} = \hbar \frac{d\delta(E)}{dE}$

Neon photoionization has been previously studied using various methods to take into account many-body correlations [1, 10]. Isinger *et al.,* [10] have addressed the "7-year old puzzle" spectrally disentangling direct 2s ionization in neon from ionization with shake-up, in which a 2p electron is ionized while a second is excited to 3p state. In the present work, the time delay has been calculated for the 2p subshells of neon using RRPA, and also 'RRPA with relaxation', and compared with the latest experimental results of Isinger *et al*., [10]. The calculated WES photoionization time delays for linearly polarized photons in the direction of the photon polarization for Ne 2*p* is shown in the figure along with the experimental results [10].

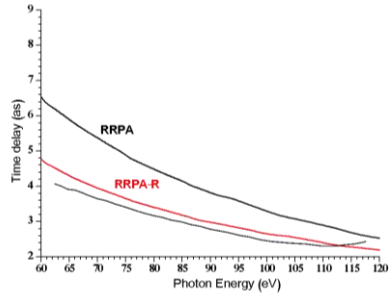

Figure 1: WES time delay for Ne 2p photoionization showing the RRPA-R and RRPA theoretical results along with experiment (dashed line) [10]

In this case, the RRPA-R calculations are seen to be in excellent agreement with the latest experimental results [10] for 2*p* WES time delay in Ne.

Keywords: WES Time Delay of Neon; Photoionization of noble gas atom; Relaxation effect

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OP25

Structural, morphological and electrical properties of Aurivillius $Bi_4Ti_3O_{12}$ and Perovskite $Bi_{0.5}Na_{0.5}TiO_3$ ferroelectrics

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Ferroelectric oxides belong to different families like perovskites, pyrochlores, illmenites, layered perovskites and Aurivillius structures. These ferroelectric materials havea wide range of applications in sensors, actuators and memories. Lead zirconate titanate (PZT) is an ideal ferroelectric material, however, its low curie temperature and toxicity of lead reduce its technological applications. The demand for high Tc and nontoxic oxide ferroelectric materials increases further interest. Bismuth-based ferroelectric materials like Aurivillius $Bi_4Ti_3O_{12}$ (BIT) having Curie temperature of 675°C and perovskite $Bi_{0.5}Na_{0.5}TiO_3$ (BNT) are potential candidates for lead-free ferroelectric materials. The BIT and BNT compounds have been synthesized by the 'solid state ball milling with subsequent sintering' method using the stoichiometric ratio of suitable precursors Bi_2O_3, Na_2CO_3, and TiO_2.The thermal behaviour of the prepared compounds is studied by Thermogravimetric and Differential Thermal Analysis (TG & DTA).Two major weight loss behaviour is seen, the first one around 100°C related to the dehydration of hydrated molecules and the second one related to the degradation of precursor compounds. There is no weight loss above 600°C in BIT and above 800°C in BNT confirming the phase formation.

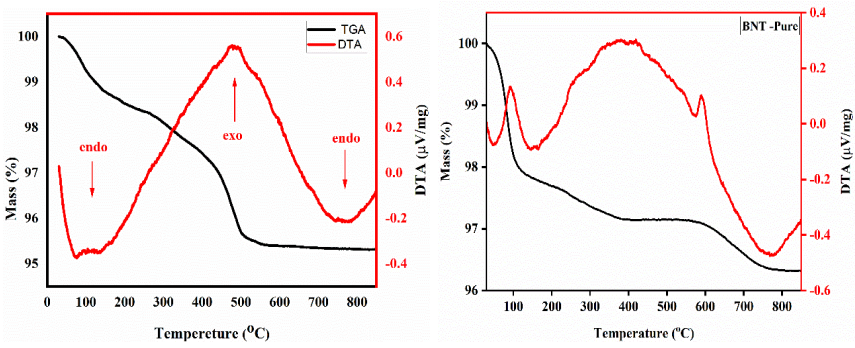

Fig1: Thermogravimetric and differential thermal analysis plots of BIT and BNT compounds

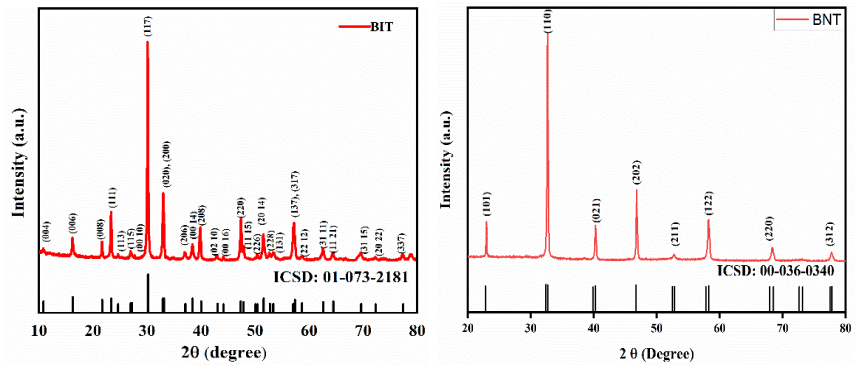

Fig2: X-ray diffraction plots of BIT and BNT compounds

BIT and BNT compounds analysed by X-ray diffraction, shown in figure 2, are characteristics of the single-phase 'BIT with Orthorhombic structure' and 'BNT with Rhombohedral structure' comparable with the ICSD data file No: 01-073-2181 and 00-036-0340 respectively. The average crystallite determined using Scherrer's formula is 24nm for BIT and 34nm for BNT.

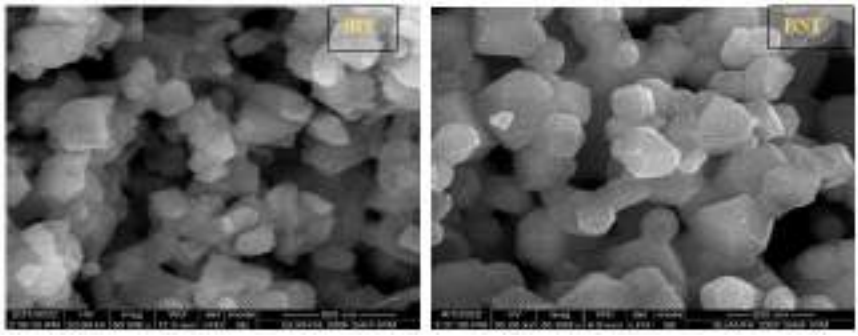

Fig3: HR-SEM images of BIT and BNT compounds

Surface morphology images of BIT and BNT obtained through High resolution scanning electron microscopy show homogeneous spherical-like particles.

Dielectric studies show the variation in dielectric constant with frequency and low dielectric loss at the higher range of frequencies.

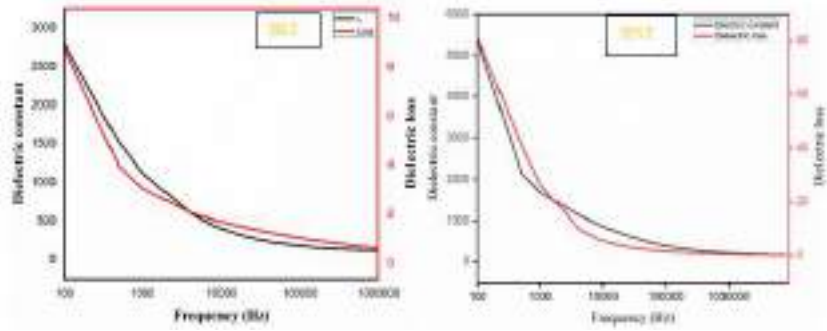

Fig4: Dielectric graph of BIT and BNT compounds

References:

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OP26

Development of Firmware for Interfacing of Underwater Inductive Modem (UIM) to the Moored Buoy Data Acquisition System

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Oceans have a significant impact on the global weather and climate patterns. The vast open ocean's isolation has made it difficult to continuously observe them earlier, but now being synchronized by in-situ and satellite-based observations. In-situ observations includes meteorological, sea surface and subsurface observations [1]. These real-time observations are necessary for precise forecast of climate variability, weather predictions, ocean state, seasonal and annual monsoons. Subsurface observations can be carried out through various communication modes like, serial cable, acoustic, optical, and induction, where cable and optical communications are limited to a small range. The acoustic communication is broadly used for underwater communication but is comparatively slower, expensive, requires more power and bulky hardware. This communication is also greatly affected by the transducer orientation, surrounding acoustic noise and communication being limited to the single instrument at a time. Therefore, according to today's advancements inductive modem technology offers a solution that is practical, affordable, dependable, and flexible, enabling to communicate multiple sensors at a time. Also, provides accurate real-time data through sub-surface data transmission

[2]. The Ocean Observation system of National Institute of Ocean Technology, India, maintains OMNI (Ocean Moored Buoys in the Northern Indian Ocean) buoy network (Fig.1) comprising of 12 buoy systems that measure surface meteorological parameters along with temperature and salinity profile measurements at discrete levels up to 500 m [3].

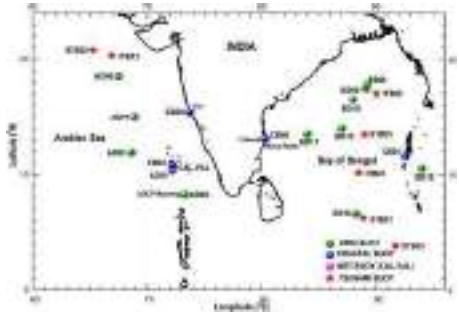


Fig.1 Indian Moored buoy network

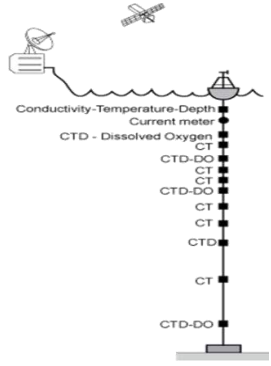
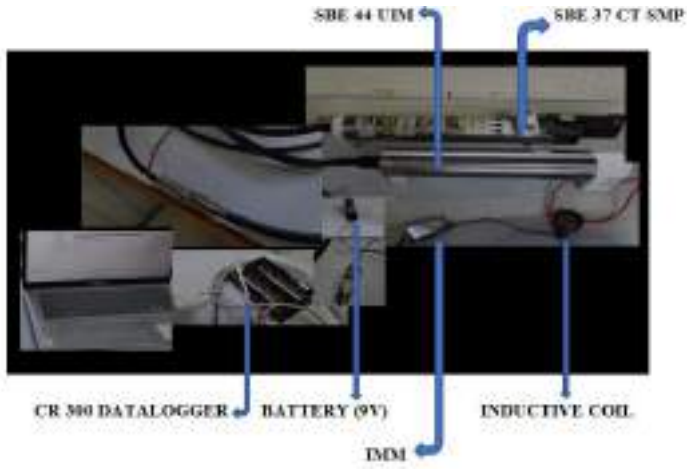


Fig.2 Inductive mooring

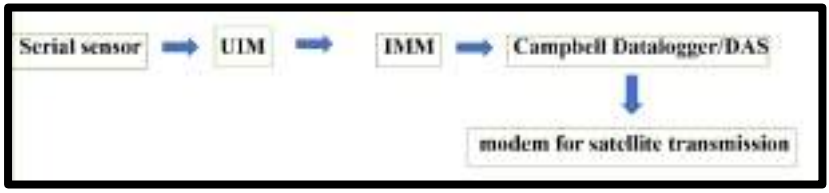
Communication is through a 500 m induction cable connecting CT (conductivity and temperature) sensors to the buoy data logger through a Surface Inductive Modem (SIM) or Inductive modem module (IMM) (Fig.2). An Underwater Inductive Modem (UIM) [4] is used to connect any serial sensor to the inductive cable. The main objective of this study

is to develop a firmware for Interfacing of UIM to the Moored Buoy Data Acquisition System. A firmware is developed by using CR basic command language and embedded in the Campbell Scientific datalogger [5]. The firmware is also successfully tested in the lab environment by using SBE 44 Underwater Inductive modem (UIM) and SBE37 SMP CT sensor [6] to retrieve data (Fig.3).

Fig 3. Experimental setup



BLOCK DIAGRAM:



Keywords: Underwater communication; In-situ Observation; Sub-surface data transmission; Moored Buoy; Data retrieval

References:

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[4]SBE 44 UNDERWATER INDUCTIVE MODEM with RS-232 Interface for Serial Instruments- https://www.seabird.com/asset-get.download.jsa?id=54627862503
[5]https://s.campbellsci.com/documents/au/manuals/cr300.pdf - CR 300 Product Manual (Campbell scientific datalogger)
[6]SBE 37-SMP Micro CAT C-T (P) Recorder-Conductivity, Temperature (pressure optional) Recorder with RS-232 Interface and integral Pump- https://www.seabird.com/asset-get.download.jsa?id=54627862349

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OP27

Co-precipitation synthesis of guava leaf extract bio-templated ZnO – CuO nanocomposite and its antimicrobial activity

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With a mounting rise in the nanotechnology domain, the search for materials that offer multi-functional properties for an advanced and wide range of applications in all realms is highly promising. The most pivotal word that is materializing today is green synthesis. This surfacing technique is opening ideas and opportunities for applications in the biomedical field in realms such as early detection of diseases and is also being much preferred because of its cost effective and eco-friendly nature. The present report is on the synthesis of ZnO, CuO and ZnO-CuO pure and bio-templated nanocomposite by the method of co-precipitation. The as-synthesized materials are characterised by XRD

studies. The crystalline structure and the lattice parameters are confirmed by XRD study and then was characterised by SEM with EDAX in order to study about the structural morphology and size of synthesized metal oxide composite and finally with FTIR to study about compound and amount of compound present in the sample from IR spectrum. Antibacterial study was done to determine the efficacy of the prepared sample on various microbes. The antibacterial activity of the as-synthesized materials against pathogenic bacteria were analysed which would find applications in the development of new antibacterial drugs.

Keywords: Guava leaf; Nanocomposite; Antimicrobial activity; Co-precipitation

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OP28

Permittivity and Loss Tangent of Barium Magnesium Tantalate at Low Frequencies

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The permittivity and the loss tangent of Barium Magnesium Tantalate ($BaMg_{1/3}Ta_{2/3}O_3$) are studied at low frequencies. A pure phase

$BaMg_{1/3}Ta_{2/3}O_3$ is grown by solid state reaction method. This is done by ball-milling the precursors and then calcining at 1400°C for 5 hrs. The calcined powders are grinded and pelletized at a pressure of 210 kg/cm^2. The observed pellets are sintered at 1500°C for 5 hrs. The phase identification is made by X-ray Diffraction and morphology studied is carried out by Scanning Electron Microscope. The real and imaginary part of permittivity and the loss tangent measurements are done at low frequencies (< 10^3 Hz).

Keywords: $Ba(Mg_{1/3}Ta_{2/3})O_3$; Permittivity; Loss tangent

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OP29

Synthesis of Pure and rare earth doped Bismuth Vanadate ($BiVO_4$) Nanoparticles for efficient Photocatalytic Application

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Because of industrial revolution and urbanization, water pollution has been increasing exponentially and its effects on humans and other living organisms are acute [1]. Continuous contamination of water resources by the release of untreated effluents from factories, organic dyes from textile industries and also contamination by infectious microorganisms have been a threat to aquatic ecosystem.

Organic dyes have a slow degradation rate under normal atmosphere and its presence on water bodies restricts penetration of sunlight into water for longer time period. Semiconductor based photocatalysts can degrade the organic dyes completely. Because of its utilization of solar energy as driving force, photocatalysis is green friendly, economical, clean and renewable waste water treatment method.

Bismuth Vanadate is visible light responsive photocatalytic material. $BiVO_4$ nanoparticles are employed for photocatalytic dye degradation because of their high surface to volume ratio, high diffusivity, high reactivity, excellent dispersibility and low cost. From the sun, the Earth surface receives about 5% ultraviolet light and 45% visible light [1]. $BiVO_4$ has an advantage of utilizing the entire region of visible light from the solar spectrum due to its narrow band gap of 2.4 – 2.8 eV. Doping of Photocatalytic material will increase the efficiency or photodegradation rate of the organic dyes.

Pure and rare earth doped $BiVO_4$ was synthesized via chemical precipitation method by taking bismuth nitrate pentahydrate and ammonium metavanadate as precursors. The structural, optical and morphological studies on pure and rare earth doped bismuth vanadate was carried out using powder XRD, UV-Visible spectroscopy and Scanning Electron Microscopy. The lattice parameters and particle size was calculated using X-Ray Diffraction. From UV-Visible spectroscopy, the optical band gap of the samples was calculated. Surface morphology was observed in SEM and the photocatalytic studies were also carried out. The reports will be presented in detail.

Keywords: Photocatalysis; $BiVO_4$

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OP30

Synthesis of Metal Nanoparticles for Cell Enhancement

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Metal nanoparticles are being used in various industries like food, textile, agriculture, cosmetics, and coating. In recent years, metal nanoparticles have shown a number of properties and it has opened numerous new pathways in the field of medicine. Metal nanoparticles like gold, silver, palladium, titanium, and zinc possess enhanced optical properties and unique characteristics like surface plasmon resonance. These properties have enabled them to be used for several biomedical applications like anticancer, antifungal, antibacterial, drug delivery, enhancement in radiotherapy, diagnosis, and many others.

In this report, a few metal nanoparticles have been synthesized using the method of chemical reduction in order to investigate the cell enhancement and biocompatibility of the nanoparticles. Characterization techniques such as UV, Raman, FTIR, and Fluorescence were carried out. As a result, the response of the cell lines on the injection of metal nanoparticles will be studied.

Keywords: Nanoparticles; Cell enhancement

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Poster Presentations

PP1

A Review on improved performance of Flexible Supercapacitors by using $SiTiO_3$ and $NiCo_2S_4$ electrodes

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A super capacitor is a specially designed device which has a very large capacitance; it combines the properties of capacitor and battery into one device. The development of modern electronic industries has put forward high requirements for flexible energy storage systems. At this point flexible supercapacitors attract much attention due to its unique advantages like long cycle life, high power density and fast charging or discharge speed etc. Research shows that the performance of flexible supercapacitor can be improved by using suitable electrode materials such as, Strontium Titanate ceramic films, MoS_2 nanosheets, $NiCo_2S_4$ nanosheets, MnO_2 nanoflakes, ultra large graphene sheets and vanadium dioxide etc. Here we will be reviewing about two such materials that can be used as electrodes. Firstly, we begin with $SrTiO_3$ which is considered as a potential energy storage material because of its good electrical conductivity properties and oxygen vacancy structure; when it's doped with ceramic films, they give good electrochemical performance and excellent specific capacitance of 2895 mF cm^{-2} at 3 mA cm^{-2}. Recently, $NiCo_2S_4$ has been extensively researched as a promising pseudo capacitor material and the reviewed result shows that $NiCo_2S_4$ nanosheets delivers the best performance with specific capacitance of 2.98 Fcm^{-2} at 1 mA cm^{-2} and a good cycling stability and when fabricated on activated carbon they possess good energy density. High performance flexible supercapacitors are getting upgraded day by day, by altering the electrode material and improvising the performance. It is still under research and let's hope to find a masterpiece in the near future.

Keywords: Flexible Supercapacitors; Electrochemical performance; electrodes; Energy density; Specific capacitance; Oxygen vacancy; Doping

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PP2

Synthesis and Characterization of ZnS thin films by Chemical bath deposition

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ZnS thin films were deposited on the glass substrate by CBD technique under our optimized conditions. From the several attempts made on the fabrication of ZnS thin films, the present optimized chemical bath conditions showed better structural and surface characteristics. The films' structure was basically amorphous or microcrystalline. After annealing, the main diffraction peaks due to ZnS (111) planes correspond to sphalerite-type ZnS. The particles on the film's surface were almost spherical and homogeneous, and there were some white spots. The resistance of the ZnS films without annealing, reduced with the increasing concentration of $ZnSO_4$.

Keywords: XRD; Solvothermal; ZnS particles

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PP3

Effect of capping agent on Tin Sulfide Nanoflower by Solvothermal method

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In this study we synthesized orthorhombic SnS nanoflower with the well - crystallized morphologies as solid flower particles via solvothermal method. The synthesized samples were characterized with UV, XRD, FTIR, PL, DLS and SEM. The SnS nanoflower structured particles have been solvothermal synthezised by using thiourea and $Sncl_2.2H_2O$ as raw materials and the solvent ethylene glycol with addition of capping agent acetic acid. The effect of capping agent on SnS nanoparticles change it morphology from sphere to flower with the size reduction of the particle.

Key Words: SnS; XRD; SEM

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PP4

Vibrational analysis and Quantum chemical study of 2,6 -Bis thieno Benzene -3- enyl-3,5- dimethyl –N-Methyl Piperidin -4-one by HF and DFT method

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In this study, we are examining vibrational, electronic and structural specifications of molecule 2,6-Bis thieno Benzene -3-enyl-3,5-dimethyl-N-Methyl Piperidin-4-one by HF and DFT method using 6-311G and 6-311++G basis sets. In the investigation of Molecular structure, the Geometrical parameters are tabulated based on the position of each atom. For analyzing molecular vibrations, the HF frequencies and the vibrations are observed and tabulated by the periodic motion of atoms. The UV analysis investigates the electronic transition of the molecule in solvent and comparing the values of excitation energies, absorption wavelength, and oscillator strength for variable excitation states and tabulated. In the HOMO-LUMO analysis, the homo lumo energy gap is obtained. In the NBO analysis, the stabilization energies are tabulated

and these energies are explaining intermolecular hydrogen bonding, intermolecular charge transfer and delocalization of electron density. The mapped ESP and ETD are differentiated the atoms by different colours. Thermodynamic parameters and the NLO parameters are calculated by HF method.

Keywords: HF; DFT; basis sets; HOMO-LUMO; NBO

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PP5

The dark story into White future

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Henri Becquerel presented the discovery of radium by Pierre and Marie Curie at the Paris Academy of science. One century later, radium has been abandoned, mainly for radiation protection difficulties. Hidden story of "Radium Girls", the women who fought for their lives in a killer work place. Guns can be used to commit crime, or stop it similarly radiation cause cancer but it is also used to treat it. Radiation therapy is efficacious for the treatment of many cancers. These technologies have provided the ability to increase radiation conformality precision, improving the outcomes for many radiation therapy patients. Radiation therapy can be used in combination with surgery and/or chemotherapy. The history of discovery and medical use of radium.

Keywords: Radium Girls; Radiation; Radiation therapy; Chemotherapy

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PP6

Growth and Characterization of N-Benzoyl Glycine Single Crystals for Optical Application

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Optically good transparent single crystals of N-Benzoyl glycine with dimension of 20 x 15 x 5 mm^3 were grown by slow evaporation solution growth technique at ambient temperature. It crystallizes in an orthorhombic system with space group $P2_12_12_1$. The functional groups were identified using FT-IR spectral analysis. The optical transmittance of the grown crystal was determined by using UV-Vis-NIR spectral analysis and it has good optical transparency in the entire visible region. Lower cut off wavelength was observed at 304 nm, it shows direct allowed transition with optical energy band gap of 4.07eV and the linear refractive index of the grown crystal was found to be 1.3703. Optical constants such as extinction coefficient and optical conductivity were calculated. The band tail energy of the grown crystal was analysed. The electronic polarizability of the grown crystal was calculated. The laser damage threshold value was tested and it was 1.8 GW/cm^2 for the title compound by using Nd:YAG laser. The second harmonic generation was tested by Kurtz-Perry powder technique and efficiency is higher than the standard potassium dihydrogen phosphate (KDP) crystals.

Keywords: Single Crystal growth; Spectral analysis; UV-Vis-NIR analysis; Laser damage threshold; SHG

Introduction

The nonlinear optical (NLO) properties of large organic molecules and polymers have been the subject of extensive theoretical and experimental investigations during the past two decades [1]. The organic NLO materials play an important role in second-harmonic generation (SHG),

frequency mixing, electro-optic modulation, optical parametric oscillation, optical bistability, etc [2]. N-Benzoylglycine is an organic compound with molecular formula $C_9H_9NO_3$ .It crystalizes in orthorhombic system with space group $P2_12_12_1$. It is an excellent crystal for second harmonic generation because of its high conversion efficiency [4]. In the present work, we have grown a good transparent single crystals of N-Benzoyl glycine by conventional method. Further it was confirmed by single crystal X-ray diffraction analysis [3]. Optical studies used to measure optical constants [5] and laser damage threshold [6] used to estimate optical tolerance of the title compound. Second Harmonic Generation (SHG) was confirmed that the material exhibits non-linear optical behavior.

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PP7

Spectroscopic Characterization of an Oxime derivative 2-Hydroxy-2-Phenylacetophenone Oxime using Quantum Computational methods

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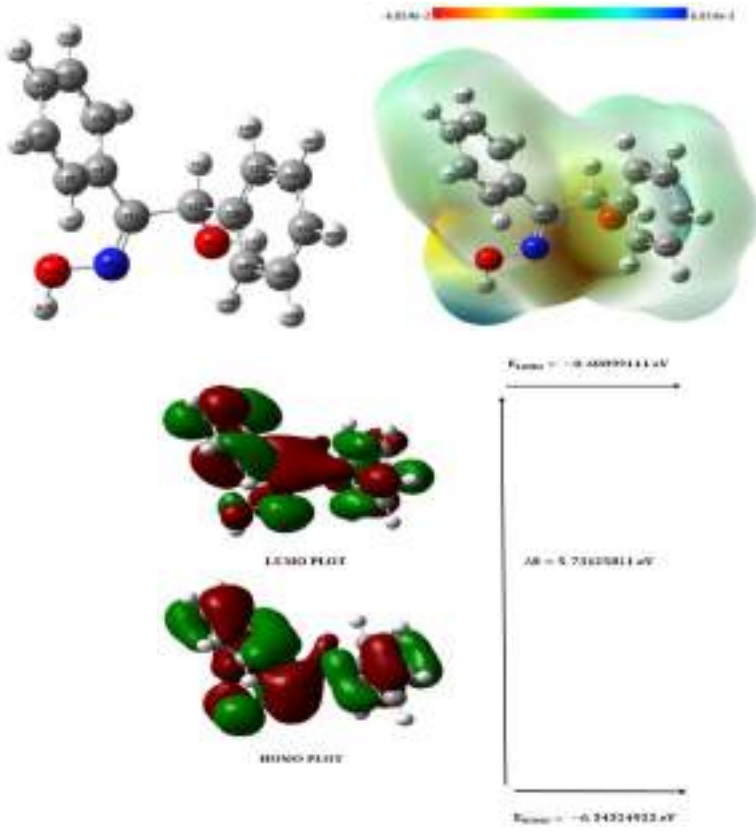
The titled compound, 2-hydroxy-2-phenylacetophenone oxime (2H2PO), is an oxime derivative used in industry, agriculture and medical instrumentations for the detection and determination of Cu, Mo, and W as well as in the extraction of tantalum, vanadium, and tungsten as chelating agents [1]. The molecular structure parameters and spectroscopic properties of 2H2PO is elucidated theoretically by B3LYP method using 6-31G** basis set. The optimised geometry of 2H2PO is shown in Figure 1. The structure shows two phenyl rings interlinked with an oxime group and a hydroxyl group oriented at a dihedral angle of 79.643A0. The theoretical and experimental values were compared, and their deviations are tabulated in Table 1. The Natural Bond Orbital analysis shows a maximum stabilization energy of 188.406 kJmol-1due to the strong intramolecular hyperconjugative interaction of *(C12-N13) with *(C4-C5) which decreases the electron density (0.357e) at *(C4-C5). The Homo-Lumo plot is shown in Figure 2.The band gap energy of one electron excitation from Homo to Lumo is calculated to be about 5.734 eV, which results in the good kinetic stability of the molecule [2]. Figure 3 shows the MEP plot of 2H2PO ranging from-6.814e^{-2} to 6.814e^{-2}, from which we conclude that the highest electronegative oxygen atom in the O-H group behaves as the electrophile region and the hydrogen atom behaves as the nucleophile region, and the region over the rings is neutral. These regions give information about intermolecular interactions [3].

Keywords: DFT; NBO; Homo-Lumo; MEP

Table 1: Optimized geometrical parameters of 2H2PO

Bond Length (A0)	**Calc. Value**	**Exp. Value**	**Bond Angle** (A0)	**Calc. Value**	**Exp. Value**
C4-C5	1.403	1.388	C4-C5-C6	118.729	118.05
C5-C12	1.490	1.482	N13-O14-H15	101.396	109.49

C12-N13	1.283	1.276	C17-O18-H19	106.681	109.33
O14-H15	0.967	0.882	**Dihedral Angle (**A0)		
C17-C20	1.528	1.513	C5-C12-N13-O14	1.733	1.00
C17-O18	1.419	1.423	C5-C12-C17-C20	79.643	74.68
O18-H19	0.967	0.825	C20-C17-O18-H19	-44.703	-53.07



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PP8

Identification of Bioactive Constituent from Methyl 18-methyl nonadecanoate

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The green synthesis of Methyl 18-methyl nonadecanoate taken from the methanol extract of calotropis gigantea flowers. FT-IR spectrum have given the active absorption of Infra-red spectra by theoretical values. The UV-Vis absorption analysis reflects the nature of charge transition, its position through experiment and calculated absorption peaks. The (HOMO) Highest Occupied Molecular Orbital and (LUMO) Lowest Unoccupied Molecular Orbital analysis reflects the charge transfer within the molecules. The energy sign transfer within the molecules confirmed in molecular electronic potential (MEP). The atomic charge have been calculated using Mullikan population analysis. The Density functional theory (DFT) used to investigate all the electronic structure of many body systems like atoms or molecules.

Keywords: FT-IR; HOMO; LUMO; MEP; DFT

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PP9

Study of $LiCoO_2$ Cathode materials for rechargeable Lithium ion batteries

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The Li-ion battery market is undergoing rapid expansion, as portable electronic devices demand a higher energy density and better cycle life. The conventional $LiCoO_2$ cathode materials have excellent electrochemical stability, good discharge capacity, longer cycle life, and high energy density, retention ratio, etc. The present investigation deals with synthesis of $LiCoO_2$ cathode materials for Lithium ion batteries using sol-gel method with citric acid as chelating agent. The $LiCoO_2$ gel precursor was studied by TG-DTA, and then it was calcined at different temperatures in the range 400-800ºC. The prepared samples crystalline structure, surface morphology and composition of the elements were analyzed using XRD, FTIR, and SEM with EDX. The SEM picture of 700ºC–$LiCoO_2$ powder revealed hexagonal structure with homogeneous and submicron particles of narrow size distribution.

Keywords: Rechargeable Battery; XRD; FTIR; SEM; EDX

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PP10

Biosynthesis of pure and Silver doped Nickel oxide nanoparticles using *Moringa oleifera* flower extract and their potential antimicrobial application

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The synthesis of pure and silver doped nickel oxide nanoparticles were prepared by green synthesis method using aqueous flower extract of *Moringa oleifera* Lam. The flower extract of *Moringa oleifera* flower contains various bio-active chemical components and so it is used as a strong reducing, stabilizing, and capping agent in the synthesis of pure and silver doped nickel oxide. The synthesized nanoparticles were characterized by various techniques like XRD, UV-Vis spectra, SEM, EDAX and FTIR spectroscopy. The XRD pattern confirms the very good crystallinity of the material and the average crystalline was found to be in the nanometer range(1-100nm) and it belongs to rhombohedron structure. The morphology of samples were studied using SEM analysis and shows spherical shape with agglomeration matrix and the presence of elements were confirmed by EDAX. FTIR study was carried out to identify the functional group present in the prepared samples extensively. The UV-Vis absorption spectra used to calculated band gap values for the synthesized nanoparticles. The antibacterial study reveals that both synthesized samples shows good antibacterial activity on both gram positive and gram- negative organisms. Hence the synthesized silver doped NiO nanoparticles can be used for biomedical applications.

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PP11

Biomaterials - A restoring function

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Biomaterials are widely used to formulate artificial organs. Biomaterials can be adopted from nature or prepared in the laboratory by using different chemical processes with incorporation of metals like polymers, ceramics or composite materials and used in medical applications as an

augment, or replacer of natural function. Biomaterials are mostly applied in Joint replacements, dental applications, Blood vessel prostheses, drug delivery, vascular grafts, Stents, Nerve conduits, contact lens and in surgery as transplant material. Cell therapy is a new and emerging approach to the repair of a damaged heart. Tissue engineering can create cardiac patches, modified and seeded with bone marrow or mesenchymal stem cells to form a near-natural repair. Natural and synthetic biomaterials are being explored in this area as well. Chitosan and fibrin are instances of natural hydrogels, while polyvinyl alcohol is a synthetic one. These are used to convey therapeutic cargo, including genetic material, proteins or cytokines, in order to treat cancers, autoimmune diseases and inflammatory airway disease.

Keywords: Artificial organs; Cell therapy; Hydrogels; Tissue engineering

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PP12

Photocatalytic Activity of Biogenic Synthesized Nickel Oxide (NiO) Nanoparticles using Catharanthus roseus Leaf Extracts

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Green synthesized catalysts serve as a sustainable technology for removal of organic pollutants by advanced oxidation processes (AOPs) in wastewater treatment [1]. An eco-friendly biosynthesis of photocatalytically active nickel oxide (NiO) nanoparticles (NPs) using the bioactives *Catharanthus roseus* leaf extracts, which acts as reducing agent and acts as a template for the biogenic synthesis of NiO NPs [2,3]. *Catharanthus roseus* belonging to Apocynaceae family is an important medicinal plant that contains the indispensable bioactive anti-cancerous

drugs like vincristine and vinblastine. The synthesized NiO NPs were characterized by various analytical and sophisticated techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS), Transmission electron microscopy (TEM). The synthesized NiO NPs were highly active towards the photocatalytic degradation of methylene blue (MB) dye with an efficiency of 98%. The NiO NPs show excellent stability and reusability up to 3 cycles without significant loss in the efficiency.

Keywords: Biogenic Synthesis; *Catharanthus roseus*; Nickel Oxide Nanoparticles; Photocatalysts; Methylene Blue

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PP13

Hydrothermally synthesized transition metal (Co, Ni) doped MoO_3 nanoparticles electrode for Supercapacitor application

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In this work, we have synthesized MoO_3 (MO), cobalt doped MoO_3 (CMO) and nickel doped MoO_3 (NMO) nanoparticles via hydrothermal method. The structural, morphology and electrochemical properties of the as-prepared samples were analysed through powder X-ray

diffractometer (XRD), Raman spectrometer, Fourier transform infrared spectrometer (FTIR), scanning electron microscopy (SEM), Energy-Dispersive X-ray spectroscopy (EDAX) and transmission electron microscopy (TEM). XRD confirmed the formation of monoclinic MoO_3, cobalt doped MoO_3 and nickel doped MoO_3 nanoparticles with an average crystalline size of 48.9nm, 39.7nm and 25.6nm respectively [1]. The nanorod-like morphology was observed for the nickel doped MoO_3 nanoparticles [2]. The electrochemical performance of the electrode materials MoO_3 (MO), cobalt doped MoO_3 (CMO) and nickel doped MoO_3 (NMO) nanoparticles was analysed using cyclic voltammetry (CV), Galvanostatic charge-discharge (GCD) and electrochemical impendence spectroscopy (EIS). The result showed that the addition of Co and Ni ions enhanced the rate of electrochemical behaviour. The high specific capacitance value of 258.38 F/g at the current density 0.5 A/g, was obtained for Ni doped MoO_3 (NMO) and its capacitive retention of 99.79 % over 5000 cycles was achieved in GCD cyclic performance at the current density 10 A/g infers the high stability of the prepared electrode material.

Keywords: Asymmetric supercapacitor; Hydrothermal method; Metal oxides; Nanorod; Specific capacitance

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PP14

Review on influence of electrolytes on fabrication of Titania Nanotubes via Anodization and its Photocatalytic application

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This study examined numerous articles of various electrolytes used in the anodization procedure to fabricate titanium dioxide nanotubes (TiO2 NTs). The properties of nanotubes, such as length, thickness, pore diameter, pore size, etc., are revealed by the fundamentals of different electrolytes. On these electrolytes, the effects of fluoride ions and water content were investigated. Taking into account the effects that other variables have on the titania nanotubes' form. Titanium dioxide nanotubes are beneficial for many different purposes, including hydrogen production, biomedical research, self-cleaning, air and water purification, antibacterial activities and many other applications as photocatalytic behavior.

Keywords: Anodization; Electrolytes; TiO_2; Morphology; Photocatalyst

Introduction

Nanotechnology is increasingly becoming the foundation of modern progress. Every application is in the hands of nanotechnology to an infinite extent. It is making progress in several areas, including the production of fuel, effective power sources, healthcare, natural preservation, security, and privacy. Depending on their shape, physical, chemical, and size, we are surrounded by several types of nanoparticles, such as ceramic, carbon-based, metallic, semiconductor, polymeric, etc. Therefore, these 1-100nm materials can power the environment around us. Nanotubes, a type of one-dimensional nanoscale material, are very useful in many fields, including magnetism, electronics, and catalysis. Work in nanotechnology based on nanotubes is currently quite active.

Carbon nanotubes were the foundation of early research. Over time, new materials for creating nanotubes started to appear. Such a substance with a variety of qualities is TiO_2. These are widely used in H-generation [1], solar cells [2], water treatment [3], CO_2 reduction [4], sensors [5], etc. because of their capabilities such as nontoxicity, wide bandgap, biocompatibility, photocatalytic ability, unique electronic and ionic properties, and high surface area. Titanium dioxide (titania) NTs can be fabricated by using different methods like sol-gel [6], the hydrothermal method [7], physical vapour deposition [8], and chemical vapour deposition [9]. Electrochemical anodization can also be considered a low-cost, effective facile method for the development of titanium dioxide nanotubes. The self-ordered TiO_2 nanotubes were initially discovered in 1999, by Zwilling et al., [10], by electrochemical anodization. He adopted fluoride-containing electrolytes for the formation of these nanotubes. Various electrolytes such as HF, NH_4F, NaF, formamide, Na_2SO_4, etc. are currently being used in this research. These electrolytes determine pore size, spacing, length, thickness, and diameter for NTs. Many other parameters also affect the morphology of titania: time, voltage, electrodes, temperature, pH value, etc.

These efficient titania nanotubes can be used in a variety of nanotechnology fields. Titanium dioxide nanotubes, which play a significant role in waste-water treatment applications, are the subject of intensive research today. The scarcity of drinking water is one of the major problems we are currently facing. Millions of people perish each year as a result of drinking water shortages. In many areas of India, drinking water is still in short supply. Water can be purified in several ways, including through boiling, filtration, distillation, chlorination, and water purification by photocatalysis. It offers a cheap, useful, and engaging one. Titania NTs, a photocatalyst that absorbs light and raises its energy, can be employed in photocatalysis. This energy is delivered to the substance that will undergo a chemical reaction. The role of photocatalytic activity in producing pure water is acceptable. Titanium dioxide nanoparticles (NTs) make an efficient photocatalyst for photocatalytic water purification.

Properties of TiO_2

Chemical formula	TiO_2
Molecular weight	233.38 g/mol
Density	4.5 g/cm^3
Boiling point	1600ºC
Molar mass	79.866 g/mol
Melting point	1580ºC
Appearance	White solid
Odour	Odourless
Solubility in water	Insoluble
Band gap	3.0 eV (rutile), 3.2 eV (anatase)

Electrolytes used for Anodization

Anodization can be thought of as a method for producing very effective nanotubes. Long nanotubes, however, require anodization to last for a longer time. Titania (TiO_2) NTs self-organize themselves when an electrochemical setup is present [11]. Essentially, it is made up of two electrodes, electrolytes, and a DC power source (Fig 1).

The initial generation of nanotubes is coated with an HF acid electrolyte. However, the length of the emerging nanotubes is only a few hundred nanometres. Mixing HF/electrolytes of various acids increase the length of nanotubes. In this case, platinum primarily serves as the counter electrode whereas titanium can be considered the working electrode (anode). They both were immersed in the same electrolyte. We can also use other kinds of counter electrodes like stainless steel, carbon, aluminium, iron, and graphene. All electrodes have their attributes in anodization.

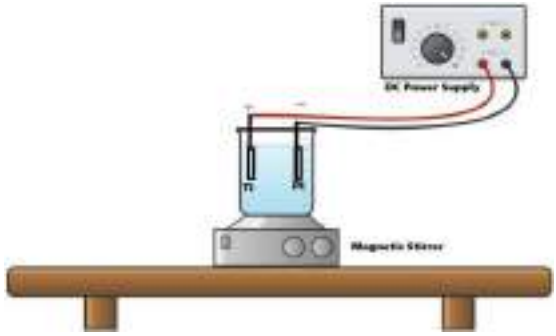

Fig 1. Anodization

The electrochemical anodization process consists mostly of three phases. such as 1.chemical etching, 2. field-assisted oxidation, and 3. field-assisted dissolution. When O^- or OH^- ions from the electrolytes interact with the titanium, titanium oxide develops on its surface. Titanium ions are transported and dispersed through the titanium's surface in the electrolyte solution. Only the electrolyte's F^- ions contribute to pore formation. This initiates the etching process and deepens the pores. When the anodization starts, the current becomes quickly decreased according to the formation of an oxide layer on the surface of the titanium. This current subsequently rises due to the pore formation by fluoride ions and then becomes the steady state only after the formation of nanotubes [12].

The current review highlights the disparate types of electrolytes used for the formation of titania NTs. According to the first generation, at low voltages with 0.5 wt% HF electrolytes provides sponge-like or similar alumina structure. Short NTs of about 200-500 nm in length were obtained by handling inorganic aqueous electrolytes (HF-based electrolytes) [14]. Beranek et. al., introduced 1M H_2SO_4 electrolyte mixed with various small amounts of HF. Current oscillation during the anodization sensitively depends on the HF concentrations. Bauer et.al., fabricated titania nanotubes by applying pH buffering electrolyte H_3PO_4 with the amount of HF. The electrolyte, which is pH buffering influenced the pore geometry of the nanotubes substantially. Length increased up to

20nm-1μm when they applied phosphoric acid mixed with HF solution [15].

Alternative HF electrolyte NaF combined with Na_2SO_4 was adopted for the second generation of titania NTs. After 6 hours of anodization at 20 V, they received nanotubes with a length of 0.5-2 μm. Pore diameter and wall thickness are decreased from 120 to 70nm and 20nm to 12nm, respectively. However, the corollary nanotubes are covered by rough walls with rings. The thickness of the tubes increases over time and inhibits up to 2.4μm, reaching only after 6h of anodization. The irregular structure was grown after this time. The use of NaF instead of HF electrolyte allowed for a thicker porous layer. The chemical etching rate of TiO_2 is become slower in neutral electrolytes than in acidic electrolytes [16] (Fig 2). Using NH_4F instead of NaF affords well-ordered titania nanotubes with up to the length of micrometer obtained. The formation of nanotubes is strictly affected by the concentration of ammonium fluoride. The diameter of the nanotubes also increases with the increasing rate of electrolyte concentrations [17] (Fig 3). Ripples or irregularities also exist in this form.

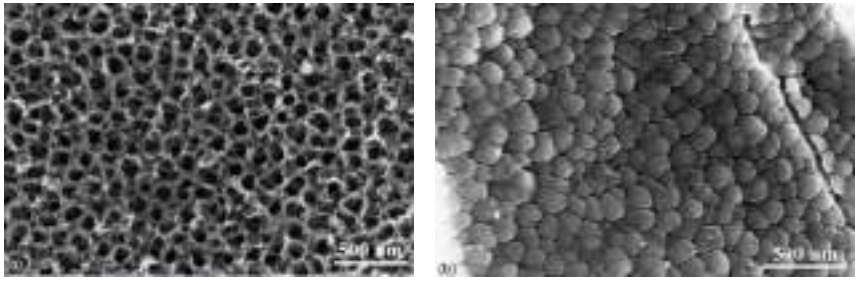

Fig. 2 - Reference [16] - top and bottom view of porous structure on sample anodized for 6 h in Na_2SO_4 (1M) + 0.5 wt % NaF

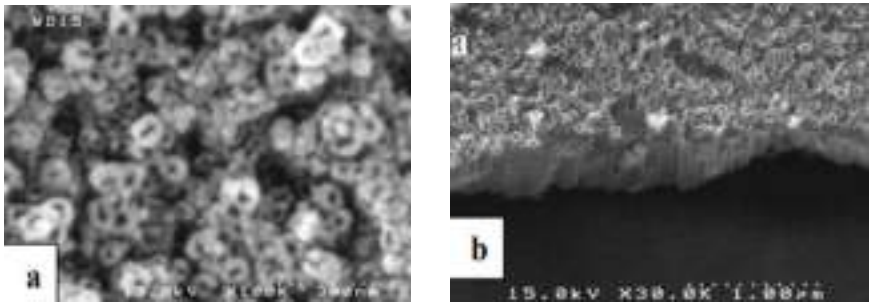

Fig. 3 - Reference [17] - FESEM image of TiO_2 nanotubes. Glycerol containing 1.5 wt% NH_4F and water (a) the top, b) the cross-sectional

Maximum nanotubes growth was attained at 60V when we applied ethylene glycol (EG) mixed electrolyte. In the case of NH_4F mixed electrolyte, the oxide dissolution increases the concentration of NH_4F, which is decreased by appending H_2O, which drives to longer nanotubes. 17h of anodization with EG containing 0.25 wt% NH_4F and 2wt% H_2O provides longer nanotubes about 134μm in length roughly [11]. The use of polar organic electrolytes was devised in the third generation of titania nanotubes. The reduction in water content reduces the chemical dissolution of oxide in the electrolyte resulting in longer nanotubes. Smooth walls of TiO_2 were obtained at a lower diffusion rate. This is achieved by a glycerol-based electrolyte that reduces the current fluctuations.

Chloride-containing electrolytes/ fluoride-free electrolytes are brought in for the fourth generation. However, the eventual result, a flower-like structure of nanotubes is detected. That is, there are passive breakdown conditions are produced. These tubes have a diameter of about 15nm, a length of 1μm, and a thickness of about 10nm. But according to this fourth generation, bundles of tubes were identified in a short time [18]. The electrolyte containing $HClO_4$ and $NaClO_4$ shows high aspect ratio bundles of tubes. These tubes are closely packed together.

So, for the fabrication of titania nanotubes, there were four generations occurred. In the first generation, aqueous HF-based electrolytes are used. Sponge-like structure converted to tapered conical-shaped nanotubes [19]. In the second-generation Cai and co-workers adjusted the pH of both KF and NaF aqueous electrolytes to reduce the chemical dissolution of oxide as a result NT length increases to several microns [20]. The third generation of titania reported by Paulose and co-workers [11], used organic electrolytes such as ethylene glycol, diethylene glycol, formamide, etc. in combination with HF, NaF, KF, NH_4F, etc. Resultant NT arrays have 1000µm length and growth rates of up to 15µm/h. Richter and co-workers [21], anodized titanium using electrolytes contains chlorine salts in combination with oxalic, formic, gluconic, hydrochloric, and sulfuric acids. Clumps of NT were obtained rather than arrays.

Table 1 – Morphology of TiO_2 NTs obtained at different generations

Generations	Electrolytes	Length (L), Thickness (T), Diameter (D)	Morphology
1	HF aqueous electrolyte	L-up to 500nm T-(10-30) nm D-(20-80) nm	Short nanotubes are obtained, when the voltage (V) is greater than 23V sponge-like structures were found.
	$HF+H_3PO_4$	L-up to 1µm D-(15-120) nm	The length of the nanotubes is increased up to 1µm.
2	NaF $+Na_2SO_4$	L-up to 2µm T-12 nm D-70 nm	Resultant nanotubes are roughly walled with rings.
	NH_4F+ Na_2SO_4	L-700 nm D-90 nm	Well-ordered nanotubes were found. When the voltage increases ripples are formed

3	NH_4F+EG	L-up to 1000µm D-(50-90) nm	Longer nanotubes are found. The reduction of water content reduced the solubility of titanium dioxide.
4	HCl electrolyte	L-up to 1µm T-10nm D-15nm	Bundles of tubes are formed in a short time.

Effects of F^- ions and H_2O content in Electrolytes

The outcomes of fluoride concentration in the electrolyte help to enhance the longer nanotube's structure [22]. The existence of fluoride ions can create a fluorine complex like TiF_6^{2-} which is water-soluble and propels fluoride ions on the surface of the titanium. Which only eases the formation of pores. Because F^- ions interact with the surface and allow the ions of electrolyte to freely penetrate the medium, the nanotubes get longer[23].

$$Ti^{4+} + 6F^- \rightarrow [TiF_6]^{2-} \quad (1)$$

$$TiO_2 + 6F^- \rightarrow [TiF_6]^{2-} + 2H_2O \quad (2)$$

Due to the low conductivity oxide that forms on the electrolyte/titanium contact, the current density in the first step drops down dramatically. The actively chemical dissolving reaction caused by F^- ions from electrolytes causes the current densities to grow [24]. This occurrence can be attributed to the surface oxidation's worm-like pores and pits that were randomly drilled. Further oxidation is driven by the greater field at the bottom of the pore, and the field also aids in dissolving. The current eventually reaches a constant condition. The rate of pore expansion is stabilized at this steady state [25].

In recent years, fluoride-free/chloride-containing electrolytes were handled for the formation of bundles of NTs, which can be explored up to rapid breakdown voltage [12]. But fluoride-containing electrolytes are

composed of ripple-free, longer, structured NTs. That is, fluoride-free electrolytes have fewer current densities than fluoride-contained electrolytes. Therefore, the oxide dissolution advanced due to these fluoride ions. During the anodization, the chemical dissolution and oxide layer formation rates are approximately equal. Fluoride ions stabilize the chemical dissolution rate, which brings the pore formation. That is the concentration of fluoride leads to surface etching, an increase in the diameter of pores, and the generation of more pores [26]. Therefore, fluoride ions are required in electrolytes for the fabrication of long titanium dioxide nanotubes [27].

In the case of water-content electrolytes, it will also affect the structure of NTs. In general, the anodization process would weaken in the absence of water in electrolytes due to a lack of H^+ ions and high viscosity of the solution, which results in the creation of titanium dioxide layers exclusively. Raja and co-workers [28], discovered that to create well-ordered titania nanotube arrays, ethylene glycol needed to include a minimum of 0.18% water. However, Ahmed El Ruby Mohamed et al. developed a preparation of titania nanotubes in viscous electrolytes, and in that research, they discovered that no nanotube arrays were generated below 2 wt% water concentration. At a water concentration of 5 wt%, well-ordered nanotube arrays started to develop. As the water content increased to 50 wt%, the nano architecture of the arrays changed as the inner diameter increased from 38 to 76 nm and the length from 250 to 900 nm. The diameter and length of nanotubes decreased to 40 nm and 424 nm, respectively, as the water content was increased further to 99.5 wt%. Due to the electrolyte's viscosity, the rise in diameter and length with water concentration between 5 and 50 wt% can be explained [29]. When the filling of water is approximately (8-25) %, which brought in the production of nanotubes and is interconnected by ripples. Nanotubes grow much more compact without water and ripples are absent. So higher nanotubes will become close-packed. concluded that there is no inner tube spacing. The length of NTs is about 100 in water content and about 200 in 0 vol% content of water [30]. Therefore, the thickness of NTs is increased in water-rich electrolytes.

Application of TiO_2 as Photocatalyst

Because of the remarkable performance of TiO_2 NTs, they can be adopted in many applications. The scopes of energy storage, extensive oxidative power, stability, high whiteness, biocompatibility, high melting and boiling point, etc. are their charming properties. Photocatalytic competencies are one of them. This demonstrates that titania can absorb light radiation and bring it to higher energy states. This energy gives to the substance which will cause the chemical reaction. Titania has chiefly three crystalline structures: anatase, rutile, and brookite. Compared to the other two forms, brookite is unstable. Anatase is mostly used for photocatalytic applications. Because they offer high oxidative power and photocatalytic capability. Compared to pure anatase, the mixture of rutile - anatase shows high photocatalytic activity [31]. When looking at the bandgap of anatase, which is merely capable of absorbing UV light, its value is about 3.2 eV [32]. To conquer this drawback, we demand to reduce the band gap of anatase. The coupling helps to keep effective titania in the visible region. Titanium dioxide is an n-type semiconductor, where most carriers are electrons that are translated into p-type by successful doping.

Titania delivers electrons and holes during photocatalysis. The leading components operating in the chemical reaction are the hydroxyl radicals. This beats the pollutants and breaks their chemical bonds to create innocuous substances [33]. There are generally two processes that occurred, redox reaction and oxidation, which is strongly explained by Honda – Fujishima [34].

The photocatalytic ability of titania points to a lot of fields. Like water splitting and hydrogen generation, self-cleaning, biomedical applications, air purification, and water purification. TiO_2 accepted for water purification has been recently practiced in several laboratories. Elemental mercury in the flue gas can be removed by the photocatalytic property of the titania nanotubes [35]. According to that experiment, titania has greater than 90% efficiency for the excellent removal of elemental mercury (Hg^0) for 100h. The efficiency became decreased when the

structure was sintered to a rod-like particle with 600ºC. Fourth-generation bundle nanotubes appear to have better photoactivity than second and third-generation nanotubes based on their band gap value and absorbance properties. [36], Fourth-generation TiO_2 nanotube arrays are an appropriate architectural design for water photoelectrolysis under solar light illumination due to the improved light absorption and propagation characteristics resulting from their carefully managed and oriented porosity. While annealed TiO_2 films exhibit a red-shift and stronger absorption in the wavelength range of 350 to 550 nm, non-annealed titania films show less adsorption in the visible light region. The anodic titania photocatalyst heat treated at 550ºC showed the highest efficiency of dye and dichloroacetic acid (DCA) degradation among the catalysts, according to the photocatalytic data. The predominant presence of the anatase-type composition in the anodic film may be responsible for the catalytic reaction's high efficiency [37].

The semiconductor photocatalytic method has demonstrated tremendous promise as a low-cost, environmentally responsible, and long-lasting treatment technology to support the "zero" waste initiative in the wastewater industry in recent years.

Modified TiO_2

The annealing process is essential for titania tubes generated by anodization. Because only the annealing process determines which crystal structure is. Without annealed titanium dioxide can never act as a proper photocatalyst in photocatalysis. The Anatase form accepts more photocatalytic strength than the rutile one. Without annealed sample/titania shows 70% of degradation of phenol [17] which allows 87% degradation by anatase and 76% degradation by rutile one.

Photocatalytic efficiency decreases due to the fast recombination rate of electron-hole pairs. To avoid this, coupling, doping, and co-doping methods are required. When we doped titania with non-metals, noble metals, transition metals, etc. There is an escalation in the specific surface area of titania. The absorption dimension of the doped catalyst

has drifted towards a longer wavelength and can be active in the visible region also [38-39]

Transition metal like iron (Fe), doping into TiO_2 for the removal of humic acids in drinking water provides the shallow trapping sites for charge carriers. That is Fe^{3+} traps electrons as well as holes which will increase the photocatalytic activity. The photocurrent of these doped media increased obviously [40]. Molybdenum (Mo) doping helps for the phase transition and allows absorption of visible light. This is done by the combined method of direct current magnetron sputtering and anodization. The bandgap of undoped- titania is 3.24 eV and it becomes 3.16, 3.14, etc. due to an increase in the concentration of doping Mo [41]. Cerium (Ce) is one of the rare earth metals that can be doped with Titania. Ce-TiO_2 activity in 2-mercaptobenzothiazole (MBT) was reported by Li et al., The 4f electronic configuration of Ce improves the absorption range and which is shifted to the 400-500 nm range. A higher concentration of Ce changes the surface of titania and converts it to rutile form. Initially, MBT degradation increases with an increase in Ce^{3+} content but it will be declined beyond the high value of cerium concentration. The result shows that 1.2% Ce^{3+}- titania gives the best performance in the UV region and 0.7% Ce^{3+} - titania performed under the visible region [42]. The case of nitrogen-doped titania shows high emission of current and excellent field emission stability [43]. N-Doped titania was obtained by using different methods like annealing titania in a nitrogen atmosphere, N- ion bombardment, plasma treatment, etc. N(2p) states of nitrogen ions are located above the valance band of titania by substituting oxygen atoms in the titania lattice. The result of mixing N(2p) with O(2p) states reduces the bandgap of N- doped titania [44]. Copper (Cu) doped titania has a great attraction in photocatalysis than pure titania [45]. It can be fabricated during the anodization process by using $HF/HNO_3/H_2O$ mixture with a ratio of about 1:4:5 in volume. For the degradation of methylene blue (MB), visible light and UV light were used, but the effective degradation only occurs in Cu-TNT with visible light. When we used Cu-TNT, the Fermi level of CuO is placed lower than titania, which leads the electrons in the valance band to jump up to

CuO and disperse to the surface of titania. Strontium (Sr) doped titania significantly improves the photoconversion efficiency and is about 0.69%, which is about 0.2% in un-doped titania [46]. Sr-doped titania was fabricated during the anodization by using anhydrous strontium hydroxide salt.

Conclusion

This article specifies titanium dioxide's efficiency in the water purification system and gives the knowledge about types of electrolytes applied for the fabrication of these NTs. Different electrolytes have different capabilities to produce TiO_2 NTs. Compared with aqueous electrolytes, organic will play a major role in the evolution of longer nanotubes. There are no nanotubes were found without F^-. When we doped titania with noble metals, non-metals, rare earth metals, etc. It brings some reduction of the crystal structure's bandgap and allows the sample surface to drive in the visible region. Therefore, water purification using photocatalysis will become effective when we use doped titania. That is, which will make the electrons easily penetrate from the valance band to the conduction band with the help of some photons with low energy and visible light can act as the light source for the photocatalysis mechanism also.

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PP15

FTIR and FT-Raman, studies of-5-(furan-2-ylmethylene) pyrimidine-2,4,6(1h,3h,5h)- Trione

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The IUPAC name of FPT crystal is 5-(furan-2-ylmethylene) pyrimidine-2,4,6 (1h,3h,5h)- trione. The FTIR-ATR spectrum of FPT compound was recorded at SAIF-SPIHER St. Peters University, Avadi-Chennai, using Perkin Elmer Spectrum The FT-RAMAN spectra have been recorded at SAIF-Indian Institute of Technology (IIT), Chennai, using BRUKER

RFS 27: Standalone FT- Raman Spectrometer at a range of 50 -4000 cm^{-1}. The most featured region of amino group N-H vibrational stretching occur at 3400 – 3500 cm^{-1}. The FTIR peaks of 3148 cm^{-1} is found to be N-H stretching vibrations and the band is found to be very weak and this is due to N-H. In this study the FTIR bands at 3040, 2852, 2323, 2080, 1911 cm^{-1} shows C-H Stretching vibrations. The band at 3040 cm^{-1} shows asymmetric stretching vibrations. In FT-RAMAN spectrum the vibrational stretching of C-H bond has been noticed at 2307, 2272, 2233, 2193, 2122 cm^{-1}. The FT-RAMAN band at 2122 cm^{-1} is found to be a weak band. In this present study the FTIR band at 1704,1743, 1650,1561 cm^{-1} indicates the presence of C=O stretching vibrations. For FT-RAMAN the C=O spectral vibrations has been registered at the region of 1796 cm^{-1}. The bands of FTIR at 1630 cm^{-1} is found to be strong band. Literature the C-N vibration stretching has been observed at the range of 1362 cm^{-1} for FTIR spectrum and has been registered as a medium band. The C-N stretching vibration for FT-RAMAN has been observed at 1360 cm^{-1}. In the present study the FTIR bands observed at 1516 and 1404 cm^{-1} are assigned to aromatic CC stretching vibrations. The FT-RAMAN bands are observed at 1516 and 1437 cm^{-1} are assigned to aromatic CC stretching vibrations.

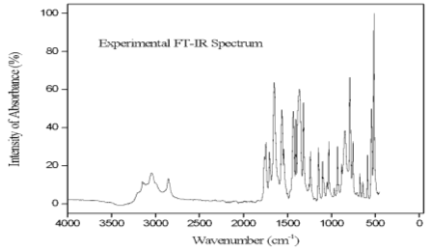

Fig.1 FTIR spectrum of FPT crystal

Keywords: FTIR; FT-Raman; Vibrational Assignments

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PP16

Synthesis of pure MgO and Carbon-based nanocomposites for Anti-Cancer, Anti-diabetic, Anti- inflammatory application

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MgO nanoparticles are potential candidate for biomedical application as they possess good biocompatible nature [1]. In this study, the pure MgO, PEG-MgO, PEG-MgO-rGO, PEG-MgO-gC_3N_4 nanocomposites are prepared successfully via Co-precipitation method and annealed at 500°C. The physcio-chemical properties such as structure, surface morphology and elemental composition were investigated through X-ray diffractometer (XRD), Scanning Electron Microscopy (SEM), Energy dispersive X-Ray analysis spectroscopy (EDAX). The XRD analysis revealed the crystal structure of the prepared sample as cubic with space group Fm3m (225) and the average crystalline size (D) is found to be 18 nm to 25 nm. From the UV-Vis analysis the absorbance was found to be 254 nm – 267 nm and the band gap ranging between the 3.5 eV- 3.7 eV for pure and composites of MgO. The characteristic metal oxide (Mg-O) vibrational peak at 470 cm^{-1} was established from the FTIR analysis. The SEM analysis revealed the clustered micro spheres morphology for both PEG-MgO-rGO and PEG-MgO- gC_3N_4. Further, the synthesized samples were subjected to anti-Cancer, anti-diabetic, anti-inflammatory activities. The high inhibition percentage of 91.18 % and 87.03 % are achieved against α-amylase and bovine serum albumin in anti- diabetic and anti-inflammatory assays respectively. The in-vitro cytotoxicity (MTT) assay revealed the IC_{50} value of 80.58 for PEG-MgO-gC_3N_4 nanocomposite, which shows the potential anti-cancer property of the prepared sample. Hence, the above results reveal that the decreased cell viability of cancer cells and the very high percentages of inhibition against α-amylase and

bovine serum albumin (BSA) shows that the synthesized Pure MgO and their composites was an effective material for bio-medical applications.

Keywords: Anti-Cancer; Anti-diabetic; Anti- inflammatory; MgO; Nano-composites

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PP17

Application of Electronic Nose in Agriculture

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An Electronic Nose (e-nose) is a group of gas sensors which finds promising applications in the field of agriculture. They are used in improving assessments of food quality characteristics compared with other traditional methods. The present review work summarizes the application of e-nose in monitoring food quality, and their operating conditions in other quality-related properties of food analysis. A comparative study is done on the working principle, applications and limitations of the different sensors employed in electronic noses. In addition, the various algorithms utilized for the same have been studied and compared.

Keywords: Electronic nose; Gas sensor; Food-quality; agriculture

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PP18

Cosmic Microwave background: How it explained our beginning

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Introduction

When the universe was only a fraction of a second old, its primary objective was expansion. At that time, it was trillions of degrees hot, blazing with an unfathomable brightness, and packed with photons. Photons lost energy to the expanding universe as the cosmos cooled. The photons changed into ultraviolet, visible, and infrared light from gamma-ray and X-ray radiation. They became cooler and less energetic as their wavelength increased, yet they never ceased to be photons. 13.7 billion years after the universe's creation, photons have moved down the spectrum and are now known as *"microwaves."* They are referred to as "Cosmic Background Radiation" or "Cosmic Microwave Background".

The Discovery

NASA's COBE Differential Microwave Radiometer (DMR) experiment discovered cosmic microwave background (CMB) anisotropies based on its first year of data. The discovery of the Cosmic Microwave Background (CMB) by Penzias and Wilson has been a 'game changer' in cosmology. Before this discovery, despite the observation of the expansion of the Universe, the steady-state model of cosmology still had a respectable group of followers. After the discovery of CMB, the Big Bang model of the universe has been established. The paper they published in 1965 in *The Astrophysical Journal* refers to the persistent puzzle of an inexplicable "excess antenna temperature," rather than the astronomical discovery of the century.

Big Bang or Steady State?

The story of the CMB, like most of modern cosmology, begins with the equations of General Relativity developed by theoretical physicist Albert Einstein (1879–1955) and published in 1916.

Solutions to Einstein's equations were found that correspond to an expanding universe and, soon thereafter, astronomers found evidence for

this expansion: distant galaxies were all moving away from our vantage point within the Milky Way Galaxy. This evidence strongly stated that the universe is denser in the past and thus proving the Big Bang model. Immediately after the discovery by Penzias and Wilson, cosmologists started to look for anisotropies in the CMB radiation. This was motivated by the assumption that structure in the Universe, galaxies, clusters, voids and filaments formed from small initial fluctuations by gravitational instability.

CMB's Future

As the Universe expands, this remnant radiation from the Big Bang is getting more redshifted and its energy is continuously diminished. The current cosmic microwave background will no longer be seen in a few trillion years since it will have redshifted into insignificance. The Universe will have greatly expanded in this far future, and even the nearest galaxies will be well out of our field of vision. There won't be any observable signs of the Big Bang or the Universe's expansion at this point.

Conclusion

The discovery of the Cosmic Microwave background has changed the course of astrophysics. Soon, physicists can search for the missing links, i.e., Dark matter and Dark energy and may even find out the driving force which initiated the Big bang. The accuracy of these experiments has helped us to estimate the parameters of the cosmological model with unprecedented precision so that in the future we shall be able to test not only cosmological models but General Relativity itself on cosmological scales.

Keywords: Big Bang; Expanding Universe; Cosmological Model.

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PP19

Construction of Radio Telescope and observe 1.42 GHz

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Examine and explore the Universe with atomic hydrogen 21 cm emission is a fascinating and challenging work in astronomy. Radio telescopes play a vital role in detecting and imaging these faint signals. Powerful radio telescopes are complex to construct and operate. We have built a parabolic dish type radio telescope primarily for educational training purposes. The design uses a parabolic dish with the diameter of 180cm, ready-to-use radio-frequency components, and a software-defined radio module. The telescope operates efficiently from a rooftop in a city environment. Using this telescope, we have conducted observations and successfully detected the 21 cm line emissions from the different directions of our galactic plane.

Keywords: Hydrogen line; Hydrogen emission; 21cm wavelength; low cost radio telescope

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PP20

Synthesis and Characteristics of Biopolymer Cellulose Acetate

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The proposed biopolymer system was synthesized using amorphous polymer polymethyl methacrylate (PMMA) with cellulose acetate (CA) in different composition as ((PMMA)X and (CA)1-X in the weight ratio of 1-x = 0.1, 0.2, 0.3, 0.4 and 0.5 mol% respectively by solution casting technique with Dimethyl formamide (DMF) as solvent. The synthesized in the form of thin films were characterized by AC impedance analysis for conductivity studies for different composition and the composition (PMMA) 0.97-(CA)0.3 was found to have a high conductivity value of 5.45610-8 Scm-1. This film is further subjected to XRD analysis and was found to be having halo pattern with peak free pattern which proves the amorphous nature of the sample.

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PP21

Synthesis and Characterization of Proton conducting membrane using PMMA/CA/NH_4SCN

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The proton conducting membrane was synthesized using polymers Poly (methyl methacrylate)–cellulose acetate (PMMA/CA) in the ratio of 97/3 mol wt% and ammonium thiocyanate is added as dopant salt in different ratios of 0.1, 0.2, 0.3, 0.4 mol wt%. The blend polymers of PMMA/ CA with ammonium thiocyanate using DiMethyl Sulfoxide (DMSO) as

solvent were prepared by solution casting technique. The PMMA/CA blend ratio was first optimized for the highest conductivity value (5.456 x 10^{-8} S/cm). The addition of ammonium salts increases the ionic conductivity because charge carriers are created by the metal ions. In our work, we used ammonium thiocyanate to the blend of PMMA/CA which increases its ionic conductivity at room temperature. By using the AC impedance studies the ionic conductivity of the prepared membranes were calculated and among them the highest ionic conductivity value was found to be 1.812 x 10^{-7} S/cm. This best conducting composition was subjected to XRD characterization which reveals the amorphous nature of the prepared membrane without any observed peaks.

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PP22

Synthesis and Characterization of Cu_2NiSnS_4/ZnO composites for Thermoelectric Applications

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Population increase has only further increased the energy demands of the world. Fossil fuels cannot drive these energy needs forever and hence; this calls for cleaner and greener forms of energy. Thermoelectric is an energy harvesting technique, wherein waste heat is utilized to produce electricity. Earth-abundant quaternary chalcogenides such as Cu_2NiSnS_4 with complex crystal structures are non-toxic and hold the potential to become thermoelectric (TE) materials [1,2,3]. Currently, polycrystalline tin copper selenide has the highest figure of merit at about 2.1 [4]. Engineering TE materials by employing the energy filtering effect with appropriate bandgap nanoparticles have proven to enhance their TE efficiency. Cu_2NiSnS_4/x wt% ZnO (x = 0.1, 0.2, 0.3, 0.4) nanocomposites

suitable for mid-temperature TE applications, in which ZnO nanoparticles are dispersed into the Cu_2NiSnS_4 matrix. X-ray Diffraction (XRD) was adopted to study the structure and morphology of synthesized nanocomposites. The incorporation of ZnO nanocomposites has resulted in simultaneous enhancement of the Seebeck coefficient (S) and a decline in electrical conductivity (σ), which is attributed to the decrement in carrier concentration (n). By increasing the wt% of the nanocomposites, n and σ decrease, which is not the ideal properties required for a high figure of merit. The highest power factor of 90.29 $\mu wm^{-1}K^{-2}$ at 573 K is recorded for 30 wt% composites. The thermal conductivity of the same composite exhibited a low value through stronger phonon scattering at the grain boundaries and interfaces formed between the CNTS matrix and ZnO nano inclusions. The novel strategy of introducing metal oxides into the host matrix for obtaining efficient TE performance could be extended to other eco-friendly quaternary chalcogenides.

Graphical abstract:

Keywords: Cu_2NiSnS_4/ZnO nanocomposites; energy filtering effect; phonon scattering; thermal conductivity; Figure of merit (zT)

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PP23

Production of Biodiesel via Transesterification of Jatropha oil in presence of MgO Impregnated Mesoporous Carbon

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An ever increasing demand of fuel has been a challenge for today's researchers. The fossil fuel resources are dwindling day by day. Biodiesel seems to be a solution for future. Biodiesel (FAME), which is derived from triglycerides by transesterification with methanol, has attracted considerable attention during past decade as a renewable, biodegradable and non-toxic fuel. Jatropha oil is used as feedstock for the production of biodiesel. Low cost Jatropha oil is considered as a potential non-edible feed stock for biodiesel production. Due to remarkable features of mesoporous carbon with respect to high surface area (856.076 m^2/g) and pore volume (1.030 cc/g), it is chosen as a support and it was prepared by hard template method using SBA-15. MgO supported on mesoporous carbon is successfully synthesized by wet impregnation method with five different weight percentages (3%, 5%, 7%, 9%, 11%) and each is carbonized under 700°C at N_2 atmosphere. Batch reaction was carried out with pre-esterified Jatropha oil (>1% FFA) with methanol and required reaction parameters were optimized using different MgO/MC. Effect of

temperature and effect of time were studied and the reaction products were analyzed using GC (Shimadzu GC 17-A). The physiochemical properties of the prepared catalysts were determined by XRD (X-ray diffraction), FT-IR (Fourier transform infrared), UV-DRS (diffraction reflectance spectroscopy), BET (Brunauer-Emmer-Teller) surface area analysis, SEM (Scanning electron microscopy) and HR-TEM (High resolution scanning electron microscopy).

Keywords: Biodiesel; Jatropha oil; Transesterification; Wet impregnation; Mesoporous Carbon

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PP24

A Novel Mesoporous Zinc ion Loaded Hydroxyapatite for Cancer Drug Delivery

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A novel mesoporous hydroxyapatite (Meso-HAP) was prepared through soft-template method using microwave heating with the aid of cationic surfactant CTAB (cetyltrimethylammonium bromide). Due to remarkable features of Meso-HAP with respect to high surface area, pore volume and tuneable pore size, it could be a suitable candidate for effective drug loading and controlled release of drug. Osteosarcoma is a common primary malignant bone tumour which results in high mortality rate and poor prognosis that leads to post-surgical therapy. As an alternative, therapy using nanomaterials provides passive accumulation of nanocarriers in tumour tissues due to their unique properties. As zinc has immense attention as antimicrobial agent property, a series of zinc (1 wt.%, 2 wt.%, 3 wt.%, 4 wt.%, 5 wt.%) ion was impregnated on the Meso-HAP. The developed Zn/Meso-HAP was characterized for its

physico-chemical properties, biocompatibility and degradation studies. Zn loaded Meso-HAP was used for loading drug methotrexate (MTX). The drug loading efficiency was found to be more than 85%. Furthermore, from drug release assay, it was found that the release of MTX was sustainable and pH dependent. Mesoporous HAP was confirmed by low-angle XRD and BET surface area analysis. All the prepared materials were also characterized by high-angle X-ray diffraction (XRD), high-resolution scanning electron microscopy (HR-SEM), Fourier transform infra-red spectroscopy (FT-IR), UV-Visible diffuse reflectance spectroscopy (UV-Vis DRS) to understand their physio-chemical properties and then the sustainable release of elements analysis by (ICP-OES).

Keywords: Hydroxyapatite; CTAB; Methotrexate; Mesoporous; Zinc; Osteosarcoma

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PP25

Facile green synthesis of Fe_2O_3 doped magnesium oxide nanoparticles using *Scoparia dulcis* leaf extract for efficient photocatalytic degradation of acetaminophen

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In recent years, increasing level of emerging contaminants appears in the aquatic environments, especially from pharmaceutical wastes and healthcare products. Even though the concentration these pollutants seem to be low, the impacts of bare contaminants as well as its degradation

products are found to be highly toxic to the environment and human beings. In this present work, photocatalytic degradation of acetaminophen (paracetamol) was carried out using magnesium oxide nanoparticles MgO (NPs) synthesized using by *Scoparia dulcis* leaf extract. The leaf of the plant is used in the treatment of abdominal pain, insect bites, fever, heart problems, liver and stomach disorders, malaria, venereal disease, and also as a general tonic. In the present study, *Scoparia dulcis* is used as a reducing agent in the synthesis of MgO. The bandgap of MgO is modified by doping with different w/w% of Fe_2O_3 to improve the efficiency towards visible light activity. The synthesized and modified nanomaterials were characterized by different analytical techniques. X-ray diffraction (XRD) to calculate the average crystal size, particle size analyser for average particle size, field emission scanning electron microscopy (FE-SEM) for morphological studies, UV-Visible diffuse reflectance (UV-DRS), photoluminence (PL) and UV-visible spectroscopy to analyse the absorption patterns. The degradation of acetaminophen (paracetamol) was carried out using UV light with 250W and 365 nm. The reaction parameters such as catalyst loading, pH of the reaction solution, and degradation time were optimized.

Keywords: Fe_2O_3 doped MgO (NPs); *Scoparia dulcis;* photocatalytic degradation; Acetaminophen

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PP26

Environmental applications of Carbon doped Titanium dioxide nanomaterials: A review

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The work describes how carbon-doped TiO_2 nanoparticles were used in for environmental applications. The characteristics of titanium dioxide

nano particles and the changes that occur to them before and after doping are discussed in the article. Additionally, a comparison of the differences in property changes between TiO_2 nanomaterials doped with metal and non-metal is displayed. The review also includes a description of the sol-gel synthesis technique used to create nanomaterials, along with a full schematic illustration of the technique. The carbon doped TiO_2 nanomaterial exhibits a wide range of characteristics, with the photocatalytic property receiving particular attention. The two applications suggested use a process called photocatalytic dye degradation to get rid of water-soluble dyes in the textile sector. Methylene blue is used to demonstrate photocatalytic dye degradation and the next application discussed is Hydrogen production by using doped TiO_2 nanoparticle as photocatalyst. Four organic fatty acids were used for analysing the result.

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PP27

Synthesis and Characterisation of zinc ferrite nanoparticles for possible Biomedical applications

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Zinc ferrite ($ZnFe_2O_4$) finds applications in various fields in both the micro and nano forms. The structure and properties of this compound in the nanoscale are different from those in the microscale. Ferrite nano particles exhibit unique chemical, electric, magnetic and thermal properties enabling them to use as catalysts, absorbents, gas sensors, and a tool to combat cancer. The properties of dust generated electric arc furnace, which can contain up to 40% zinc, substantially in the form of

$ZnFe_2O_4$ are studied. In the present work, zinc ferrite nanoparticles have been synthesized by chemical co-precipitation method with chloride precursor. Prepared samples were characterized by FTIR and XRD to study its chemical and structural properties. Transition metal ferrite nanoparticles are of great concern because of their unique properties that enable them to be used in fields such as magnetic storage, biomedicine, ferrofluids, catalysis and magnetic refrigeration system. Zinc ferrites are found to have high electric resistivity, low eddy current loss, moderate thermal expansion coefficients, magneto-optic and magneto-resistive behaviour. These properties make zinc ferrite suitable for numerous device applications such as sensors, anode materials for batteries, catalysts, lasers, microwave and electrochemical devices.

Keywords: Zinc ferrite; Co-Precipitation; Biomedicine

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PP28

Role of an Energy Filtering Effect on the Thermoelectric Performance of Cu_2NiSnS_4/CdO Nanocomposites

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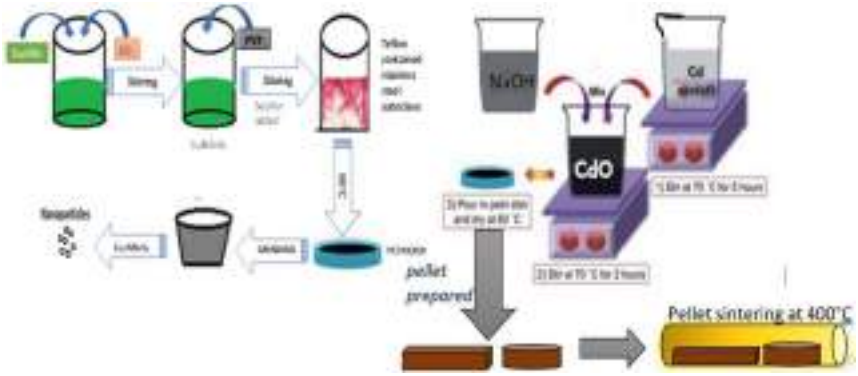
The rapidly increasing energy demand, the rise in the cost of energy, and the global warming issues are well-known critical problems for the modern world. Fossil fuels (coal, oil, and natural gas) which are the major energy source for the world, lead to inevitable carbon dioxide pollution and anthropogenic global warming. Every year, about 474 EJ (1 EJ = 10^{18}J) of energy are generated, out of which 340 EJ are rejected as waste heat, which reveals about 70% of the global energy is lost to

the environment without being utilized [1]. Thermoelectricity is one of the promising technologies (direct energy conversion by electrons in solids) to convert waste heat into electricity and can cool materials without an exchange media like a freon gas possessing various advantages in harmony with the environment. By recycling the waste heat, one can be able to control CO_2 emissions up to a certain extent, which leads to a greener environment. The loss of heat happens in different sectors, with a wide range of temperatures from 100 to 1000 °C [2]. There are several waste heat sources that emit low grade to medium-to-high-temperature heat. For example, the industrial steam/water boilers, food, paper, and textile industries generate low-grade waste heat at temperatures of 100 to 200 °C; chemical and other industries usually produce waste heat up to 500 °C; and most of the metal and glass industries generate waste heat in the high-temperature range of 500–1000 °C [2]. From a viewpoint of basic science, thermoelectric power is an entropy (or heat) carried by an electron. This is controversial terminology, because entropy and heat are concepts in the macroscopic world, whereas the electron is a concept in the microscopic world. Thus, a new thermoelectric effect is lying near the boundary between microscopic and macroscopic worlds, which will give a new insight or direction to condensed matter science. Therefore, semiconductor-based thermoelectric materials have been extensively investigated, especially in recent decades. Earth-abundant quaternary chalcogenides such as Cu_2NiSnS_4 with complex crystal structures hold the potential to become non-toxic and economically viable thermoelectric (TE) materials. Engineering TE materials by employing the energy filtering effect through hybridization with appropriate bandgap nanoparticles have proven to enhance their TE efficiency. In the present work, CNTS-CdO nanocomposites were prepared by the
solvothermal method. Cu_2NiSnS_4/x wt% CdO (x =0.1 %, 0.2 %, 0.3 %, and 0.4 %) nanocomposites suitable for mid-temperature TE applications, in which CdO nanoparticles are dispersed into the Cu_2NiSnS_4 matrix. X-ray diffraction (XRD) was used to study the structure and morphology of synthesized nanocomposites. The

incorporation of CdO has resulted in the simultaneous enhancement of the Seebeck coefficient (S) and a decline in electrical conductivity (σ), which is attributed to the decrease in carrier concentration (n). By increasing the weight percentage of the nanocomposites, n and σ decrease, which is in good agreement with the increase in energy bandgap.

Graphical abstract



The highest power factor of 90.29 $\mu Wm^{-1}K^{-2}$at 573 K is recorded for 30 wt% composites. The thermal conductivity of the same composite exhibited a low value of stronger phonon scattering at the grain boundaries and interfaces formed between the CNTS matrix and CdO nano inclusions. The novel strategy of introducing metal oxides into the host matrix for obtaining efficient TE performance could be extended to other eco-friendly quaternary chalcogenides.

Keywords: Cu_2NiSnS_4/CdO; Nanocomposites; Energy filtering effect; Phonon scattering; Thermal conductivity

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PP29

Ancient society's Nanotechnology

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Nanoscience and Nanotechnologies though seem to be new concept developed at the end of 20th century yet usage of metallic nanoparticles dates from ancient times. The gadgets that were used for various applications in diverse fields made use of nanotechnology. To cite a few example, Damascus Swords is one of the amazing applications of nanotechnology in 18th century. The shields of the swords reveal that the blades were made from nanowires, carbon nanotubes. The Lycurgus cup used by the Romans in the 4th century exhibited different colors under different conditions. The glass cup was made of nano sized gold and silver particles that display red and green color when light was made to pass through it in different directions. Apart from it, ancient history made use of nanotechnology for treatment of various ailments in human body. Moreover, there are many literary evidences which speak out the significance of nanoscience and nanotechnology. Anu kolgai (Atomic theory and Repeated Fissions) is mentioned in "tirumandhiram" Avvaiyar says:

"அணுவில் அணுவினை ஆதிப் பிரானை அணுவில் அணுவினி ஆயிரம் கூறிட்டு அணுவில் அணுவை அணுக வல்லார்கட்கு அணுவில் அணுவை அணுகவும் ஆமே "-திருமந்திரம். இதன் பொருளை விளக்க முடியுமா?".

In this regard, a review work has been carried out to present an overview about nanotechnologies with applications from ancient times till date in varied field.

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PP30

Pulse Oximeters using Embedded Systems

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Pulse oximeters are electronic devices which involve a non-invasive test that monitors the saturation of oxygen in our red blood cells. It can be attached to fingers, earlobes, toes, forehead, foot or nose. The main function is to determine the oxygen level in the blood through which professionals can predict how healthy the patient is during the ventilation or after trauma. These oximeters make use of embedded signal processing technique to sense oxygen saturation (SpO_2) level in the blood and beats per minute (BPM) of the heart. It uses Infrared (IR) and red light to detect the oxygenated and deoxygenated haemoglobin in blood. A photodiode senses the light and the obtained signal is filtered and its respective data is sent to the microcontroller for communication with other parts of the device and for display. The entire setup mentioned above is constructed using embedded systems. Having known the importance of pulse oximeter in the medical field, in the present work an attempt has been made to compare various pulse oximeters using embedded systems and the most efficient, accurate and economical one is recommended.

Keywords: Embedded system; Microcontroller; SpO_2; BPM

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PP31

Biomaterials for Dental Implantology: "Titanium" and other materials ahead

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A brief introduction:

A dental implant is an artificial tooth root (which is in the shape of a root) placed in the jaw to provide support for a replacement tooth (the crown)[1]. A dental implant could be screw type or cylindrical. Dental implants have been in practice from the ancient of times. Many materials have been used till now for osteointegration. Osteointegration is the attachment between the implant and the jawbone by mechanical interlocking. While various scientists tested different materials, the Branemark system of dental implants introduced us to this "space age metal" – Titanium.

Titanium as a dental implant:

Titanium gets firmly anchored to the bone, making it hard to remove it and most importantly, there is no inflammation in the peri-implant bone due to the metal. Branemark during his testing of the metal, observed soft tissue being formed attaching the bone and the metal (osteointegration). Titanium is considered one of the best metals for osseointegration. It has a tensile strength between 30,000 and 200,000 lbs per square inch[2]. It has incompletely filled d-shell electronic structure. In the elemental

form, it has hcp arrangement (hexagonal closed packed crystal structure, termed ∝) and bcc (body centered cubic structure, termed β) above 883. Titanium is corrosion-resistant in many conditions because of the formation of a passive oxide surface film (*Ti*) which makes it suitable for alloying[3]. Elements that stabilize -phase are called ∝-stabilizers (including aluminium, oxygen, nitrogen and carbon) and elements that stabilize -phase are called β-stabilizers (including vanadium, iron, cobalt, silicon, manganese and even more). β-alloys are more useful due to low elastic modulus and superior corrosion resistance.

Over these years, dental implants have usually been made from commercially pure Titanium with varying degrees of purity out of which Grade 4 cpTi is most commonly used owing to its strength[4]. Modifying the surface of biomaterials (surface modifications) plays an important role in determining the outcomes of biological-material interactions. With the appropriate method, we can improve biocompatibility (ability of a material to perform with an appropriate host response in a specific application)[5], adhesion and cell interactions. Surface modifications include Titanium surface roughening and Titanium surface coating[6]. The most common methods are Titanium plasma spraying, grit blasting (blasting with ceramic particles), etching with strong acids and anodization of Titanium in strong acids at high current density or potential. Surface coating techniques like HA coated implants (hydroxyapetite) poses clinical problems as it causes inflammatory reaction and loosening of coating when implanted. However, ion implantations, especially CO implantation, have modified the outer surface oxide in such a way that promotes bone formation and osseointegration. This method has been recommended for future investigations.

Drawback of Titanium implants and upcoming ideas:

Titanium has had a success rate of 98.8% from the last fifteen years. There has been an aesthetic challenge with the fact that it is gray in colour not mimicking the exact natural teeth. It is no longer considered as a completely bio-inert material as studies have found its traces in lymph nodes, serum and urine which could pose health issues to the

patient. There is a huge demand for completely metal free dental implants [7].

Ceramic materials like Zirconia have better mechanical and tribological properties but its hardness, in vivo failures and lack of enough scientific data still keeps it under trials and testing. Addition of Zirconium to Titanium decreases its melting temperature, thus decreasing the cost. The alloy exhibits properties like low cytotoxic effects, great stability, low corrosion rates and long range availability. Many other alloys like Ti-6Al-4V, Zirconia toughened alumina, Poly-ether-ether-ketone and even more have found to be promising. Continuous tests and research works will give us even better biomaterials in the near future.

Keywords: Osteointegration; Surface modifications; alloys

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PP32

Proton Therapy: Delivery Technology and Challenges Ahead

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Introduction

Proton therapy has become a subject of considerable interest in the radiation oncology community and it is expected that there will be a substantial growth in proton treatment facilities during the next decade. Over the last decade, the number of proton therapy facilities has risen at increasing speed, from approximately 20 centres in 2007 to >100 today. Although the advantageous properties of a proton beam for radiation therapy have generally been accepted since its early application in the 1960s, commercial solutions for proton therapy only became available at the end of the 1990s. The commercial availability probably linked to the breakthrough of intensity modulated radiotherapy technology with photons at the end of the 1990s and the belief that dose distributions would be even better with proton beams, triggered greater interest in proton. A high demand set into motion a process addressing a large hurdle in making this technology available to a large number of patients, namely its cost. Technological development is focusing on making proton therapy more efficient and versatile to serve a broader group of oncology patients with improved radiation therapy. Not only has the technique to irradiate target volumes with a proton beam evolved, but the layout of proton therapy facilities and their integration into existing hospital facilities has changed.

Proton therapy delivery technology

A particle accelerator, be it a cyclotron or a synchrotron, delivers a narrow particle beam, typically a few millimetres in diameter. This narrow beam is transported through a beam-line to the treatment room, where it is fed to the last part of the beam-line, the so-called 'nozzle'.

The function of the nozzle is to change the properties of the beam in such a way that a target volume of a few centimetres up to a few tens of centimetres in diameter can be irradiated with a therapeutic high dose level while sparing surrounding tissue. The nozzle is a cascade of beam-modifying devices and detectors. Its design and the production of secondary stray radiation differ depending on the technique used. Proton therapy as a treatment modality is undergoing a transition between two delivery techniques at present, moving from passive scattering to pencil-beam scanning.

Passive scattering has been the main delivery technology for the past two decades, and is applied in the majority of cases treated with proton therapy today. The technique creates a wide proton beam, making use of one or multiple scatterers designed geometrically and in composition to produce a wide beam with homogeneous intensity. Active pencil-beam scanning does not require scattering/flattening devices, compensators, or beam-shaping apparatus in the beam. The beam modifier cascade is replaced in the nozzle by a pair of scanning magnets. The scanning beam approach is applied to cover a target volume of up to tens of centimetres with a fine pencil beam, steering a large number of these beam spot dose depositions to a grid of locations in the target. The range of each beam spot is adjusted through energy switching in the energy selection system (ESS), which can be placed upstream in the beam-line at a considerable distance from the patient. Pencil-beam scanning results in a considerably lower neutron background compared with passive scattering, as the main source of secondary radiation is the interaction of the proton beam with the patient, which is obviously inevitable. A major advantage of pencil-beam scanning compared with passive scattering is the improved quality of the dose distribution. In passive scattering, some tissues proximal to the target will receive the same dose as the target volume itself. In pencil-beam scanning, this can be avoided and the dose to these tissues can be reduced.

The promises and challenges for proton therapy

The proton beams need to be used optimally. If used inappropriately, proton dose distributions may be no better, or even worse, than those for

photon intensity modulated treatments. The cost of proton therapy is high**.** Most of the costs of proton therapy (capital and personnel) are fixed, therefore proton therapy must be made more efficient so that more patients can be treated and the fixed costs can be spread among a greater number of patients. The IMPT efficiency needs to be optimized. IMPT will result in improved dose distributions and neutrons produced will be lesser than when passive scattering techniques are used. Clinical investigations need to be conducted in those disease sites that have not yet been shown to be better treated using proton beams. Physicians, physicists, therapists and dosimetrists need to be trained in proton therapy. There is a substantial shortage of personnel that are experienced in proton therapy. More proton therapy facilities need to be built. For many disease sites there is no justification for using photons if proton beams are available-this is especially true for paediatric patients. Proton therapy is often not available to patients who can benefit from this important treatment modality. Clinical trials that compare protons and carbon ions need to be conducted. It has not been definitively shown that carbon ions result in improved clinical outcomes over those that can be achieved using proton beams. The physical dose distributions of carbon ions and protons are qualitatively very similar. Carbon ions may offer a biological advantage over proton ions; however, they will be more expensive. Before building many carbon ion facilities we must determine that they will improve clinical outcomes. We do, however, need to build a few carbon ion facilities in order to conduct the necessary clinical research.

Keywords: Proton therapy; Passive scattering; Pencil-beam scanning

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PP33

Mapping Dynamical Systems onto 2D – Applications in Macromolecular dynamics

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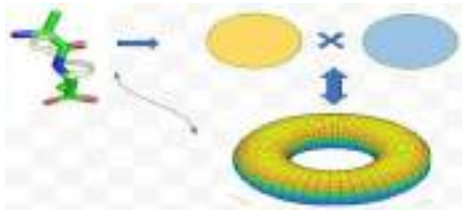
We propose a conjecture between a variant of Monte-Carlo method and flat-space decomposition of dynamics of Homopolymer systems, by Constructing Geometrical Poincare Sections. The method works by capturing the global dynamics and is proven to be efficient for dimensions that scales to utmost 20. We apply the method to model Homopolymer systems using Mutual Orthogonal Latin Squares (MOLS) and illustrate that Scrambling the sequences in MOLS method[1–3] improves the convergence at Atomistic Scales.

Graphical Abstract:



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PP34

Review on helioseismology using time-distance technique

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On the surface of the Sun, resonant vibrations can be produced by sound waves created in the solar convection zone. With helioseismology, we may examine them to gain a deeper understanding of the solar interior. The Sun's core appears to rotate more quickly than its surface. Discoveries about the complicated movement of the Sun's active regions as well as the corona's and heliospheric impact on its magnetic field is revealed through Helioseismology.

Global modes can therefore be used to measure solar oscillations. The frequency of these modes reveals information about the Sun's structure and spin. However, these cannot be seen in a three-dimensional image. Local helioseismology paves a pathway for this by examination of the regional modes. In addition, local modes can be used to estimate the depth of subsurface penetration. Direct modelling, Fourier-Hankel decomposition, ring-diagram analysis, time-distance helioseismology, helioseismic holography, and helioseismology are some of the key techniques used to study local helioseismology. In this article, we will be discussing in detail about the time-distance methodology of local helioseismology and their fascinating discoveries.

Keywords: Vibrations; solar interior**;** Convection zone; Local helioseismology; Time-distance methodology; Sun's structure

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PP35

Preparation and structural analysis of TiO_2 nanofiller incorporated PEO- $AgCF_3SO_3$ polymer electrolyte

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Polymer electrolytes are compounds developed by the dissolution of salt into polar and excessive molecular weight polymers [1]. PEO is widely used as a common host polymer because of its ability to dissolve a wide variety of metal salts, and also exhibits good mechanical properties compared with those of other polymer hosts [2,3]. The main drawback of PEO based electrolytes is their low conductivity value (10^{-9}-10^{-7} Scm^{-1}) at the ambient temperature, and this restricts their use in commercial devices [4,5]. To overcome this disadvantage, a few methods are suggested that would change the morphology of the host by the addition of nanofillers, plasticizers, ionic liquid and salt with large anion within the polymer matrix [6].

The present work is, therefore undertaken to explore the development of silver-ion conducting nanocomposite polymer electrolyte systems based on PEO-$AgCF_3SO_3$ incorporated with nano-sized inorganic TiO_2 fillers in order to arrive at a polymer electrolyte system with better performance. Thin films of nearly 100 microns thickness containing Polyethylene oxide (PEO) and Silver trifluromethane Sulphonate or Silver triflate ($AgCF_3SO_3$) were prepared by solution casting technique. The films were air-dried at room temperature and pressure. Fourier transform infrared (FTIR) spectroscopy has been carried out on the complexes containing PEO and $AgCF_3SO_3$ salt and also on the electrolytes incorporated with 5 % TiO_2. Spectral analysis of the samples by Fourier Transform Infra-Red (FTIR) spectroscopy has revealed the complexation of silver ions with oxygen in PEO. The room temperature X-ray diffraction studies have shown the presence of the two

characteristic peaks of PEO. Also, the complexation of the salt and nanofiller within the polymer matrix is revealed by the reduced intensity of the PEO peaks. This promising approach of dispersing nano-sized filler has proved to influence the materialistic property of the electrolyte system as reported in literature [7-9].

Keywords: Polymer electrolytes; PEO; Silver triflate; Nano TiO_2; Structural changes

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PP36

Energy storage for a Greener future: Comprehensive timeline of materials and technologies

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It's time to harness wind water and sun. Our continued reliance on fossil fuels is unsustainable. If we are to avoid an energy crisis in the future, we must shift to renewable energy sources and storage devices. The world's energy needs are getting out of hand, fossil fuel resources are running out, and existing energy conversion technologies are inefficient. Energy materials and storage devices must meet certain requirements to achieve a sustainable energy development. These requirements include increase in the energy density, lifetime, and safety of energy storage devices, as well as reducing their cost and environmental impact. Lithium-ion batteries, sodium-ion batteries, supercapacitors, metal oxide electrode materials, graphene-based mesoporous materials, and lithium-sulphur batteries are examples of materials that offer specific advantages in each area. Advances in energy storage, such as batteries and supercapacitors, have the potential to revolutionise the way we use and store energy. This article examines the timeline of energy materials and their storage methods. Future research will concentrate on graphene-based metal oxide electrodes with high storage capacitance and heterovalent doping, resulting in ultrahigh energy storage density in multilayer capacitors.

Keywords: Graphene; Batteries; Perovskite; Electrodes; Supercapacitor

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PP37

Characterization of Microplastics in estuarine surface sediments from Estuaries on the southwest coast of Kerala

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Plastic pollution is a rapidly worsening environmental problem, especially in oceanic habitats. The ubiquity of microplastics in aquatic and terrestrial environments and related ecological impacts have gained global attention. The impact of microplastic pollution on the environment and biota is not well known. In this context, to examine the occurrence of microplastic particles (MPs) on the southwest coast, samples were collected from five sites from Chandragiri and Kavvayi backwaters and processed for microplastic extraction through density separation. Identification of the polymer components of MPs was carried out using Raman spectroscopy and the surface characteristics of microplastics and the morphological alteration in microplastics were done using a Scanning electron microscope (SEM). This will help further to use this technique, which is becoming especially relevant in microplastic analysis.

Keywords: microplastics; Density separation; Polymer composition; Raman spectroscopy; Scanning electron microscope

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Natural radioactivity assessment of surface sediments from the selected estuaries in Northern Kerala

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The Present study is emphasized to assess the radiation hazards from the selected estuaries in Northern Kerala using the activities of natural radionuclides ^{238}U, ^{232}Th, and ^{40}K. In order to achieve the aim of the study 12 sediment samples were collected in two estuaries. 4 from Chandragiri estuary and 8 from Kavvayi estuary. Textural analysis was carried out to determine the percentage of sand, silt and clay. The activity concentrations of the radionuclides were determined using gamma ray

spectrometry The of activities of ^{238}U, ^{232}Th, and ^{40}K ranges from 27 to 55, 17 to 24, and 197 to 440 Bq kg−1, respectively in Chandragiri backwater, and in Kavvayi activities of ^{238}U, ^{232}Th, and ^{40}K ranges from 43 to 67, 10 to 23, and 255 to 535 Bq kg−1, respectively which were comparable to values of other regions in the world. The radium equivalent activity was less than the recommended limit of 370 Bq kg−1; therefore, the sediment in this area can be safely used for reclamation.

Keywords: Radiation; Radionuclides; Estuaries; Kerala; Backwater

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PP39

Phytochemical Analysis and Molecular Docking studies of pomegranate fruit peel against cervical cancer

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Since ancient times, secondary metabolites obtained from plant sources have been used by humans for therapeutic purposes, even though the mechanism involved in the process of curing the ailment was not known. Different phytoconstituents like flavonoids, terpenoids, and antioxidants of many plant species are used to wound-repair and for treating inflammations, tumors and viral and fungal infections (1,2). India is home to thousands of species of plant that find use as medicines in Siddha, Ayurveda and Unani system of medicines. Currently, medicines based on such traditional knowledge systems are gaining popularity because of many advantages like safety, lower side-effects, cost-efficacy and easy availability.

In view of this, in the current work, it is proposed to analyze the phytoconstituents of the peel of the fruit pomegranate. While the pulp of

the fruit is consumed widely, its skin or peel, in spite of having high content of valuable phytoconstituents, is generally discarded. Recent research has revealed that peels too contain valuable phytochemicals, with a number of therapeutic uses (3, 4). So, in the current work, a thorough investigation of the phytochemicals present in the peel of pomegranate fruit using spectroscopic tools was done and docking studies of selected phytochemicals from the peels against a cancer that afflict women, namely cervical cancer. According to reports by WHO, cervical cancer is the 4th most common cancer among women. In India alone, about 2% of the female population in the 0 to 74 years age group is in the cervical cancer risk group. About 90% of the new cases and deaths world-wide in 2020 occurred in middle-income country like ours. Two Human Papillomavirus (HPV) types (16 and 18) are responsible for nearly 50% of cervical cancers (5, 6). Cervical cancer is caused by the Human Papilloma Virus (HPV), and can be prevented by vaccination and early detection. But, once the cervical region becomes cancerous, treatment becomes very painful, with chemotherapy or radiation therapy. The main disadvantage is the severe side-effects of chemotherapy, making the patient completely lose a good life-style.

FTIR spectra of the ethyl acetate extract of pomegranate peel was recorded, analyzed and assignments of the various functional groups was done based on data already available. The GC-MS spectra was recorded and the various compounds that were observed were identified from data readily available in the National Institute of Standards and Technology (NIST) library. Two of the compounds identified from GC-MS analyses of the peel extract, namely, o-cymene and D-limonene were studied for their activity against cervical cancer using Auto Dock Vina software (7). The three-dimensional structure of phytocompounds were optimized for docking conformation study. The structure-based molecular docking was performed to study the protein-ligand interactions of the phytochemicals with target proteins obtained from databases available (for example, Research Collaboratory for Structural Bioinformatics (RCSB) data bank).

The best binding conformation of phytochemicals against target proteins was determined based on lowest total binding energy among different conformations generated. For O-cymene, the binding affinity with E6 protein of the Human Papilloma virus was found to be -6.1 kcal/mol and for E7 protein it was found to be -4.2 kcal/mol So, pomegranate peel extract is better inhibitor of the E6 protein. Further, relative strengths of the binding interactions of best identified phytocompound, ligand efficiency were also analysed using AutoDock Vina.

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PP40

Density functional theory studies on structural, electronic, and optical properties of double perovskite $K_2AgInCl_6$ using wien2k

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The double perovskites are potential sources of clean and sustainable energy. The cubic phase double perovskite $K_2AgInCl_6$ crystal structure has a lattice constant of 9.9638 Å and a space group of $Fm\bar{3}m(225)$. The structural, electrical, and optical characteristics of the double perovskite $K_2AgInCl_6$ have been investigated using density functional theory. $K_2AgInCl_6$ possesses an extremely stable crystal structure with a straight band gap, both of which are necessary for inter-band transitions and recombination. The band gap of 2.880 eV was estimated from the band structure of $K_2AgInCl_6$. The optimized lattice constants are used to calculate the optical properties of K2AgInCl6, including the dielectric constant, refractive index, optical loss, optical conductivity, etc.

Keywords: Double Perovskites; Density Functional Theory; Dielectric constant; Optical conductivity

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PP41

The First Principle Calculations on Structural, Electronic, and Optical Properties of Ternary semiconductor $AgInS_2$

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Density Functional Theory has been used to calculate the structural, electrical, and optical characteristics of $AgInS_2$. The Self Consistent Field is obtained using the Full Potential Linear Augmented Plane Wave (FPLAPW) technique. The space group I-42d and the lattice parameters of the tetragonal crystal structure of $AgInS_2$ are a = b = 5.986 Å and c = 11.509 Å. $AgInS_2$ core/shell configurations in chalcopyrite

semiconductors provide strong narrow-band photoluminescence that result from a band-edge transition. According to the total and partial state densities, the compound's state significantly contributes to the valance band in the energy range from -10 to 0.0 eV. $AgInS_2$, a ternary semiconductor, has an electronic band gap of 2.0 eV. Using optimal lattice parameters, it has been possible to explore the optical properties of $AgInS_2$, including its dielectric constant, refractive index, optical loss, optical conductivity, etc. $AgInS_2$ is a direct band gap semiconductor at Γ - Γ point.

Keywords: Density Functional Theory; Full Potential Linear Augmented Plane Wave; Chalcopyrite; Dielectric constant; refractive index

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PP42

Artificial Leaf like Photonic Crystals of g-C_3N_4 Hydrogel using Polyvinyl Alcohol for Photocatalytic H_2-Generation (PVA@g-C_3N_4 Hydrogel)

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"In the 20th century, global average temperature has increased by 0.7˚C" [1]. Hence there arise a need for clean and green method, one of the ways to limit the greenhouse gases is generation of hydrogen fuels which is now a developing area of interest, and can be seen as future fuels as they do not pollute air, which led to the discovery of photocatalytic activity of TiO_2. Various semiconductor photocatalyst materials have been observed for producing H_2 gas efficiently. This study cooperatively discloses the basic introduction of photocatalysis and its working principle of PVA@g-C_3N_4 Hydrogel. Among the materials used in photocatalysis for the application of H_2- Generation, g-C_3N_4 (graphitic carbon nitride) has gained attention due to its combined property of its electronic structure,

its notable high physiochemical stability (among organic materials) and its suitable band position (E_g = 2.7-2.8 eV) which further supports the photocatalytic water splitting activity even in the visible light absorption of around 450-460 nm.

In this paper g-C_3N_4 are improvised as photonic crystals mostly used for photocatalysis possess inverse opal structure. This array of air spheres within the matrix of respective photocatalytic material upon being periodic on the same length scale as light, influence the propagation of light by trapping photons in them. This modification overcomes the disability of pure g-C_3N_4 as poor light absorber. This paper continues to discuss the production of H_2-Generation effectively done by g-C_3N_4 embedded with PVA (Polyvinyl Alcohol) films that serves as polymeric solvents for water splitting. The main focus of this study is to fabricate a freestanding graphitic carbon nitride g-C_3N_4@PVA films of dimensions (1×1, 2×2, 3×3 etc.) for enhanced photocatalytic water splitting. The details regarding the synthesis and main principle on which it works along with its application is briefly studied in this paper.

Keywords: PVA-g-C_3N_4 hydrogel; water splitting activity; Photocatalytic H_2-generation.

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PP43

Effect of Mg substituted in p-type Manganese telluride for thermoelectric application

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Manganese Telluride (MnTe) is one of the emerging thermoelectric materials in recent days and wonderful material for energy conversion and storage purpose. Pristine MnTe is a p-type semiconducting material with low carrier concentration and low electrical conductivity. Magnesium is incorporated with MnTe in stoichiometric ratio of $Mn_{1.12-x}Mg_xTe$ (x=0, 0.01, 0.025, 0.05, 0.075) via Vacuum sealing and hot press methods. The structural, electrical and thermoelectric properties of Mg substituted MnTe has been studied. Morphology of the samples was analyzed by HRSEM and HRTEM. Seebeck coefficient, electrical conductivity and thermal conductivity were measured in the temperature range of 303-753 K. The power factor and figure of merit (zT) were estimated for the data. The maximum power factor of $361\mu W/mK^2$ is achieved at 753 K for $Mn_{1.07}Mg_{0.05}Te$. The maximum zT of 0.27 is obtained at 753 K for $Mn_{1.07}Mg_{0.05}Te$. In this study the electrical conductivity and thermoelectrics property of the material is enhanced via Mg substitution.

Keywords: MnTe; Mg substitution; Power factor; Seebeck coefficient; Thermoelectrics property

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PP44

Review on Treatment of organic pollutants using titanium dioxide as Photocatalyst

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Photocatalyst has been proposed as an efficient solution in dealing with degradation of organic pollutants in air, water contamination and has also been proposed to be used in degradation of oil spills. Titanium dioxide as a photocatalyst has shown promising results in water purification. Different phases of TiO_2 like anatase phase has high photoactivity whereas the rutile phase of TiO_2 has chemical stability. However the energy band width of titanium dioxide is large which limits the absorption light range from visible light to UV which constitutes less than 5% of the solar spectrum. Also, the recombination rate of titanium dioxide is fast which limits its photocatalytic activity. In order to overcome these disadvantages, titanium dioxide is doped with different types of dopants {Semiconductor doping (CdS, Cu_2O, Fe_2O_3, WO_3, etc.), metal doping (Cr^{3+}, Fe^{3+}), and non-metal doping (N, S and C)} and their efficiency is studied.

Keywords: Titanium dioxide; Photocatalyst; Organic pollutants; Oil degradation; Doping

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PP45

The Structural, Electronic and Optical properties of ternary semiconductor using wien2k code

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The structural, Electronic and optical properties have been calculated for $AgInSe_2$ using Density Functional Theory (DFT). $AgInSe_2$ is one of the potential compounds of this family of alloys due to its wide band gap of around 1.2eV. This chalcopyrite structure is closely related to the zinc blend structure. It forms the crystal structure with the space group I 42d. Its lattice parameters are a=5.85438Å, b=5.85438Å and c=11.45789Å. It shows the direct energy gap with Eg~1.2eV. The electrical studies of this compound gives a wide range of conductivity and it also dominated by shallow donors. The optical band gap lies between 0.8 and 2.0eV. The total and partial density of states indicates the state of compound have the strong contribution of valance band in the energy range from 1.873eV to 1.92eV. The dielectric constant, refractive index, optical loss, optical conductivity and other Properties of $AgInSe_2$ are calculated using optimized lattice constants.

Keywords: Density functional theory; Optical conductivity; Optical loss; Refractive index; Dielectric constant; chalcopyrite structure

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PP46

One Step Green Way Synthesis of Cu_2O Nanoparticles using Citrus limon Pulp Extract: Antimicrobial Evaluation

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Cuprous oxide is a most promising material for different applications due to its interesting characteristics such as low-cost, abundant availability and nontoxic nature. Green route synthesis of metal oxide nanoparticles provides an extensive, reliable, sustainable, cost-effective and eco-friendly protocol. We report a facile one-step green synthesis of cuprous oxide nanospheres by reducing Cu^{2+} ions using Citrus limon (lemon). The pulp extract serves both as reducing and stabilizing agent under ambient temperature. The face centered cubic phase with space group pn3m is confirmed from X-ray diffractograms. SEM micrographs reveal well defined spherical shaped nanoparticles having higher tendency for agglomeration. The two absorption peaks at 311 nm and 383 nm in the UV-Vis absorption spectrum confirm the formation of CU_2O nanoparticles. FTIR supports the presence of L-ascorbic acid which plays a significant role in reduction of copper ions. Good zones of inhibition obtained on assays of bacterial and fungal strains establish the prepared cuprous oxide nanoparticles to be an effective antimicrobial agent.

Keywords: Green route; Nanoparticles; Metal Oxide; Spherical

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PP47

Structural and Optical properties of rare earth doped ZnO Nanoparticles

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ZnO, a compound semiconductor with a large dielectric band gap, has several uses in photonics, optoelectronics, and photocatalysis. Using the precursors of Zinc acetate dihydrate and Gadolinium trinitrate in different ratios (0 mol - 3 mol%), the simple co-precipitation technique was used for the synthesis of Pure and Gadolinium (Gd) doped Zinc Oxide (ZnO) nanoparticles (NPs). X-Ray Diffraction analysis of the structural characteristics of as prepared pure and Gd doped ZnO NPs revealed the sample to have a high degree of crystallinity [1]. The diffraction peaks (100), (002), and (101) are indexed to the hexagonal wurtzite structure, and the produced NPs' lattice characteristics and crystallite size were investigated. From UV-Visible spectrum used to determine the optical studies of the nanoparticles, such as absorption and transmission of the Gd doped ZnO (GZO) nanoparticle [2-3]. The morphological studies of the shape of the nanoparticles and their size distribution were observed using SEM analysis.

Keywords: Gd; ZnO; Co-precipitation; Nanoparticles

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Women's Christian College, the first private college for women in Chennai was established in the year 1915. The college aims to provide a complete, meaningful and relevant education to women so that they are intellectually well-trained, morally upright, socially aware and spiritually inspired. The college has been an autonomous institution for 40 years, affiliated to the University of Madras. The National Assessment and Accreditation Council (NAAC) accredited the college with Grade 'A+' in 2019. The College has been awarded with 'Potential for Excellence' status by the UGC in 2016. The college has tie-ups with many state, central and private industries and institutes. The college has many collaborations with universities overseas - Liverpool Hope University, (U.K.), LeTourneau University, (Texas, U.S.A), Ginling College, Nanjing Normal University (People's Republic of China) and Binary University, (Malaysia).

The Department of Physics, established in 1916, has been offering the B.Sc. Program since 1953 in the government aided stream and the M.Sc. Program was started in 1999 under the self-financed stream. The department provides a vibrant and conducive environment to kindle students' curiosity in theoretical and experimental Physics as well as research, imparting strong foundation under the guidance of well experienced and qualified faculty. Original research and creativity are encouraged and nurtured to enable students to pursue a career in Physics and other related fields.

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