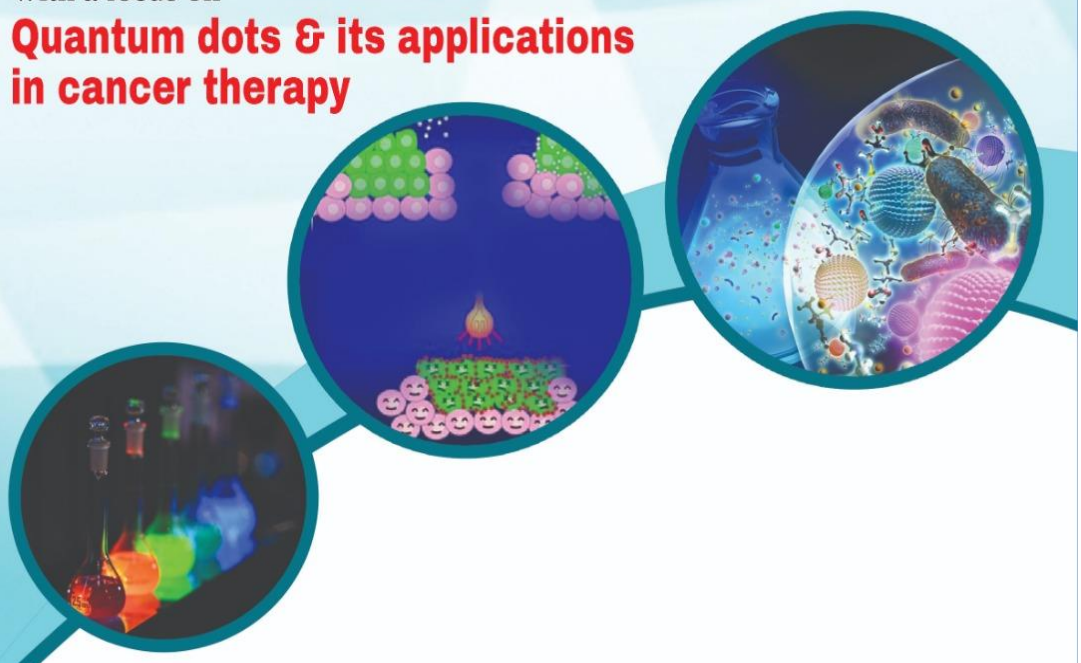
iCNMS 2023

INTERNATIONAL CONFERENCE ON NANOTECHNOLOGY AND MATERIALS SCIENCE

With a focus on

Quantum dots & its applications in cancer therapy



PROCEEDINGS

Organized by

PG & Research Department of Chemistry
Mar Ivanios College (Autonomous)
Thiruvananthapuram

December 18 & 19, 2023

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International Conference on Nanotechnology and Materials Science

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Mar Ivanios College (Autonomous)

Nalanchira, Thiruvananthapuram-695015

Kerala, India

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About the College

The College was established in 1949 and pursues excellence upholding the far-sighted vision of our revered Founder, Servant of God Archbishop Mar Ivanios. The College currently offers 18 Under Graduate degree programmes and 9 post-graduate programmes. Upholding academic excellence, the Institution has established six research centers. Initially, a college affiliated with the erstwhile University of Travancore, the College has been affiliated with the University of Kerala since 1957. Mar Ivanios College is the first Institution in the University of Kerala to receive accreditation from the National Assessment and Accreditation Council (NAAC) in 1999. The College was also the first to be re-assessed and re-accredited with an "A" Grade by NAAC in 2004. In 2011 the College was re-assessed by the NAAC Peer team as part of the Third Cycle of the re-accreditation process with an "A" grade. Mar Ivanios College became the first private college affiliated with the University of Kerala to receive the status of College with Potential for Excellence (CPE) from the UGC. The College has been conferred Autonomy status by the UGC since June 2014. In 2019 the College underwent the 4^{th} cycle of the re-assessment process by NAAC to obtain an "A^{+}" grade. The National Institutional Ranking Framework (NIRF) ranked the college at 36^{th}, 29^{th}, 48^{th}, 44^{th} 50^{th} and 45^{th} positions in the NIRF Rankings (for Arts & Science Colleges) 2017, 2018, 2019, 2021, 2022 and 2023 respectively. In 2019 the college has conferred the status of a UGC-Paramarsh Mentor College.

About the Department

The Department of Chemistry was established in 1957 and the post-graduate course was started in 1964. A research centre in Chemistry was established in the College in 1976, with a view to promote research interests, both among the students and the teachers of the Department. Currently the Department offers under-graduate courses, post-graduate courses and research programmes. The Department is an approved research center for Chemistry under the University of Kerala. Chemistry is offered as a complementary course to the UG students of Physics, Botany and Zoology. From its inception, the Department also offers various add on-courses such diploma in Pharmaceutical Chemistry, Certificate courses in Principles of Phytochemistry and Instrumental Methods of Analysis. The galaxy of eminent alumni bears ample testimony to the Department's excellence because of the hard work and dedication of a team of committed faculty members, guided by able administrators. The Department is a DST-FIST supported Department. The golden jubilee of the PG Department of Chemistry was celebrated in the academic year 2015-16. The Department has produced several nationally and internationally renowned scientists and professors who are

holding positions of high esteem. The Department provides consultancy services to IGNOU and undertakes projects from various industries.

About the Conference

Quantum dots, sometimes called artificial atoms, are precise nanocrystals made of silicon and other semiconductor materials that are just a few nanometres wide — small enough to exhibit quantum properties just as individual atoms do, although they are a hundred to a few thousand atoms in size. Because electrons can be trapped at certain energy levels within them, the nanocrystals can emit only certain wavelengths of light. By controlling the size of the particles, researchers can program precisely what colour the quantum dots will flash when stimulated. Researchers can precisely determine what colour of light will emerge from the quantum dots simply by regulating their size. That offers a huge advantage over the use of other kinds of fluorescent molecules, for which a new type of molecule is needed for every distinct colour. This advantage in controllability isn't limited to the colour of quantum dots. By adjusting the size of the nanoparticles, researchers can also adjust their electrical, optical and magnetic effects, as well as physical properties like their melting point or how they influence chemical reactions. The conference intends to bring together experts in the area of nanotechnology and material Sciences. Deliberations and discussions on these important areas of research will be conducted.

FOCUS AREA OF THE CONFERENCE

- Biomaterials
- Ceramics
- Electronic materials
- Luminescence and fluorescent materials
- Magnetic materials
- Materials for energy and the environment
- Nano electronics and photonics
- Nano toxicology
- Nanocomposites
- Nanomaterials
- Nanomechanics
- Semiconductors
- Superconductors

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Abstracts Edited by

Dr. R. Selwin Joseyphus

December 2023

Printed in India: Designed by S.A. Solutions, Malamukal, Thiruvananthapuram, Kerala

Published by

Department of Chemistry, Publication Division, Mar Ivanios College (Autonomous), Nalanchira, Thiruvananthapuram, Kerala, India

INVITED SPEAKERS

Prof. (Dr.) Mohanan Kunnummal
Hon` Vice-Chancellor, Kerala University of Health Sciences & University of Kerala, Thiruvananthapuram

Prof. (Dr.) Vasudevan Pillai Biju
Hokkaido University, Japan

Prof. (Dr.) Jarugu Narasimha Moorthy
Director, IISER, Thiruvananthapuram

Prof. (Dr.) Suresh Das
IISER, Thiruvananthapuram

Prof. (Dr.) Kuruvilla Joseph
IIST, Thiruvananthapuram

Prof. (Dr.) I Hubert Joe
University of Kerala, Thiruvananthapuram

INVITED SPEAKERS

Prof. (Dr.) R. Justin Joseyphus
NIT, Tiruchirappalli

Dr. Reji Varghese
IISER, Thiruvananthapuram

Dr. G. Antilen Jacob
London Center for Nanotechnology, UK

Prof. (Dr.) G.M. Nair
Director, CLIF
University of Kerala

INVITED SPEAKERS

Prof. Zeena S. Pillai
Amrita Vishwa Vidyapeetham
Amritapuri, Kollam

Prof. George Lukose
Mar Ivanios College (Autonomous)
Thiruvananthapuram

Dr. T. R. Satyakeerthy
Assistant Regional Director, IGNOU Regional Centre
Thiruvananthapuram

PROGRAM SCHEDULE

Day 1- Monday, December 18, 2023

Registration	**8.00 am – 8.45 am**
Welcome address	**Dr. Suju C. Joseph** *Head & Coordinator, Department of Chemistry* *Mar Ivanios College (Autonomous)*
Presidential Address	**Rev. Fr. Vincy Varghese** Principal *Mar Ivanios College (Autonomous)*
Inaugural Lecture	08.45 am -09.45 am
Introducing the Session	**Dr. Suju C. Joseph** *Head & Coordinator, Department of Chemistry* *Mar Ivanios College (Autonomous)*
	"***Molecules to Materials: Porous Organic Polymers (POPs) by Bottom-UP De Novo Design***" **Prof. (Dr.) Jarugu Narasimha Moorthy** *Director, IISER TVM*
Plenary Lecture- I	09.45 am-10.45 am
Introducing the Session	**Dr. Suja Mathai** *Assistant Professor, Mar Ivanios College (Autonomous)*
	"***Advances in Magnetic Nanoparticle Theranostics***" **Dr. R. Justin Joseyphus** *Professor & Head, Department of Physics* *National Institute of Technology (NIT), Tiruchirappalli*
TEA BREAK	10.45 am -11.00 am

Plenary Lecture- II	11.00 am-12.00 pm
Introducing the Session	**Dr. Jinu M. John** Co-convener ICNMS 2023 *Mar Ivanios College (Autonomous)*
	"***Silicon quantum dots as spin qubits***" **Dr. G. Antilen Jacob** *London Center for Nanotechnology, United Kingdom*
Plenary Lecture- III	1**2.00 pm -01.00 pm**
Introducing the Session	**Dr. R. Selwin Joseyphus** *Convener ICNMS 2023* *Mar Ivanios College (Autonomous)*
	"In-vitro and In-vivo Studies of Folate Decorated Fe_3O_4 @AU-DEX-CP Nano Formulation for Targeted Drug Delivery in Colorectal Cancer Therapy" **Dr. I. Hubert Joe** *Professor & Head* *Department of Nanoscience and Nanotechnology* *University of Kerala, Thiruvananthapuram*
LUNCH BREAK	01.00 pm - 1.45 pm
Plenary Lecture- IV	01.45 pm-2.45 pm
Introducing the Session	**Dr. Sajith Kurian** *Assistant Professor, Mar Ivanios College (Autonomous)*
	Dr. Vasudevan Pillai Biju *Professor, Graduate School of Environmental Science* *Hokkaido University, Japan*
Plenary Lecture-V	02.45 pm - 03.15 pm
Introducing the Session	**Dr. Suju C. Joseph** *Head & Coordinator, Department of Chemistry* *Mar Ivanios College (Autonomous)*

	"***Photodynamic Therapy -Paradigm Shift in Cancer Treatment***" **Dr. Zeena S. Pillai** *Professor* *Amrita Vishwa Vidyapeetham, Kollam*
Research Poster Presentations	03.15 pm -04.00 pm
TEA BREAK	04.00 pm -04.15 pm

Day 2- Tuesday, December 19, 2023

INAUGURAL SESSION	**9.30 am-10.30 am**
TEA BREAK	10.30 am – 10.45 am
Plenary Lecture-VI	10.45 -11.45 am
Introducing the Session	**Dr. Sonia Mol Joseph** *Organizing Secretary ICNMS 2023* *Mar Ivanios College (Autonomous)*
	"***Responsive DNA nanostructures for cancer therapy***" **Dr. Reji Varghese** *Associate Professor (Chemistry)* *IISER TVM*
Research Oral Presentations	11.45 am-01.15 pm
LUNCH BREAK	**01.15 pm -01.45 pm**
Plenary Lecture- VII	01.45 pm - 02.45 pm
Introducing the Session	**Dr. Rabin Rajan J Methikkalam** *Assistant Professor, Mar Ivanios College (Autonomous)*
	Dr. Kuruvilla Joseph *Outstanding Professor, Registrar & Dean* *IIST, Thiruvananthapuram*
TEA BREAK	02.45 pm to 03.00 pm

December 19, 2023

INAUGURAL SESSION

(9.30 am-10.30 am)

Prayer Song	
Anthem	*Kerala University of Health Sciences*
Welcome Address	**Dr. Suju C. Joseph** *Head & Coordinator, Department of Chemistry* Mar Ivanios College (Autonomous)
Theme of the Conference	**Dr. Sonia Mol Joseph** *Organizing Secretary, ICNMS 2023*
Presidential Address	**Rev. Fr. Vincy Varghese** *Principal, Mar Ivanios College (Autonomous)*
Benedictory Address	***His Excellency Most Rev. Dr. Mathews Mar Polycarpos*** *Auxiliary Bishop of the Major Archeparchy of Trivandrum*
Inauguration	**Prof. (Dr.) Mohanan Kunnummal** *Hon` Vice-Chancellor* *Kerala University of Health Sciences &* *University of Kerala*
Keynote Address	**Prof. (Dr.) G. M. Nair** *CLIF Director, University of Kerala*
Felicitations	**Shri. Abey George** *General Secretary, Swasthi Foundation*
Vote of Thanks	**Dr. R. Selwin Joseyphus** *Convener, ICNMS 2023*

National Anthem

December 19, 2023

VALEDICTORY SESSION

(3.00 pm to 4.00 pm)

Silent Prayer Song	
Welcome Address	**Dr. Sonia Mol Joseph** Organizing Secretary, ICNMS 2023
Chief Guest	**Prof. (Dr.) Kuruvilla Joseph** *IIST, Thiruvananthapuram*
Presidential Address	**Rev. Fr. Vincy Varghese** *Principal, Mar Ivanios College (Autonomous)*
Felicitations	**Dr. Suju C. Joseph** Head & Coordinator, Department of Chemistry Mar Ivanios College (Autonomous) **Prof. K. V. Thomaskutty** Secretary, MSC Colleges
Award Distribution *Ceremony*	**Mr. Jiffin Sam** Co-convener, ICNMS 2023
Summing up	**Dr. Jinu M. John** Co-convener, ICNMS 2023
Feedback	Participants
Vote of Thanks	**Dr. R. Selwin Joseyphus** *Convener, ICNMS 2023*

NATIONAL ANTHEM

* * *

PLENARY LECTURES

PL-01

Advances in Magnetic Nanoparticle Theranostics

R. Justin Joseyphus

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Abstract

Magnetic nanoparticles are useful for biomedical applications such as magnetic nanoparticle hyperthermia, drug delivery, magnetic particle imaging, and magnetic resonance imaging (MRI) contrast agents. The utilization of magnetic nanoparticles for specific applications primarily depends on the particle size, morphology, coercivity and saturation magnetization. The diagnosis and therapy of cancer are presently undertaken using separate techniques such as MRI, radiography, surgery, and chemotherapy. It was shown that magnetic nanoparticles could be employed for diagnosis and therapy, minimizing the hospitalization time, and reducing the side effects compared to conventional treatment methodologies. We present potential spinel ferrite-based magnetic nanoparticles that deliver high specific loss power for magnetic nanoparticle hyperthermia. The heat generated by the magnetic nanoparticles is investigated using non-contact infrared thermography that could also be utilized to investigate subsurface thermal profiles. The physics behind heat generation by magnetic nanoparticles and the mechanism based on the material characteristics shall be presented.

PL-02

In-vitro and In-vivo Studies of Folate Decorated FE_3O_4@AU-DEX-CP Nano Formulation for Targeted Drug Delivery in Colorectal Cancer Therapy

I. Hubert Joe

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Abstract

Targeted drug delivery using magnetic nanoparticles is a great option for cancer treatment due to its site specificity, high encapsulation capacity, and biosafety compared with typical drug delivery systems. Fe_3O_4@Au core–shell nanoparticles were synthesized by pulsed laser ablation technique in liquid. Further, dextran was coated by encapsulating cisplatin and surface functionalizing it with folic acid for targeted drug delivery to treat colon cancer. Dynamic light scattering, field-emission scanning electron microscopy, high-resolution transmission electron microscopy, atomic force microscopy, ultraviolet-visible spectroscopy, X-ray diffraction, and vibrating sample magnetometry techniques have been performed to evaluate the prepared compound Fe_3O_4@Au-DEX-CP-FA. The average size, zeta potential, and polydispersity of Fe_3O_4@Au-DEX-CP-FA were 64 ± 2 nm, −48 ± 9 mV, and 0.040, respectively. The capacity of the drug delivery system was evaluated using loading efficiency and release profile tests. MTT assay of cisplatin loaded Fe_3O_4@Au-DEX-FA nanoparticles on the SW480 cell line revealed that it could diminish cell viability compared with the cisplatin alone. The outcome of apoptosis induction showed that Fe_3O_4@Au-DEX-CP-FA could kill cancer cells via the apoptosis route. Real-time PCR evaluation indicated an enhancement in NF1 gene and a reduction in Wnt-1 gene. In-vivo studies showed that this core–shell drug system dramatically reduced tumor volume in mice and can be used as a potential drug delivery system for clinical colon cancer treatment.

PL-03

Responsive DNA Nanostructures for Cancer Therapy

Reji Varghese

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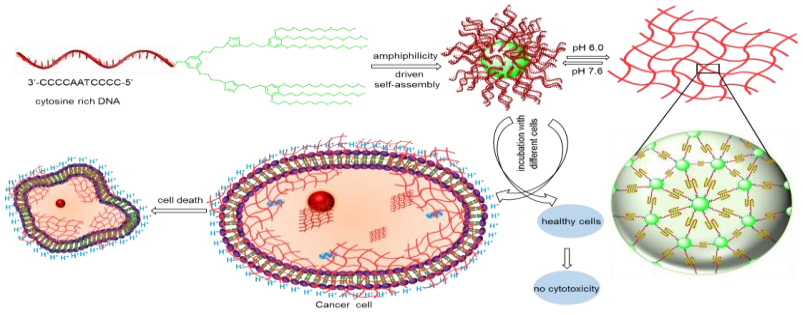
Abstract

Improving the effectiveness of the anticancer drugs while minimizing their side effects is a great challenge in cancer research. Recent research efforts in this direction have shown that encapsulating the cell in a gel network can lead to the cell death. Considering the high proton gradient along the cancer cells membrane, we have designed a pH responsive DNA based smart material which contains C-rich DNA as hydrophilic domain and glycol dendron as a hydrophobic domain, which will self-assemble into micellar nanostructure in basic environment, on acidification cytosine gets protonated and forms inter molecular i-motif, which brings them together and leads to the formation of entangled network. These networks could entrap water molecule which leads to the formation hydrogel. The pH triggered i-motif formation and the fusion of the micelles have been characterized using different spectroscopic and microscopic analysis. The hypothesis was examined using three different cell lines, HeLa, A549 and HEK, where HeLa and A549 cell lines are cancer cell line and HEK is healthy cell line. MTT assay analysis reveals that pH responsive hydrogel is highly cytotoxic for the cancer cell lines and biocompatible for the healthy cell lines. Moreover, CLSM analysis on HeLa cell line showed an extra cellular gelation. Our results suggested that pH responsive hydrogel is a good candidate for the selective inhibition of cancer growth (Scheme 1). Details of these results will be presented.



Scheme 1. *Design of a pH responsive hydrogel for the selective inhibition of cancer growth.*

PL-04

Silicon Quantum Dots as Spin Qubits

G. Antilen Jacob

Quantum Engineering with Solid State Technology (QuES2T), London Centre for Nanotechnology, UCL

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Abstract

The demand for faster and efficient calculations than classical computer has fueled intense research in the quest for robust and scalable qubits. Among various qubit candidates, spin qubits in silicon quantum dots nanostructures have emerged as a compelling platform, combining the advantages of long coherence times with the well-established CMOS technology. Recent breakthroughs in fabrication processes have allowed for precise control over the number of electrons confined within these quantum dots, enabling the creation of well-defined spin qubits. Additionally, advances in material engineering have significantly extended the coherence times of these qubits, a critical factor for error correction and fault-tolerant quantum computation. The integration of silicon quantum dots into scalable architectures is a pivotal aspect of realizing practical quantum processors. Various techniques, such as gate-defined quantum dots and donor-based qubits, are explored for achieving reliable and scalable qubit coupling. Moreover, the development of sophisticated control and readout mechanisms is essential to manipulate and measure the quantum states of these silicon-based spin qubits accurately. In this talk I will provide a glimpse into the recent progress made in leveraging silicon for quantum information processing, emphasizing the potential for transformative advancements in quantum computing.

PL-05

Photodynamic Therapy-Paradigm Shift in Cancer Treatment

Zeena S. Pillai

Amrita Vishwa Vidyapeetham, Kollam

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Owing to its spatiotemporal selectivity and noninvasive nature, photodynamic therapy (PDT) has become a clinically promising approach for the treatment of a wide range of cancers and other diseases. However, the full potential of PDT has not been achieved so far due to the lack of optimal photosensitizers (PSs) and/or smart transport/activation strategies. These problems, which unfortunately lie at the core of the PDT paradigm, include the oxygen reliance limits, the effect of PDT on hypoxic tumors, limitations of light penetration, and undesired skin photosensitization induced by PSs. Recently, supramolecular approaches, which rely on the use of non-covalent interactions to construct biomedical active materials, have become suitable methods for developing innovative PSs. Non-covalent interactions enable supramolecular PSs to have sensitive and controllable photoactivities. In addition, versatile supramolecular PS-assemblies can be designed so that PDT occurs synergistically with other therapeutic modalities

PL-06

Tannin based biomaterials and their applications: A Review

T R Satyakeerthy[a*], Raju Bolla[b] , Devina Devarajan[a]

[a]*IGNOU Regional Centre Trivandrum, Kerala, India*
[b]*IGNOU Regional Centre Hyderabad, Telangana, India*

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Abstract

Tannins are natural polyphenols found in vascular plants acting as defence agents against herbivores, fungi, and other microorganisms. They are mainly of two types condensed and hydolysable. Tannins are highly reactive and the condensed tannins are more reactive than the hydrolysable tannins. Tannic acid (TA), as a polyphenolic phytochemical with high level of galloyl groups, interacts with various substances (proteins, polysaccharides, and metals) through several modes including hydrogen bonding, hydrophobic and electrostatic interactions. Such hybrid or hybrid-like systems allow the preparation of various advanced materials with promising applications. Tannins find many applications in several areas. Condensed tannins are used in tanning hide to prepare leather. The tannins bind with collagen eliminating water preventing bacterial growth. They are also used in preservation of fishing nets preventing degradation of cellulose by bacteria and fungi. Tannins are better anti fouling agents and so can be used in surface coating. Condensed tannins, also known as proanthocyanidins**,** have been added as functional additives to acrylic-based clear coatings to promote polymer coating longevity and also stabilize timber colour on accelerated and exterior weathering. Polymeric surface coatings based on chitosan and tannins are used as antimicrobial agents in corn production. Tannin aminated-Tannin surface coating for particle boards for better cross linking are developed. Tannins are also extensively used in the preparation of bio-based adhesives for sustainability. Tannins are known bactericides because they react with proteins irreversibly, thus complexing within bacterial membranes, neutralizing their activity and therefore tannin-based pharmaceuticals to cure intestine infections have long-time been marketed. They have effective anticaries properties. Tannins or tannic acid can chelate diverse metal ions through coordination bonds and rapidly form a steady

five-element ring complex with these ions. Tannin based biomaterials have great potential in the treatment of different inflammatory and related diseases that are associated with ROS overproduction. Tannin based biological materials have been increasingly studied in the context of IBD, liver injury prevention, ischemic stroke, cognitive impairment, anti-UV skin protection, bone renovation and regeneration and osteoarthritis.

Tannins combine with metal ions, such as Al^{3+}, Fe^{2+}, Fe^{3+}, Cu^{2+}, and Zn^{2+}, can reduce metal elements' toxicity and improve metal drugs' biocompatibility. Tannins are also widely used as water-reducing agents, oil drilling fluid viscosity-reducing agents, pharmaceutical, mineral processing, water treatment, gas desulfurization, metal anticorrosion, wood anticorrosion, printing and dyeing, liquor clarification, oil antioxidant, daily chemical products and other products preparation. Tannins also form hybrids like tannin-metal hybrid, tannin-noble metal hybrid, tannin based metal-carbon hybrid, tannin-ceramic hybrid, tannin-titania hybrid, tannin-zirconia hybrid, tannin based nano composites, and tannin based polyelectrolytes. All these hybrids have exceptional potential as absorbent materials for various applications including 3D and 4D printing.

ORAL PRESENTATIONS

OP-01

Anticorrosion Performance of Zinc Complex of Carboxymethyl Chitosan in Neutral Medium

Nayana Senan V[a], Beena Kumari K.S[*, b], Lekshmy O[a]

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Abstract

Corrosion is one of the most common problems found in everyday life, especially in the oil and gas processing industry. Corrosion can be prevented or controlled by using corrosion inhibitors. Chitosan can be regarded as a biocompatible, non-toxic, environmentally friendly, and cost-effective alternative at the place of synthetic polymers. Chitosan and its derivatives are widely used as corrosion inhibitors. The anti-corrosive applications of chitosan and chemically modified chitosan are demonstrated for different metal/electrolyte systems. The corrosion resistance of the metal complex is improved by introducing polyvinyl pyrrolidone (PVP) as binder. In this work, zinc-based metal complex of Carboxymethylchitosan/PVP (ZCM/PVP) based coatings were investigated for the protection of copper substrates in neutral media. Coated and uncoated copper substrates were characterized by electrochemical techniques, SEM and EDX. Coating on copper substrate was performed by spin coating technique. Potentiodynamic polarization measurements show that the ZCM/PVP acts as a good inhibitor for corrosion. The inhibition efficiency for ZCM/PVP coating is calculated as 92%. The investigated inhibitor has shown good inhibition performance in 3.5% NaCl solution.

Key words: Copper, PVP, SEM, NaCl, Polymer

Reference

1. Zhang, Q.H; Hou B.S.; Li, Y.Y.; Zhu, J.Y.; Liu, H.F; Zhang, G.A, Corrosion Science, ; **2020,** 164, 108346.

OP-02

Unveiling the Molecular Structure and Antimicrobial Potential of a Novel Compound: Insights from Theoretical and Experimental Investigations on DDAPDP

S. Anila Raj, V. G. Vidya

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Abstract

The single crystal 1,5-dimethyl-4-[(2-oxo-1,2-diphenylethylidene) amine]-2-phenyl-1,2-dihydro-3H-pyrazol-3-one[1] [DDAPDP] designed to enhance antimicrobial activity using benzil and 4 aminoantipyrine. Density Functional Theory calculations of DDAPDP were done with Gaussian 16W program employing hybrid functional B3LYP with 6-311++G (d,p) basis set for geometry optimization without symmetry constraints. The single crystal was studied based on theoretical aspects such as Frontier Molecular Orbital (FMO) (Fig. 1), Natural Bond Orbital **(**NBO), Mullikan atomic charge and Molecular Electrostatic Potential (MEP) using density functional method. The experimental and theoretical spectral analysis of the electronic structure was investigated using FTIR, Raman, UV -visible, ^{1}H NMR and ^{13}C NMR techniques. Positive electrostatic potential regions dispersed throughout the rings and represent possible nucleophilic attack sites, whereas negative electrostatic potential regions are typically grouped around the CO group. Energy gap -3.776391 eV, confirmed by the estimated HOMO and LUMO energies. Natural bond orbital analysis (NBO) was used to assess the molecule's stability because of charge delocalization and hyper conjugation. Electron population of each atom was calculated by Mulliken atomic charge distribution analysis. The bacterium E. coli and the organism Staphylococcus aureus, together with a standard medication, were used to study and assess the compounds' antimicrobial activity in vitro. Which reveals that the antibacterial and antifungal activities with DDAPDP compound.

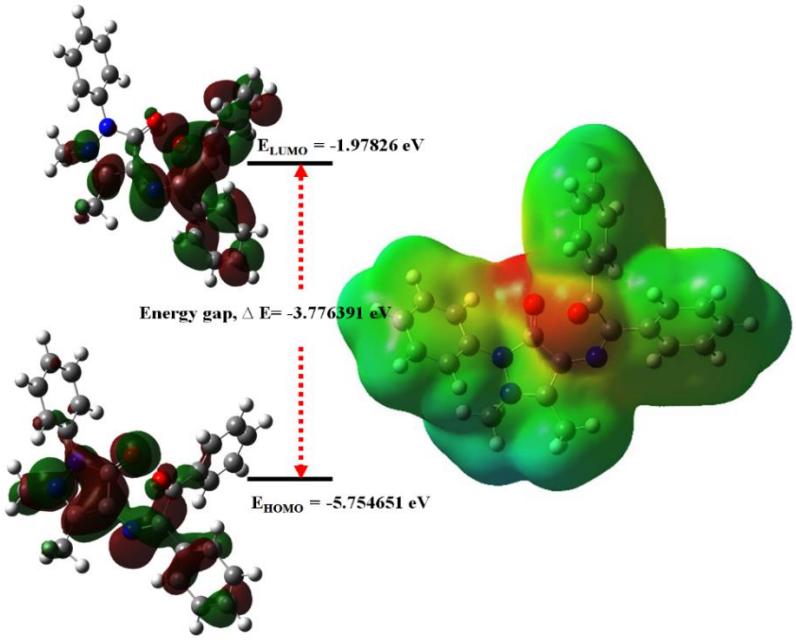

Fig. 1 The 3D plots of the frontier molecular orbitals HOMO and LUMO of the DDAPDP compound.

Keywords: Aminoantipyrine, Benzil, Density Functional Theory, Single Crystal XRD, Antimicrobial activity

References

1. Raj, S. A., Vidya, V. G., Preethi, V., & Kumar, V. V. *Results in Chemistry*, *4*, (**2022**) 100665.

OP-03

Synthesis and Characterization of Polypyrrole@Aluminium- Iron Fumarate Metal Organic Frame Work for The Adsorption of Methyl Orange from Aqueous Solution

Darsana S, Radhakrishnan P.G.
Department of Chemistry, University college Thiruvananthapuram, Kerala, India
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Abstract

A novel aluminium-iron fumarate metal organic framework (AlFeFu-MOF) was synthesized by hydrothermal method and polypyrrole@aluminium-iron fumarate metal organic framework composite was prepared by polymerizing pyrrole over AlFeFu-MOF. The prepared composite was used as an adsorbent for the removal of methyl orange (MO) from aqueous solutions. The synthesized adsorbent was well characterized by FT-IR, XRD, SEM, EDS, BET and TG techniques. pH has a substantial influence on the adsorption of MO and maximum adsorption occurred at pH 4.0. The adsorption of MO on polypyrrole@aluminium-iron fumarate metal organic framework in aqueous solutions at different temperature and pH was investigated to evaluate the operational parameters influencing adsorption. The MO adsorption decreased with increase in pH and temperature. Langmuir-SCA and Freundlich SCA models were used to fit the sorption data at different pH and temperature. The changes in thermodynamic parameters such as ΔG^0, ΔH^0 and ΔS^0 were evaluated from thermodynamic studies. The adsorption is spontaneous and is exothermic in nature.

Keywords: AlFeFu- MOF, Methyl Orange, Isotherm, SCA models, Polypyrrole.

OP-04

Optical Properties of Some Pyrimidine Schiff Bases and their Zinc(II) Complexes

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Abstract

Although transition metal complexes of Schiff bases have been extensively investigated, less attention has been given to optical properties of their metal complexes. A series of zinc(II) complexes of Schiff bases derived from 2-hydroxy-1-naphthaldehyde and aminopyrimidine or its derivatives have been synthesized under microwave assisted solvent free condition. The ligands and metal complexes have been characterized based on elemental analysis, molar conductance measurements, magnetic susceptibility data, UV-Visible, infrared, ^{1}H and ^{13}C NMR spectral studies. The spectral data reveal that the ligands act as monobasic bidentate, coordinating to the metal ion through the deprotonated naphtholate oxygen and azomethine nitrogen. Molar conductance values adequately support the non-electrolytic nature of the complexes. A tetrahedral geometry has been proposed for all the zinc(II) complexes. The Schiff bases under investigation have been studied in both polar and non-polar solvents by UV-Visible spectroscopic technique. Similar spectral features were observed for all the ligands in methanol. The fluorescent properties of the Schiff bases have been studied in different solvents of varying polarity. In the present study the ligands showed fluorescence enhancement on complexation with zinc(II) ion. Enhancement of fluorescence through complexation is of much interest as it opens the opportunity for photochemical applications of these complexes. Besides, at room temperature excited sate intramolecular proton transfer is observed in different solvents, which suggests that the compounds studied are a new class of fluorescent materials.

Keywords: Optical properties, fluorescence enhancement, monobasic bidentate.

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OP-05

Preparation of Novel Green Synthesized Copper Oxide Loaded MOF-74/rGO/PAM Fenton Like Catalyst and Study of Influence of Operational Parameters for the Photocatalytic Degradation of Methylene Blue

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Abstract

A novel light sensitive Fenton like catalyst of green synthesized CuO decorated MOF-74/rGO/PAM composite was prepared by solvothermal method. The metal oxide MOF composite has been characterized by FTIR, XRD, SEM and EDX techniques. The applicability of this metal oxide MOF composite towards the photocatalytic degradation of methylene blue has been explored in the presence of green oxidant H_2O_2. The effect of various operational parameters like concentration of methylene blue, H_2O_2, pH, temperature, influence of different scavengers, catalytic amount was studied as a function of time. The kinetic data were fitted into the pseudo-first-order equation and rate constants were determined. The temperature has a positive impact on the degradation of methylene blue and the activation parameters relating to degradation were calculated. The hydroxyl radicals are responsible for the degradation of methylene blue. Thus, from the above studies, it is found that the novel CuO loaded MOF-74/rGO/PAM composite shows very remarkable Fenton like catalytic property towards the degradation of methylene blue.

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OP-06

Study of Corrosion Inhibition Properties of Nickel Titanate Produced Using New Technology

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Abstract

The corrosion rate of mild steel varies with respect to the environment in which it is exposing, structure and design of the material and the physical, chemical, and electrochemical factors associated with it. A new method of corrosion prevention of mild steel was developed by in-situ deposition of nickel titanate on the surface of it. Nickel titanate coating was designed to be economical and applicable to many surfaces due to high durability and high resistant to oxidizing atmosphere. The specimens were characterized by using XRD and FTIR techniques. The corrosion inhibition tendency of nickel titanate coating was evaluated by weight loss methods, open circuit potential measurements and potentiostatic polarization techniques.

Keywords: Nickel titanate, Corrosion Inhibition, Mild steel, Polarization

OP-07

Thermal Performance of Solar Collector with Different Materials Using Thermosyphon Method

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Abstract

The solar collector is the widest application that had been used in commercial and residential area.[1] To ensure a high heat storage during solar radiation, a thermal performance of solar collector is conducted using thermosyphon method. The thermosyphon method is a natural circulation process that happens due to the density difference between the fluid in the collector and the storage tank.[2] The main objective of the present work is to carry out the thermal performance of solar collector using the materials namely copper, aluminum and plastic. The materials were chosen based on the cost analysis.[3] Initially, the thermal performance of solar collector with high-cost copper risers were experimented. The initial and final temperatures were tabulated.[4] Secondly, the thermal performance of solar collector with medium cost aluminium risers were experimented and the corresponding initial and final temperatures were tabulated.[5] Finally, the thermal performance of solar collector with low-cost plastic risers were experimented. The initial and final temperatures were noted. During the testing of solar collectors with different materials, a maximum temperature of 46.9 ℃ at the outlet from copper risers, 44.7 ℃ at the outlet from aluminium risers and 38.9 ℃ from plastic risers has been achieved. It can be concluded that the copper risers have high thermal performance when compared to aluminium and plastic risers.

Keywords: Solar Collector, Thermal Performance, Copper, Aluminium, Plastic.

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OP-08

Development of Bismuth-Doped Iron Vanadate Zinc Phosphate Coatings for High NIR Reflectance and Corrosion Resistance

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Abstract

The present work investigated the role of bismuth-doped iron vanadate in zinc phosphate coatings for enhancing the NIR reflectance and corrosion-resistance through a morphological change in their hopeite crystals. The phase, morphology, elemental composition, topography and surface roughness of the developed coatings were evaluated through various analytical techniques. A new mechanism has been proposed to explain the nucleation growth kinetics in the developed zinc phosphate coatings, which favors the enhancement of NIR reflectance and corrosion-resistance[1,2]. The high charge transfer resistance (908.4 Ω cm^2**)** and low double layer capacitance (4.490×10^{-12}) obtained from the EIS analysis as well as high E_{corr} (-1192.75 mV) and low i_{corr} (0.89×10^{-3} µA/cm^2) from the Tafel polarization studies confirmed the high corrosion resistance characteristics of the BFV incorporated ZP coating[3]. These coatings also exhibited 83% NIR reflectance, indicating increased crystal nucleation sites and crystal grain boundaries through the proposed mechanism.

Keywords: Zinc phosphate coating; Bismuth-doped iron vanadate; NIR reflectance; Corrosion resistance; hopeite crystals

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OP-09

Synthesis of β- Phase ZnO/PVDF Nanofibers; A Potential Material for Piezoelectric Nanogenerators for Energy Harvesting Applications

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Abstract

In view of the rapid growth of the Internet of Thing (IoT), enormous low power consuming (micro watt or milli watt) electronics devices such as sensors, actuators, and wireless transmitters have been integrated into every corner of this world for a variety of applications. Mechanical energy, such as sound wave, body movement and mechanical vibration, is a potential green power source. It spreads widely in surrounding environment and human bodies and contains small kinetic energies ranging from milli- to tens of watts. It is difficult for conventional mechanical electric generators to harvest these small kinetic energies, but possible for piezoelectric nanogenerators which are made by piezoelectric materials with micro- or nano-structures. Poly vinylidene fluoride (PVDF) has been successfully employed in energy harvesting systems due to its exceptional properties. In the β-phase of PVDF, all its dipoles align in the same direction, exhibiting the property of polarization and hence PVDF β-phase produces spontaneous polarization and exhibits strong piezoelectric characteristics. In the present work, we have developed a composite ZnO/PVDF piezo electric nano fiber, envisaging its very high energy conversion efficiency. The ZnO nanoparticles were synthesized through a novel single step combustion method followed by low temperature annealing. The morphology and formation kinetics of the nanoparticles were studied by transmission electron microscopic imaging and FWHM measurement from the XRD peaks, respectively. ZnO/PVDF nano fibres of optimised diameter ~ 238.6 nm were fabricated through electrospinning technique. The morphology of the PVDF/ZnO nanofibers were examined by FESEM. The β-phase and the functional group exist in the composite were analysed by FTIR spectroscopy.

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OP-10

Co-Precipitation Synthesis of Lithium Nickel Cobalt Aluminium Oxide (8:1:1) Cathodes for Lithium-Ion Batteries

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Abstract

The Li-ion secondary battery is highly recommended as a power source for highly advanced battery electric vehicles. Among various types, the lithium nickel cobalt aluminum oxide (NCA) battery is suitable for high energy and power applications. This study produced the NCA cathode material $LiNi_8$ $CoAlO_2$ via the hydroxide co-precipitation technique to reduce production costs and process complexity. The $LiNi_8$ $CoAlO_2$ (NCA) cathode material was prepared by co-precipitation and calcination at 700 ºC. The structure of NCA was investigated by X-ray diffraction and scanning electron microscopy. The absence of additional peaks in the XRD spectra indicated no change in the crystalline structure of the NCA material after processing. The XRD patterns of NCA show a hexagonal layered structure with no impurities detected. Based on the FT-IR spectra, all precursor samples exhibit two functional groups of hydroxide and carbonate. Based on the SEM images, reveal a uniform distribution of the co-precipitated metal cations. Segregation of particles is due to the difficulty in the precipitation of aluminum. Cyclic voltammetry is used to analyze the cell reaction.

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OP-11

Synthesis and Characterization of $Zn_{2-x}Cu_xV_2O_7(x = 0{\sim}2)$ Nanostructured Ceramics for LTCC Applications

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Abstract

Low Temperature Co-fired Ceramic (LTCC) is a multilayer ceramic technology wherein several ceramic layers with printed conductors are laminated and co-fired with metal electrode at temperatures lesser than 1000 ℃ to form a multilayer interconnection circuit. Nano size $Zn_{2-x}Cu_xV_2O_7(x = 0{\sim}2)$ ceramics ideal for LTCC applications were prepared through a single step modified combustion method and were sintered at a relatively lower temperature for the first time. The powder X-ray diffraction (XRD) analysis of the samples confirmed that the compositions crystalized in monoclinic structure. X-ray Photoelectron Spectroscopy was employed to investigate the oxidation states of the various elements in the compositions. The samples were sintered at a relatively lower temperature to their optimum densities. The microstructural study on the sintered pellets conducted using Scanning Electron Microscopy (SEM) confirmed their compactness. The overall results suggest that these nanostructured ceramics could be used as substrate materials for LTCC applications.

Keywords: LTCC, Combustion synthesis, XPS, SEM

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OP-12

Fabrication of Nanofibrous Microporous Polymer/Ceramic Composite Mat for Tissue Regeneration

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Abstract

Electrospun nanofibrous polyvinyl alcohol (PVA) structures, found to have numerous biomedical applications. They show excellent biocompatibility, flexibility and biodegradability. Highly porous biocompatible structures with adequate strength are required for tissue regeneration applications. Hydroxyapatite (HA) is the main natural inorganic mineral present in human bone as well as teeth. It has high calcium mineralization and collagen deposition capabilities.(1) Reports show that the presence of Al_2O_3 improves the osteogenic properties of HA. This paper reports the incorporation of HA/Al_2O_3 nanocomposites in PVA matrix by the method of electrospinning.(2) An auto-ignited combustion technique was used to synthesize nanostructured HA and Al_2O_3. X-ray diffraction technique was used to confirm crystalline phases present in the samples. The crystalline phases obtained from the ICDD file for HA was hexagonal and for Al_2O_3 was cubic. The crystallite size estimated using XRD was 26 nm for HA and 5 nm for Al_2O_3. HA and Al_2O_3 were mixed with an 80:20 proportions to form HA/Al_2O_3 nanocomposites and dispersed well in 10% (w/v) PVA solution. The spinning parameters were optimized to fabricate highly porous nanofibrous PVA/HA/Al_2O_3 mats. The FTIR spectra conforms its composition. Morphology of the electrospun fibers was studied using Scanning Electron Microscopy. The incorporation of HA/Al_2O_3 in PVA matrix is expected to improve the mechanical and biological properties of the nanofibrous structures, and can be used for bone tissue regeneration applications.

Keywords: Electrospinning, Auto-ignited combustion technique, osteogenic properties, Bone tissue regeneration.

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OP-13

Amide Functionalized Triazine-Based Covalent Organic Polymers for Selective CO_2 Capture

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Abstract

Triazine-based covalent organic polymers are an emerging class of porous organic materials that have been significantly investigated during the last two decades due to their structural characteristics, such as nitrogen-rich structure, chemical stability, fully conjugated skeleton, and high surface areas. All these unique properties make conjugated triazine polymers attractive for widespread applications in gas storage, separation, optoelectronics, and catalysis.[1, 2] The selective removal of the primary greenhouse gas, carbon dioxide, and its separation is crucially important for environmental remediation. Thus, the design and synthesis of covalent triazine materials having high porosity, high specific surface area, and large CO_2 uptake capacity is an emerging field of research.[3]

In this study, amide-functionalized covalent triazine organic polymers (**TAP** and **TAmP**) were synthesized for selective CO_2 adsorption. The porous polymers were characterized by powder XRD analysis, XPS measurement, CHN analysis, solid-state ^{13}C-NMR, and FT-IR spectroscopic tools. The Thermal stability and morphology of the materials were studied by TGA measurements and SEM analysis. Textural characterization and CO_2 adsorption studies of the synthesized materials were carried out via sorption analysis. We do believe that the prepared nitrogen-rich functional materials can serve as excellent materials for capturing greenhouse gases.

Keywords: Porous materials, Covalent triazine polymers, CO_2 adsorption.

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OP-14

Development of a 'turn-on' sensor for the selective sensing of pesticides in aqueous medium

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Abstract

Coordination polymers or Metal organic frameworks are a wide variety of molecules comprised of both organic and inorganic moieties. They are formed by the coordination of the ligand to metal center and repeating coordination entities extending in one, two or three dimensions. A wide variety of CPs or MOFs with structural diversity can be optimized using variety of metal centers and functionalized ligands under different synthetic conditions. The symmetry and rigidity of the ligands play an important role in the properties of the resulting CPs or MOFs. Introduction of these molecules opened a new era in the field of catalysis, separation of gases, electronic and optoelectronic device applications, photochemical sensing and biosensing, luminescent sensing, antimicrobial applications etc. Due to the rapid growth of population and economic development, an increase in the demand for agricultural products has become a challenge to humankind. This challenge results in an appreciable change in agricultural productivity by introducing hybrid and genetically modified seeds, advanced agricultural strategies and tools, proper water management systems, utilization of potent pesticides etc. Pesticides are inevitable component in agriculture because approximately one third of global agricultural production depends on such pesticides. Generally, pesticides are highly toxic and hence its detection is highly significant. The present work mainly focuses on the development of a turn-on sensor for the selective sensing of pesticides in water.

Keywords: Metal organic framework, Luminescent, Pesticides, Turn-on sensor

OP-15

Synthesis of porous organic polymers via novel Cu(II) mediated oxidative coupling polymerisation for CO_2 capture

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Abstract

Synthesis of porous organic polymers through a relatively simple method can reduce the time lag in utilising such materials in various applications [1]. There exist many conventional and non-conventional methods to synthesise POPs, making them a key platform for developing new porous materials [2]. Synthetic methods for preparing POPs include Sonogashira reaction, Heck coupling, Suzuki reaction, Oxidative coupling, Yamamoto reaction and Cyano cyclotrimerisation, which requires expensive catalysts such as Pd [3]. Herein, we report a novel, simple, and affordable synthetic method for oxidative coupling polymerisation to manufacture POPs, which can replace the current techniques. The porous organic polymers prepared in this study using a unique Cu(II) mediated oxidative coupling polymerisation method have a fair yield and the findings are comparable to those of existing organic polymeric networks. The FT-IR, XRD, SEM, EDS, XPS, and TGA were used to characterise the polymeric networks. Porosity and surface area characterisation were carried out via N_2 sorption analysis. The polymers were found to adsorb carbon dioxide at ambient temperatures. Due to the dipole-quadrupole interaction between nitrogen atoms and CO_2 as well as coordination with metal ions, the nitrogen-containing conjugated porous polymers can potentially increase the affinity with CO_2 and metal ions, hence increasing the adsorption capacity.

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OP-16

Fabrication of HA - CeO_2 Nano Composite for Biomedical Engineering

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Abstract

Hydroxyapatite (HA) is a promising material for biomedical applications due to its biocompatibility and osteoconductivity. Nano-HA has improved properties compared to normal HA, making it a promising material for biomedical applications such as bone tissue engineering, dental implants, and drug delivery systems.[1,2] However, its low density and poor mechanical properties limit its use in load-bearing applications. Cerium oxide (CeO_2) has antioxidant and antibacterial properties and can improve HA's density, mechanical properties, and bioactivity. HA-CeO_2 composites are expected to combine the beneficial properties of both materials, making them promising for biomedical applications. This study aims to synthesize nanostructured HA and CeO_2 by a one-step, self-ignited combustion synthesis and to investigate the effects of different sintering temperatures on the microstructure, mechanical properties, and bioactivity of nano HA-CeO_2 composites.[3] Nano HA-CeO_2 composites with a 20 wt% CeO_2 concentration were prepared using self-ignited combustion and sintered at different temperatures. The microstructure was examined using X-ray diffraction, and the functional groups were identified using Fourier transform infrared spectroscopy. The crystallite size of the samples was estimated using the Scherrer formula and found to be 19 nm for HA and 10 nm for CeO_2. Composites of HA-CeO_2 were prepared by mixing HA and CeO_2 in an 80:20 ratio and hydraulically pressed into pellets of 2 mm thickness and 12 mm diameter. The pellets were sintered using the conventional sintering technique at different temperatures for a soaking period of 2 hours. The composite samples sintered at 1250°C showed improved biological properties compared to HA.[4] Results show that the composites exhibited increased crystallinity and density with higher sintering temperatures. The presence of characteristic functional groups of HA and CeO_2 was confirmed in the composites. The study demonstrates that the self-ignited combustion method effectively prepares nano HA-CeO_2 composites with improved biological properties. The composites show potential as hard tissue substitutes with enhanced biological properties.

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OP-17

'A Docking Study of Covid 19 With Various Quercetin Derivatives and Antimicrobial Anlalysis by Quercetin Dihydrate'

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Abstract

Computational docking methodology for finding drugs for treating various harmful disease is very fruitful nowadays. Before applying drug in to animals including human, it should confirm many times and many ways that less hazardous. This method of testing drug computationally helps to decrease wastage of time, wastage of money, wastage of manpower and handling carcinogenic or toxic materials in laboratories. Covid 19 is a worldwide threat faced the whole world and people facing many health problems due to variant formation and ineffective use of antibiotic. Whole people above 15 years got vaccinated but still it is a threat for children below 15 years all over the world. Like a world war, covid is also a war by pathogenic virous against all living organism including human. Covid also a threat that affect the health of next generation in the whole world. The present study focusses on the effectiveness of binding of covid spike protein ID 6VYO with various quercetin derivatives as all fruits and vegetables contains quercetin which is very important antiviral agent. Hence the present study is very significant.

OP-18

Synthesis and Characterization of Benzoic Acid Functionalized Silver and Copper Nanoparticles

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Abstract

In the present study, benzoic acid functionalized silver and copper nanomaterials were synthesized, where benzoic acid acts as a better reducing agent for the synthesis of corresponding nanomaterials. Characterization studies of the synthesized benzoic acid- Ag and Cu nanoparticles were carried out by Fourier Transform Infrared Spectroscopy, XRD, and SEM techniques. FT-IR results of synthesized nanomaterials indicated the binding interaction of benzoic acid with the Nps. The enlarged SEM images of sample showed the agglomeration of the silver and copper nanoparticles which shows the spherical nature of particles. By using X ray diffraction method the crystalline structure and the lattice characteristics of synthesized nanoparticles were studied. The synthesis was carried out since many existing studies reported the antibacterial action of nanomaterials especially silver nanomaterials**.** Along with silver nanoparticles, Copper nanoparticles were also synthesized in the study and compared the effects of both on the functionalization with benzoic acid. The ultimate aim on the prescribed topic is to analyze whether synthesized nanomaterials has improved its efficiency of antibacterial activity or not when compared to the existing studies. Development of nanomaterials which are having capacity to adsorb toxic chemicals and other wastes, to remove foul odour and colour will definitely open a way to surmount the difficulties of waste water treatment..

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OP-19

Green Synthesis and Characterization of Polyacrylicacid Based Silvernanocomposite Using Lawsonia Inermis Leaf Extract.

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Abstract

The world of nanocomposites has opened a new platform for the nanomaterials to exult its properties in combination with polymer based and non-polymer based matrix (metal- metal nanocomposites, metal-ceramic nanocomposites and ceramic-ceramic nanocomposites). Nanocomposites are formed by the combination of two or more materials, which are put together to get the best properties of both the components and at least one component having nanometer dimension. In this work, poly acrylic acid is taken as the matrix. It is a nontoxic and water soluble polymer. The Green Synthesis approach is an excellent way for synthesizing polymer nanocomposites. Green synthesis research is progressing taking account of its reliable, sustainable, cost-effective and eco-friendly nature. In this work, Polyacrylic acid-based silver nanocomposite is synthesized with the help of Lawsonia inermis (mehandi) leaf extract and is named PAMH. It is then characterized by UV-Visible spectroscopy, Fourier transform infrared spectroscopy, Scanning Electron Microscopy, XRD, and Thermogravimetric and Differential Thermal Analysis analysis. The antibacterial activity against both Gram-positive and Gram-negative bacteria is studied. The scope of the study is to utilize the PAMH in producing biomedicines and wastewater treatment.

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OP-20

Synthesis and Characterization of Nickel and Cobalt Doped L-Proline Cadmium Chloride Semi-Organic Nonlinear Optical Single Crystal

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Abstract

Due to the wide range applications such as optical switching, frequency conversion, optical data storage, etc. many researchers digging the new horizons of non-linear optical materials. Amino acids and their complexes belong to a family of organic materials that have potential applications. L-Proline cadmium chloride is one such semi-organic material crystallizing in the crystal form of orthorhombic crystal system with space group $P2_12_12_1$. Literature survey shows that no effective result while doping with zinc in L-proline cadmium chloride. So, we are attempting to conduct effects of dopants like cobalt and nickel in L-proline cadmium chloride. Cobalt and nickel exhibit different stereo chemical requirements for the set of chloride and L- Proline ligands, due to their bivalency. Single crystals of cobalt chloride doped with proline cadmium chloride and nickel chloride doped with proline cadmium chloride were synthesized by method of slow evaporation. Single crystal X-Ray diffraction, Powder XRD, FT-IR were done to study more about the structure of grown crystal. The internalization of cobalt chloride and nickel chloride as dopants into proline cadmium chloride were confirmed by EDAX analysis. UV-VIS spectral analysis was also done.

Keywords: Dopants; slow evaporation; L-proline

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OP-21

Synthesis of Nickel Oxide Nanoparticles Through Sol Gel Method

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Abstract

Nickel nitrate added ammonium metavanadate were synthesized using an aqueous precipitation at room temperature the obtained particle were characterized using SEM, UV, EDAX using SOL-Gel synthesis. In EDAX calculated the peak intensity of SEM the image of nickel nitrate. The sample is mainly composed of Ni and O elements. The amounts of NiO particles were found to vary between 91% oxygen and 9% nickel. UV –Visible studies of nickel oxide.

OP-22

A Docking Study of Covid 19 with Various Quercetin Derivatives

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Abstract

Computational docking methodology for finding drugs for treating various harmful disease is very fruitful nowadays. Before applying drug in to animals including human, it should confirm many times and many ways that less hazardous. This method of testing drug computationally helps to decrease wastage of time, wastage of money, wastage of manpower and handling carcinogenic or toxic materials in laboratories. Covid 19 is a worldwide threat faced the whole world and people facing many health problems due to variant formation and ineffective use of antibiotic. Whole people above 15 years got vaccinated but still it is a threat for children below 15 years all over the world. Like a world war, Covid is also a war by pathogenic virus against all living organism including human. Covid also a threat that affect the health of next generation in the whole world.

Quercetin is a polyphenol under the class of flavonoids present in all fruits and vegetables. Flavonoid contained fruits and vegetables have antimicrobial, anti-viral, anti-fungal activities. It also has medicinal applications. Flavonoids have a wide range of pharmacological activities that include anti-oxidant, antimicrobial, anti-inflammatory, antimutagenic, antitumour, antidiabetic Vaso-relaxant, immunomodulatory and both oestrogenic and anti-oestrogenic activities. The present study focusses on the effectiveness of binding of covid spike protein ID 6VYO with various quercetin derivatives as all fruits and vegetables contains quercetin which is very important antiviral agent. Hence the present study is very significant.

Key words: Docking, Anti-viral, covid 19, Computational, toxicity etc.

OP-23

Green Synthesis of Copper Oxide Nanoparticles Using Orange Peel Extract

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Abstract

Reducing water pollution and the development of a cost-effective and sustainable platform for its abatement are incessant challenges in today's world. In this regard, the current study describes the formation of copper oxide nanoparticles (CuO NPs) via a green/sustainable, cost-effective approach using orange peel and their photocatalytic activity to counter the above-stated problem. The shape, structure, crystallite size, and optical properties of the NPs were determined using various characterizations. The synthesized nanoparticles were characterized by Ultraviolet–Visible spectroscopy (UV–Vis), Fourier Transform Infrared Spectroscopy (FT-IR), X-Ray Diffraction analysis (XRD). UV–Vis spectra showed typical absorption peaks due to their large excitation binding energy at room temperature. Chemical bond formations of copper oxide were confirmed by FT-IR analyses.

Keywords: CuO NPs, UV–Vis, FT-IR, XRD

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OP-24

Synthesis, Characterization and Cytotoxicity studies on Amino derivatives of Embelin

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Abstract

Embelin, (2,5-dihydroxy-3-undecyl-1,4-benzoquinone) with molecular formula $C_{17}H_{26}O_4$ is an orange coloured solid isolated from the fruits of *Embelia ribes.* It is an alkyl substituted hydroxy benzoquinone and possess a broad spectrum of biological activities. In the present study, three different amino derivatives of embelin namely 5-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-ylamino)-2-hydroxy-3-undecyl-[1,4]benzoquinone (EAP), 2-(4-hydroxy-3,6-dioxo-5-undecyl-cyclohexa-1,4-dienylamino)-benzoic acid (EAA) and N'-(5-hydroxy-6-undecyl-p-benzoquinone-2-yl) isonicotinoylhydrazide (EIN) were synthesized and characterized by various physicochemical techniques including ^{1}H NMR, ^{13}C NMR and single crystal XRD. The cytotoxicity effect of Embelin and its amino derivatives were evaluated on L 929 fibroblast cell lines. This was done to determine the concentration dependent toxicity of each compound on normal cells. 5-flurouracil (5–FU) was taken as the standard. LD 50 values were plotted graphically and calculated using ED50 PLUS V1.0 software. The study reveals that the cytotoxicity of Embelin has decreased remarkably with its structural modification. The result obtained for EAP regarding cytotoxicity is very promising even though the cytotoxicity of the standard drug 5-FU is uncomparably low with respect to EMB as well as its amino derivatives taken for the present study.

OP-25

Design and Evaluation of Si-GO/AuNp-g-BuMAA/AMPS Molecularly Imprinted Polymer for Enhanced Photocatalytic Applications: Synthesis, Characterization, and Photocatalytic Studies

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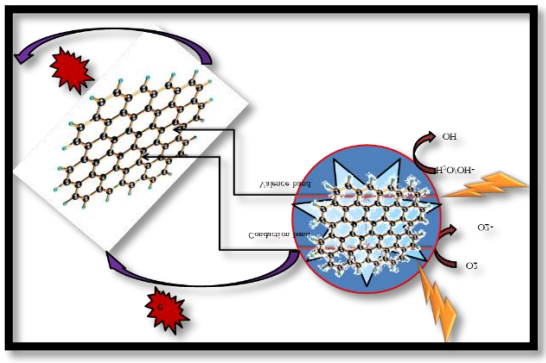
Abstract

The contamination of water in poultry fields, resulting from the excessive use of hazardous pharmaceutical compounds, notably antibiotics like Enrofloxacin (EF), has caused aesthetic pollution, eutrophication, and disruptions in aquatic ecosystems. Although EF is widely utilized in poultry for promoting animal growth and demonstrates efficient tissue penetration, it poses significant toxicity risks to humans.To mitigate this issue, a comprehensive approach was employed, integrating adsorption and photocatalysis techniques for the concurrent removal and degradation of EF from water. Adsorption, a recognized method for eliminating organic pollutants, was combined with advanced oxidation processes (AOPs), with a specific emphasis on photocatalysis. Photocatalysts, particularly graphene oxide (GO), played a pivotal role in generating reactive species like hydroxyl radicals (OH•), essential for the oxidation of organic pollutants.



Photocatalytic degradation process in EF

Graphite, a commonly used photocatalytic filler, was explored in its oxidized form, graphene oxide (GO), owing to its improved dispersion capacity in hydrophilic media. GO, with its single-atom thickness, sp^2 bonded carbon atoms, and honeycomb arrangement, exhibited compatibility with various polymers and materials. Its band gap of 1.8 eV and electron acceptor properties contributed to

efficient photocatalytic performance under visible light. In this work, synthesising a polymer Silylated Graphene Oxide/Gold nanoparticle -grafted-Butyl methacrylate/2-Acryl amido-2-methyl propane sulphonic acid[Si-GO/AuNp-g-BuMAA/AMPS] was successfully synthesized, and the photodegradation of EF from water under visible light was systematically investigated. The band gap of Sil-GO/AuNp was determined to be 2.82 eV, falling within the visible region. Characterization techniques such as FTIR, XRD, SEM, EDS, and DRS were employed. Experimental factors were scrutinized, including contact time, antibiotic concentration, temperature, and pH. The optimum pH for adsorption photocatalytic degradation was identified as 5.0. Adsorption kinetic data exhibited a good fit with the pseudo-second-order kinetic model, indicating the interaction of EF with the polymer. Photodegradation kinetics followed a first-order kinetic model. Regeneration and reusability tests of EF on the molecularly imprinted polymer (MIP) were conducted for five cycles, demonstrating high efficiency in antibiotic removal from poultry-based wastewater. The results suggest that the synthesized polymer holds promise as a proficient material for the successful adsorption and photodegradation of EF from aqueous solutions.

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POSTER PRESENTATIONS

PP-01

Electrospun $SrTi_{1-x}Fe_xO_3$ Nano Fiber Composite Cathodes for Solid Oxide Fuel Cell Applications

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Abstract

Polymer matrix composites with nano fillers were gaining attention in various fields including biomedical materials, nano sensors, and microelectronic devices, energy conversion etc for the past few decades, since they are less expensive, light weight, and having excellent physicochemical properties. We have used PVA, water-soluble clear polymer which is extensively used due to the good chemical and physical properties, non-toxicity, better film formation capacity, better chemical resistance, biodegradability, biocompatibility, semi crystalline linear synthetic polymer as the matrix and Fe doped $SrTiO_3$ as the filler. The Fe doped $SrTiO_3$ nanoparticles were synthesized via a single step combustion method. The structure of the nanoparticles was estimated using powder X-ray analysis and by measuring FWHM of the XRD peaks. $SrTi_{1-x}Fe_xO_3$ nano fibres of optimised diameter has been fabricated through electrospinning technique. Morphological properties of pure and crosslinked $SrTi_{1-x}Fe_xO_3$ nanofibers were examined by scanning electron microscopy, whereas the average diameter of pure and crosslinked $SrTi_{1-x}Fe_xO_3$ nanofibers were recorded around 100 nm.

Key words: Nano fibres, cross linked polymers, SOFC, Cathode

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PP-02

Investigation of LiNiMn Oxide for Li-ion Batteries

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Abstract

Lithium – rich cathode material, $Li_{1.5}Ni_{0.25}Mn_{0.75}O_{2.5}$ (LNMO) with ordered layered structure is synthesized using a simple carbonate co precipitation method[1,2] followed by calcination at 900˚C for varying time, 10 and 12 h, respectively. The crystal structure of the sample was studied by X-Ray Diffraction, morphology and elemental composition was studied by SEM-EDAX. SEM analysis of the material revealed cylinder-shaped particles. FT- IR analysis of the sample was also done. The cyclic voltammetry of the sample calcined at 900˚C for 12 h was done and the oxidation and reduction behaviour of the Li-NMO sample was found out.

Keywords: Li-ion batteries, Lithium rich cathode materials, Co-orecipitation

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PP-03

Cobalt Doped Titania Nanoparticles: Photocatalytic Studies

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Abstract

Titanium dioxide (TiO_2) has been widely used as a photocatalyst in many environmental and energy applications due to its efficient photo activity, high stability, low cost and safety to the environment and human[1,2]. Visible light-responsive photocatalyst are the most promising candidates for green bioremediation processes that will degrade toxic organic waste into harmless compounds. To improve the photocatalytic property of TiO_2, that is to improve its visible light response towards photocatalysis, titanium hydroxide as titanium source, cobalt carbonate as cobalt source, undoped and cobalt doped TiO_2 (Cox $(TiO_2)_{1-x}$, where x = 0.1, 0.2, 0.3 and 0.5 wt. %) nanoparticles (NPs) were prepared *via* co-precipitation method. Irrespective of the cobalt concentration, TiO_2 NPs were in the anatase phase when calcined at 800˚C. Based on the photocatalytic decomposition of methylene blue dye under UV light and visible light, the effect of cobalt doping on the photocatalytic activity of nano TiO_2 is studied. The results showed that cobalt doping in TiO_2 NPs could increase its photocatalytic activity and make them sensitive to visible radiation due to the decrease in the optical band gap energy of TiO_2 NPs on cobalt doping. Co-TiO_2 sample with 0.5 wt. % of cobalt, exhibited maximum photocatalytic activity under visible light compared to the undoped TiO_2 NPs.

Keywords: TiO_2, Photocatalyst, Nanoparticles, Cobalt, Dye Degradation

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PP-04

An insight into molecular structure of a novel hydrogel, its theoretical calculations

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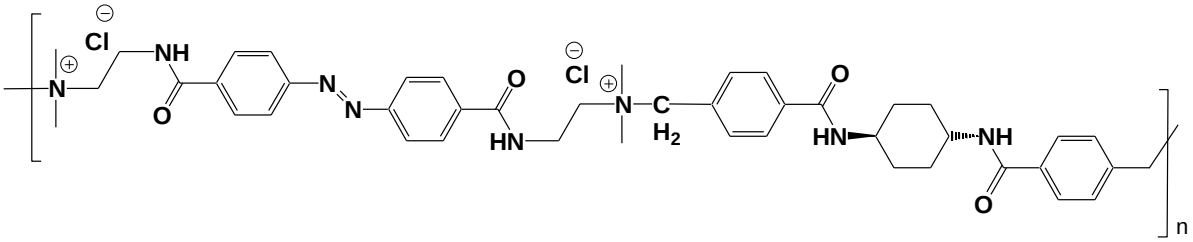
Abstract

The theoretical approach for geometry optimization, vibrational band assignments, frontier molecular orbitals, absorption spectrum and molecular parameters of the polymeric hydrogel was investigated by DFT/B3LYP/6–311+g(d,p) methods. The theoretical infrared and ultraviolet spectrum of the synthesized polymer molecule was obtained both in a vacuum state and in a solvent medium.



Keywords: Hydrogels, Azobenzene, Gelator, DFT, Gaussian 09, B3LYP.

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PP-05

Crystal Growth of a Novel Semicarbazone: Its Biological Applications in Chemistry

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Abstract

Semicarbazones are compounds of considerable interest because of their biological relevance and versatile structural features. They can coordinate to the metal either as a neutral ligand or as a deprotonated anion. The biological activities of these ligands are considered to be related to their ability to form chelates with metals. Single crystals of semicarbazone have been grown following the slow evaporation technique and unit cell parameters have been evaluated by X-ray diffraction studies. The elemental analyses, UV-Visible, FT-IR, magnetic susceptibility and conductivity measurements have been recorded to characterize the grown crystals and the structure of $[Co(HL)_2(CH_3OH)_2](NO_3)_2$, [HL=acetone-*N*(4)-phenylsemicarbazone] was confirmed by single crystal X-ray crystallography. The magnetic susceptibility measurement indicates that the Co(II) complex is paramagnetic. The bidentate nature of the ligand is inferred from IR spectrum. The ligand is coordinated to the cobalt atom through the carbonyl-oxygen and the azomethine-nitrogen, and so acts as a neutral bidentate ligand with the NO donors. The two NO_3^- anions are localized in the outer coordination sphere of the metal. Intermolecular hydrogen bonding and C–H···π interactions combine to stabilize the crystal structure. The Co(II) complex was screened for its antibacterial and cytotoxic activity

Keywords: Semicarbazone; Cobalt(II); X-ray diffraction; Magnetic susceptibility measurements; Antimicrobial studies, Cytotoxicity.

PP-06

Design of Novel Ligand Ethylenediamine-N,N,N',N'-TETRAKIS-4-Methyl- Benzoic Acid

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Abstract

A new aromatic carboxylate ligand, *ethylenediamine-N,N,N',N'-tetrakis-4-methyl benzoic acid* (HL), has been synthesized by replacement of the hydrogen of ethylene diammine with methyl-4-bromomethyl-benzoate moiety. The anion derived from HL has been used for the synthesis of lanthanide coordination compounds.

Keywords: lanthanide ions, carboxylate ligand, luminescence.

PP-07

A Comparative Analysis of Chemical and Plant-Derived Gold Nanoparticles and Their Potential Applications in Drug Delivery

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Abstract

Over the past few decades, plant-derived gold nanoparticles (AuNPs) have emerged as suitable candidates for applications in clinical diagnostics and cancer drug delivery. In the present study we have compared the application potential of plant-derived as well as chemically-synthesized gold nanoparticles as carriers in drug delivery and analysed the cytotoxicity profile against liver cancer cells. Aqueous solution of Auric chloride (AuCl) containing Au^{4+} ions was treated with the seed extract of the plant, *Solanum nigrum Linn* for preparing plant-derived AuNPs and with sodium citrate solution for preparing chemical mediated AuNPs. Characterization of plant derived AuNPs by FTIR analysis showed the presence of (-SH, -NH) functional groups, which were absent in chemically derived AuNPs. The presence of functional groups (-SH, -NH) in the plant-derived AuNPs enables them to act as reducing and capping agents, which in turn renders the conjugation of these AuNPs to anti-cancer drugs much easier than that of chemically synthesized AuNPs (Figure 1).[1] Thus, the current study emphasizes the potential of plant-derived gold nanoparticles as promising candidate carriers for drug delivery applications.[2]

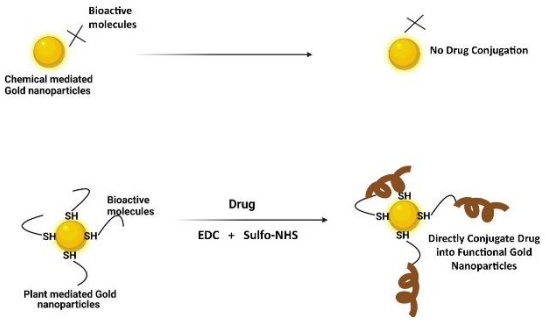

Figure 1. Schematic representation of the supremacy of plant-derived AuNPs over chemically synthesized AuNPs for drug delivery applications.

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PP-08

A Study on the Properties of Biosynthesized Tin Oxide Nanoparticles

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Abstract

Nanomaterial synthesis using a greener route has received massive attention as a sustainable, feasible, reliable, cost-effective, wealthy and environmentally friendly paradigm. The present study emphasizes a simple, efficient, and clean biogenic method to synthesize SnO_2 nanoparticles.[1] The obtained nanoparticles have been characterized by XRD (Figure 1) and TEM measurements to analyze the structural and morphological properties. The particle size is determined by Debye-Scherrer formula and morphological observations were made. The IR bands confirm the formation of SnO_2 nanoparticles which can be correlated with the XRD results. Biosynthesized SnO_2 nanoparticles exhibited enhanced thermal conductivity and antioxidant activity, which suggests its multifaceted applications.[2]

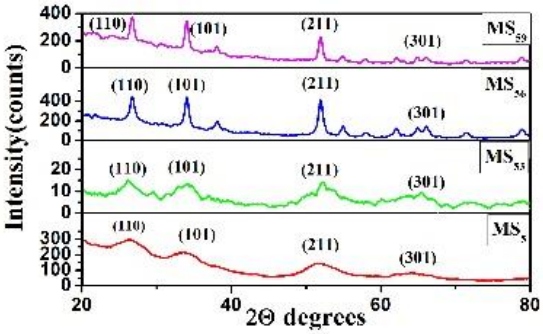

Figure.1

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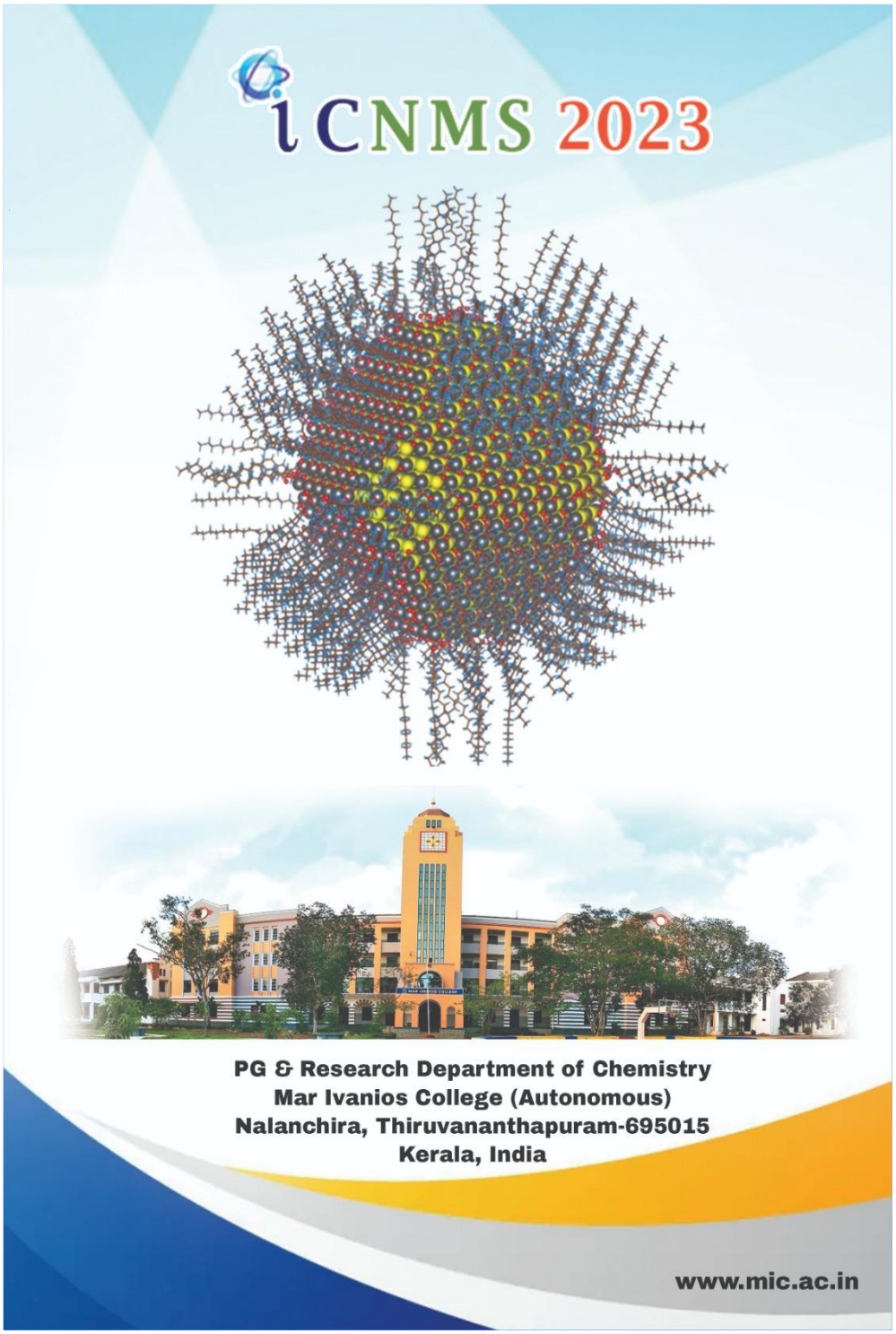
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