

National Conference On
**IMPACT OF PHYSICS
IN MEDICAL AND ENVIRONMENTAL
RESEARCH**

iPhyMER
06.03.20



SOUVENIR

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Department of Physics

Department of Physics
Indo-American College
Cheyar - 604 407, Tamil Nadu, India

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National Conference On

**IMPACT OF PHYSICS
IN MEDICAL
AND
ENVIRONMENTAL RESEARCH
(iPhyMER-20)**

Organized by



Department of Physics
Indo-American College
Cheyyar – 604407, Tamil Nadu, India

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Dr. J. EZILARASI

Principal / Convener

Indo-American College

Cheygar – 604407, Tamil Nadu, India



Message

Dear All,

I am indeed happy to give a note of appreciation to the Department of Physics for organizing a National Conference on “the Impact of Physics in Medical and Environmental Research” and presenting a collection of technical papers in the proceedings. I hope that a discussion on this idea would perpetuate the participants to think on this line which is really a dire need at this juncture. I congratulate the Staff for their endeavor in releasing this Conference Proceedings at this occasion.

I also congratulate the Head, staff members, students of the Department of Physics, participants from our and other colleges for their efforts in organizing and participating in this National Conference. I wish the conference a success.

I welcome the delegates and the resource persons who are here to stir the intellectual caliber of young minds. I wish them a great time over here.

My Hearty Congratulations!

Dr. J. Ezilarasi

Principal / Convener

Mr.R. SIVARAJAN

Vice Principal / Co-Convener

Indo-American College

Cheyyar – 604407, Tamil Nadu, India



Message

Dear All,

It is really a great opportunity for me to wish the Department of Physics and its associates for their endeavor in organizing a National Conference on “the Impact of Physics in Medical and Environmental Research” and releasing a Conference Proceeding at this juncture. I am optimistic that this platform would bring out novel ideas that could enhance the intellectual capacity of the participants and the presenters a level ahead. I hope this Conference Proceeding could contain a collection of scholarly, insightful and technical papers. I congratulate the Staff for their endeavor in releasing this Conference Proceedings at this occasion.

I expect that a discourse on this line would really motivate and catalyze young minds to think towards constructive research.

I welcome the subject experts to our campus to have a nice time with our staff, guests and students.

I wish all the participants and presenters a great time over here.

Congratulations!

MMr.R. Sivarajan
Vice-Principal

Ms. P. UMADEVI

Head of the Department

Department of Physics

Indo-American College

Cheyar – 604407, Tamil Nadu, India



Message

It is a great honor for me to address on the occasion of National conference being organized by our department on 06.03.2020 on Impact of Physics in Medical and Environmental Research (iPhyMER20) The Department is enact to add value to intellectual, moral, social and research capabilities of a student. This Conference is an effort in the direction to give an exposure to the academicians on the recent development in our field. This conference also provides a platform to our students to exhibit their inherent talents both as participants and organizers. I place on records with appreciation the hard work, involvement and effort taken by the team of staff and students in organizing this conference. I congratulate all the concerned with gratitude and wish the conference a grand success.



Ms. P. Umadevi
Head of the Department

Dr. S. SELVARAJ

Department of Physics

Indo-American College

Cheyar – 604407, Tamil Nadu, India

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Message

The goals of this conference are worthy and inspiring a celebration of advancement of Physics in the field of medical and environmental research. There is a good quote of Mahatma Gandhi that “*In a gentle way, you can shake the world*”. I believe that, “National Conference On Impact of Physics in Medical and Environmental Research” will bringing all the experts and researchers in one forum to exchange knowledge and identify areas for further research. I am very happy to note that many scientific papers revived for oral and poster presentations. I am sure that there will be useful deliberations and researchers particularly the young scientists working in medical and environmental research will be highly benefitted. I extend my heartfelt wishes for this memorable event where we can breathe and exchange our views.

Dr. S. Selvaraj

Editor (iPhyMER-20)

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Message

I am glad that the Department of Physics of Indo-American College, Cheyyar – 604407 is organizing a National Conference on **“IMPACT OF PHYSICS IN MEDICAL AND ENVIRONMENTAL RESEARCH (iPhyMER-2020)”**. Physicists are challenged to develop highly selective, energy efficient and environmentally benign new synthetic methods. Physicists in Cooperation with other scientists need to develop a better understanding of the atmosphere and the biosphere so that we can maintain a lively environment.

Physics provides all the basic necessities of life and addresses the challenges facing mankind- renewable energy resources, energy efficient fuels, new model materials, new drug to name a few... A galaxy of eminent experts will discuss these issues and I am sure all the participants will be greatly benefitted from their interactions with the learned faculty of the Conference.

It is our responsibility to know and explore the issues and put into effect the solutions and strategies which will move us forward. I believe that this Conference will do just that. On this occasion I congratulate the Convener, HOD, Principal, all faculty members and Students for their hard work to organize the Conference in a grand manner.

B.  24/02/20

Dr. N. HARIKRISHNAN, PhD.,
Assistant Professor

Dr. ARPAN KUMAR NAYAK

Assistant Professor, Department of Physics
School of Advanced Sciences
Vellore Institute of Technology
Vellore-632014



Message

I would be like to express my heartfelt congratulations and sincere thanks to the organizers for holding the National Conference on Impact of Physics in Medical and Environmental Research (iPhyMER–20) at on 06th March 2020 at Department of Physics, Indo-American College, Cheyyar - 604407. The goal of this conference are worthy and inspiring a celebration of excellence in Applied sciences, including physics, chemistry, nano science, materials science and different branches of engineering. I believe that this conference will assemble many distinguished scientists, academicians, young talented researchers, PhD students, UG and PG students. The various scientific informations and advanced knowledge to help to building a better world. I hope this conference will be an excellent forum to discuss on research innovations and current affairs in the field of medical and environmental sciences. I am sure that all the participants will be benefited immensely from the speeches being presented in the conference and young researchers will be encouraged. I am excited to visit the Department of Physics, Indo-American College on 06th March 2020. I send my warmest good wishes for a successful and productive conference.

Dr. Arpan Kumar Nayak
Assistant Professor, Department of Physics

Dr. P. SATHIYARAJ, PhD.,

Assistant Professor cum Medical Physicist

Department of Radiation Physics

KIDWAI Memorial Institute of Oncology

Bangalore, Karnataka, India

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MESSAGE

I am happy to learn that Department of Physics is organizing a National Conference on **“IMPACT OF PHYSICS IN MEDICAL AND ENVIRONMENTAL RESEARCH (iPhyMER-2020)”** organized at Indo-American College, Cheyyar, Tamilnadu – 604407 during March, 06 - 2020. The increasing demand for research in the areas of medicine, environment, industries, agriculture and in basic science encourage academic institutions to take up research in this field. I am glad that more than 250 delegates and students will attend the conference including many distinguished faculty from various colleges and universities in Tamilnadu.

Hence, the deliberations in this conference will give the academicians an opportunity to interact with the many counterparts of the people so that they can get their programmes more focused towards societal benefit. I am sure that the young research scholars will be benefited from the discussions during the conference.

I wish the conference grand success.

Dr. P. SATHIYARAJ, PhD.,

Assistant Professor cum Medical Physicist

PROGRAM SCHEDULE

Registration	:	9.00 – 9.30A.M
Inauguration	:	9.30 – 10.30 A.M
Welcome Address	:	Mrs. P. Umadevi <i>HOD / Organizing Secretary</i>
Presidential Address	:	Dr. J. Ezhilarasi <i>Principal / Convener</i>
Special Address	:	Mr. A. Radhakrishnan <i>Vice President / Chief Patron</i>
Felicitation	:	Mr. R. Sivarajan <i>Vice Principal / Co-Convener</i>
Session - I	:	10.30 A.M – 11.20 A.M
Resource Person	:	Dr. N. Harikrishnan <i>Department of Physics, Shanmuga Industries Arts & Science College, Tiruvannamalai, Tamil Nadu, India</i>
Tea Break	:	11.20 A.M – 11.30 A.M
Session - II	:	11.30 A.M – 12.20 P.M
Resource Person	:	Dr. Arpan Kumar Nayak <i>Department of Physics, Vellore Institute of Technology, Vellore, Tamil Nadu, India</i>
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Session - III	:	12.50 P.M – 1.40 P.M
Resource Person	:	Dr. P. Sathiyaraj <i>Department of Radiation Physics, KIDWAI Memorial Institute of Oncology, Bangalore, Karnataka, India</i>
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INVITED TALK

IT-01

APPLICATION OF SPECTROSCOPIC STUDIES FOR ENVIRONMENTAL RESEARCH FOR IDENTIFICATION OF POLLUTION INDEX

Dr. N. Harikrishnan

*PG and Research Department of Physics, Shanmuga Industries Arts and Science College,
Tiruvannamalai – 606603, Tami Nadu, India*

ABSTRACT

FTIR Spectroscopy is a technique based on the determination of the interaction between an IR radiation and a sample that can be solid, liquid or gaseous. It measures the frequencies at which the sample absorbs, and also the intensities of these absorptions. The frequencies are helpful for the identification of the sample's chemical make-up due to the fact that chemical functional groups are responsible for the absorption of radiation at different frequencies. The concentration of component can be determined based on the intensity of the absorption. Water analysis is a hot topic in our eco-friendly world and the truth water contamination is of central importance to environmental safety. Not only is UV-VIS spectroscopy an affordable method of water analysis but also it has many applications in the world of environmental science. Heavy metals get into the environment: water, soil, air and land through activities like intense agriculture, power generation, industrial discharges, seepage of municipal landfills, septic tank effluents e.t.c. Several spectroscopic methods have been used to monitor the levels of heavy metals in man, fossil fuels and environment. They include; flame atomic absorption spectrometry (AAS) AND atomic emission spectroscopy (AES).

Keywords: FTIR, UV-VIS spectroscopy, Atomic absorption spectrometry and Pollution Index.

IT-02**BANDGAP ENGINEERING NANOSTRUCTURED MATERIALS FOR ENVIRONMENT AND ENERGY APPLICATIONS****Dr. Arpan Kumar Nayak***Department of Physics, School of Advance Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu, India***ABSTRACT**

Nanomaterials are an important class of materials because they possess several enhanced physicochemical properties as compared to their bulk counterparts. Herein, the synthesis, characterization, and a few applications of metal oxides and sulfides-based nanomaterials are reported. Tunable bandgap and expose crystal facets of nanostructuring have generated interest of research community for their applications in chromism, water splitting, photodegradation of organic contaminants, supercapacitor, and sensing. Here, the phase and size-controlled synthesis of oxides, sulfides and nanocomposites are demonstrated via simple precipitation, hydrothermal/solvothermal and microwave assisted hydrothermal method. The as-synthesized nanostructures are employed for the photocatalytic reduction of Cr(VI), photocatalytic degradation of organic dyes under visible light irradiation and adsorption of methylene blue. The nanomaterials with different morphologies are also tested as electrocatalysts for hydrogen evolution reaction and as anode materials for photoelectrocatalytic (PEC) water splitting reaction. Furthermore, a facile and green solvothermal approach is employed to synthesize nanocomposites as an active electrode material for supercapacitor and gas sensing applications. Here we primarily emphasize on the synthesis of nanomaterials and their applications in environment remediation and electrochemical energy conversion/storage.

Keywords: Metal oxides; nanostructures; organic dye; Cr (VI) detoxification; hydrogen evolution; water splitting; asymmetric supercapacitor

IT-03

FEASIBILITY STUDY OF BASIC CHARACTERIZATION OF MAGAT POLYMER GEL USING CBCT ATTACHED IN LINEAR ACCELERATOR: PRELIMINARY STUDY

Dr. P. Sathiyaraj

Department of Radiation Physics, KIDWAI Memorial Institute of Oncology, Bangalore, Karnataka, India

ABSTRACT

The aim of this study is to evaluate the methacrylic acid, gelatin and tetrakis (hydroxymethyl) phosphonium chloride gel (MAGAT) by cone beam computed [tomography](#) (CBCT) attached with modern [linear accelerator](#). To compare the results of standard diagnostic computed tomography (CT) with CBCT, different parameters such as linearity, sensitivity and temporal stability were checked. MAGAT gel showed good linearity for both diagnostic CT and CBCT measurements. Sensitivity and temporal stability were also comparable with diagnostic CT measurements. In both the modalities, the sensitivity of the MAGAT increased to 4 days and decreased till the 10th day of post irradiation. Since all measurements (linearity, sensitivity and temporal stability) from diagnostic CT and CBCT were comparable, CBCT could be a potential tool for dose analysis study for polymer gel [dosimeter](#).

Keywords: Polymer gel, MAGAT, CBCT and Temporal stability.

CONTRIBUTED ABSTRACTS

AT-01

GREEN SYNTHESIS, CHARACTERIZATION AND LARVICIDAL ACTIVITY OF SILVER NANOPARTICLES SYNTHESIZED USING LEAF EXTRACTS OF *RAPHANUS SATIVUS* TO CONTROL *Aedes Aegypti* (DIPTERA: CULICIDAE)

Abirami.E* , Malathi.S

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ABSTRACT

Silver nanoparticle play an important role in controlling mosquito population as well as multi drug resistant pathogens without causing much harm to humans. In the present study was focused on Silver nanoparticles (AgNPs) were synthesized using leaf *Raphanus sativus* L extract that acts against dengue causing vector (*Aedes aegypti*) that affecting humans. AgNPs formation was observed as a colour change of the mixture from light yellow to dark-brownish. synthesized Silver Nanoparticles of plant materials were characterized by using UV–visible spectroscopy, Scanning electron microscopy(SEM), XRD, Fourier transform infra red (FTIR) . The synthesizes silver nanoparticles were treated to third instar larvae of *Aedes aegypti* with different concentration. This result recommended that the aqueous leaf extract of *Raphanus sativus* and green synthesis of silver nanoparticles have the potential to be used as an ideal eco-friendly approach for the control of *Aedes agypti*

Key words: *Raphanus sativus* L , green synthesis, Silver nanoparticles and ,*Aedes aegypti*

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AT-02

NANOCRYSTALLINE Bi_2S_3 THICK FILMS FOR Low-Dose X-ray DETECTION**Ajith Kumar B.S., T. Prakash****National Centre for Nanoscience and Nanotechnology,
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Nanomaterials have become highly important in the development of low dose X-ray sensing. Bismuth chalcogenides have been extensively studied in X-ray imaging and cancer therapy due to its high-Z number [1]. Among the bismuth derivatives, the n-type semiconductor bismuth sulfide (Bi_2S_3) with different morphologies was studied in X-ray sensing [2] and chemotherapy applications. Bi_2S_3 nano crystals synthesized from solid state reaction calcined at two different temperature was made in the form of thick films is used to fabricate the X-ray sensor. The synthesized material was characterized for its structural property using powder X-ray diffraction, the surface and compositional property was studied using SEM and EDS, Raman spectroscopy was carried out further to validate the composition of the sample. The X-ray sensing behavior of the Bi_2S_3 thick films were tested using intra oral pulsed 70kV AC X-ray machine (Gnatus 70E Timex, Brazil). The attenuation property of bulk and nano structured orthorhombic Bi_2S_3 exhibits higher sensitivity response to X-rays at lower bias voltage [3].

Keywords: Nanocrystalline Bi_2S_3 thick film, X-ray sensor, Solid state reaction.

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AT-03

MOLECULAR STRUCTURE ,SPECTROSCOPIC STUDIES AND QUANTUM CHEMICAL COMPUTATION OF 2- BROMO-4- FLUOROACETANILIDE.

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ABSTRACT

Acetanilide have been played an inescapable role in treating the therapeutic effects [1,2]. In this research assessment, the molecular conformation and vibrational analysis of 2-Bromo-4-fluoroacetanilide (2B4FA) were presented using experimental techniques (FT-IR, FT-Raman, UV and NMR) and density functional theory (DFT) employing B3LYP exchange correlation with the 6-311++G(d,P) basis set showed good agreement with the observed spectra. The complete vibrational assignments of wave numbers using potential energy distribution (PED) was calculated with scaled quantum mechanics. The optimized geometrical structure (fig 1), frontier molecular orbital, natural bond orbital, non linear optical effects, electron localization function, molecular electrostatic potential and thermodynamic properties (heat capacity (C), entropy (S) and enthalpy changes (H)) were included in the computational analyses. The Mulliken atomic charges and Fukui functions were also performed by the NBO investigation. The sites for nucleophilic and electrophilic attack were predicted. The linear polarizability and first order hyperpolarizability were predicted as NLO candidate. A pertinent study of molecular docking was carried out as an important part of this exploration. The ligand was docked into active sites of proteins 1H5U which belongs to the class of proteins exhibiting the property as anti-diabetic symptomatic (fig 2). A minimum binding energy and RMSD values were also explored. Thus the result confirmed anti-diabetic properties of the title compound.

Summary and conclusions (i). The theoretical, structural and vibrational assignments of the title compound which were successfully performed by FT-IR, FT-Raman, UV, ¹H and ¹³C NMR, and their quantum computations were reported in this current work, by using B3LYP/6-311++G(d,p) basis set. (ii) The intermolecular interaction of the title compound were established using NBO analyses and their MEP shows the possible reactive sites of electrophilic and nucleophilic attacks. The calculated electrophilic index found to be 2.853. (iii) The title compound's polarizability calculations leads to an effective NLO material. (iv) The HOMO-LUMO energy gap values (5.392 eV) have influence on the molecule. (v) The thermodynamic properties were calculated and the Mulliken atomic charges were linked with natural atomic charges. (vi) The 2-bromo-4-fluoroacetanilide were docked with different protein/enzyme for free binding energy (-4.43 Kcal/mol) and RMSD values calculations were approved.

AT-04

**“EFFECTS OF INTEGRATED USE OF ORGANIC AND INORGANIC
NUTRIENT SOURCES WITH EFFECTIVE MICROORGANISMS (EM)
ON SELECTED VEGETABLES GROWTH AND YIELD IN
TAMIL NADU, INDIA.”**

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ABSTRACT

Mineral fertilizers have significant effects on food production in the world, and are an indispensable component of today's agriculture. A field experiment was conducted in the research area of Cheyyar, Tiruvannamalai, Tamilnadu. The surface soil (0–15 cm) of the experimental site had pH 7.65, E_{Ce} 1.32 dS m⁻¹, organic matter 4.6 g kg⁻¹, total N 0.41 g kg⁻¹, available P 6.2 mg kg⁻¹ and exchangeable K 78.4 mg kg⁻¹. The experiment involved the treatments: T0: control; T1: 10 Mg ha⁻¹ organic material (OM, dry weight basis), i.e. farmyard manure (FYM) + poultry manure (PM) + sugarcane filter cake (SFC) in the ratio of 4:3:3; T2: extended effective microorganisms (EM), i.e. mixture of basic EM, molasses and water in the ratio of 1:1:20; T3: OM + EM; T4: full recommended NPK fertilizer (N 170:P 37:K 50 kg ha⁻¹); T5: 1/2 recommended NPK fertilizer + EM; T6: 1/2 recommended NPK fertilizer + OM + EM; T7: full recommended NPK fertilizer + OM + EM. EM was applied at the rate of 2.5 L ha⁻¹ as recommended. Effective microorganisms (EM) was a mixed culture of beneficial microorganisms including a predominant population of lactic acid bacteria (*Lactobacillus sp.*) and yeast (*Saccharomyces sp.*), and a small proportion of photosynthetic bacteria (*Pseudomonas sp.*), actinomycetes and fermenting fungi. NPK analysis were performed. As a final result, EM were showed better yield compare to others.

AT-05

**REDUCIBLE REPRESENTATION OF MOLECULAR PARAMETERS
OF MICRO MOLECULES USING NCA****E.Balumahindran^{1,*}, S.Saranyadevi¹, J. Kishor Kumar¹, S.Selvaraj², S. Kumaresan¹**

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ABSTRACT

All atoms in a molecule are continuously vibrating. Each atom position is specified by displacement coordinates. Based on the displacement coordinate described the vibrating atom based on its symmetry. Due to vibration motion of an atom in a molecule, stability of an atom is alters. This can be confirmed by moment of inertia. Based on the group theory the atom is described and its operation is determined by symmetry operations. These symmetry operations are expressed in matrix form. The matrix representation for some simple micro molecules is obtained. The matrix representation for diatomic, triatomic and tetra atomic molecules are obtained. In a diatomic and triatomic molecule C_2 symmetry operation occurs. In tetra atomic molecule C_3 symmetry operation occurs. Symmetry operations occur in $D_{\infty h}$, C_{2v} , \square_d point group symmetry belonging molecules Cl_2 , SO_2 , PCl_3 are expressed in reducible representations.

Keywords: Matrix representation; Coordinate displacement; molecular parameters, Cartesian coordinates, Molecular geomantary

AT-06

SPECTROSCOPIC AND COMPUTATIONAL INVESTIGATIONS ON MOLECULAR STRUCTURE OF ISOMERS OF TRICHLOROANILINE

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ABSTRACT

Spectroscopic and structural properties of isomers of trichloroaniline have been investigated experimentally and theoretically. The vibrational spectra of isomers of trichloroaniline have been recorded by FT-IR and FT-Raman techniques in the mid IR region. The ¹H and ¹³C NMR chemical shifts of isomers of trichloroaniline have been recorded at 300 K in DMSO solution. The UV-Visible spectra of isomers of trichloroaniline were recorded in the region of 1100-190 nm and the electronic properties such as frontier molecular orbitals and band gap energies were measured by TD-DFT approach. The theoretical chemical shifts of isomers of trichloroaniline were calculated by GIAO shielding tensors and compared with experimental findings. The molecular geometry, vibrational spectra, chemical shifts and electronic spectra were calculated for isomers of trichloroaniline using Density Functional Theory (DFT) based on B3LYP/6-311++G(d,p) basis set. The molecular geometry optimization, vibrational frequencies, chemical shifts and electronic transitions were clearly discussed. The obtained experimental and theoretical finding shows a good conformity, which gives the structural contribution for the better understanding in the field of analytical chemistry.

Keywords

FT-IR, FT-Raman, NMR, UV-Vis, DFT

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AT-07

**FLUORESCENCE AND ULTRAVISIBLE SPECTROSCOPIC STUDIES
OXYBENZONE - UAA & UVB BLOCKERS ABOBENZONE - UVA
BLOCKERS**

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ABSTRACT

The Fourier transform infrared (FT-Raman spectra of 2-hydroxy-3-(2-methoxyphenoxy) propyl carbamate (HMPC) of muscle relaxant agent were recorded in the region $4000-450\text{ cm}^{-1}$ and $4000-50\text{ cm}^{-1}$ respectively. Density functional theory (DFT) has been used to calculate the optimized geometrical parameter, electronic energies, and vibrational wave numbers and intensity of the vibrational bands. The computed vibrational wave numbers were compared with the FT-IR and FT-Raman experimental data. The computational calculations at DFT/3LYP level with 6-31G(d,p) and 6-31++G(d,p) basis sets. The complete vibrational assignments were performed on the basis of the potential energy distribution (PED) of the vibrational modes calculated using Vibrational energy distribution analysis (VEDA 4) program. UV-visible spectrum of the compound was recorded and the electronic properties, such as HOMO and LUMO energies were performed by time-dependent DFT (TD-DFT) approach. The calculated HOMO-LUMO energy gap revealed that charge transfer occurs within the molecule. The first order hyperpolarizability and Molecular Electrostatic Potential (MEP) of the molecule are computed using DFT calculations.

KEYWORDS: DFT, MEP, PED, FT-IR, HOMO-LUMO

AT-08

ESTIMATION OF GAMMA RADIATION DOSE INDICES NEAR LEATHER TANNERIES IN NORTHERN REGION OF VELLORE DISTRICT.

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ABSTRACT

Background: outdoor gamma radiation exposure levels were measured in a total of 30 randomly selected sewage water (tannery) and sewage dump (leather and tannery) across Ambur and Ranipet to determine the annual effective doses. **Materials and Methods:** All radiation measurements were taken using a Geiger Muller detector and a GPS for geographical coordinates of sample points. Equal number (30) sample point measurements were carried out for outdoor measurements. Measurements at each location point were performed holding the survey meter at 1 m above ground surface or floor to avoid unwanted effects of radiation from sewage or tannery. The detector was also held at least six to seven meters away from tannery nearby in order to avoid unwanted effects of the tannery materials on outdoor measurements. Each measurement was repeated six times and the average was taken to represent the value for a sample point.

Results: The average outdoor dose rates were determined as $6.29 \pm 1.37 \mu\text{Svh}^{-1}$ and $3.80 \pm 6.17 \mu\text{Svh}^{-1}$ respectively. The highest contribution to the total outdoor dose was from the tannery contributed the least dose. The average annual effective dose was calculated as $0.08 \pm 0.02 \text{ mSv}$, which is higher than the world average value (0.31 mSv).

Conclusion: In view of the potential radiation resulting from tannery waste and sewage water from tannery, comprehensive assessment of natural radiations in such materials is required.

AT-09

GREEN SYNTHESIS AND CHARACTERIZATION OF ZINC OXIDE NANOPARTICLES USING LEAF EXTRACT OF OCIMUM TENUIFLORUM AND ITS ANTIMICROBIAL ACTIVITY

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ABSTRACT

The synthesis of metal and semiconductor nanoparticles is an expanding research area due to the potential applications in the development of novel technologies. Especially, biologically synthesized nanomaterial has become an important branch of nanotechnology. The present work, describes the green synthesis of Zinc oxide nanoparticles (ZnO NPs) using leaf aqueous extract of *Ocimum Tenuiflorum* and its antimicrobial activities. The synthesized nanoparticles are confirmed by obtain UV- visible spectroscopy. The presences of functional groups are identified using Fourier transform infrared spectroscopy technique (FTIR). And further X-ray Diffraction studies of synthesized nanoparticles were analyzed. In this study we also investigated antimicrobial activity of green synthesized ZnO NPs. The results depicted concentration of ZnO NPs was increased (50, 100, 200 $\mu\text{g/ml}$) and also increase in antimicrobial activities was due to the increase of H_2O_2 concentration from the surface of ZnO. And this confirms synthesized ZnO nanoparticles acts against microorganism such as bacteria, fungi, etc. Finally we conclude that synthesized zinc oxide nanoparticles exhibits interesting antimicrobial activity with both gram positive and gram negative bacterial and yeast at micromolar concentration.

AT-10

X-ray ATTENUATING NATURE OF CuI

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ABSTRACT

Nanotechnology paved path to discover a superior functional property of various nanomaterials. Copper compounds have been studied because of their unique optical properties [1] and non-toxic nature [2]. In this present study, nanocrystalline Copper iodide (CuI) was synthesized by Precipitation, then processed at 150°C for 15 min under nitrogen (N₂) atmosphere. Then, the structural and optical properties were analyzed using XRD and UV-VIS respectively. The obtained results reveal that the sample exists in cubic phase with band gap of 2.9 eV. Further, X-ray attenuating and sensing nature of CuI was examined using an intra-oral diagnostic X-ray machine interfaced with Suniray X-ray image sensor.

The performance of CuI thick film coated on interdigitated electrode was assessed under various micron meter thickness. The photocurrent measurement was carried out using a Keithley source meter at biased condition. The overall dose-sensitivity plot obtained for different thickness was explained by the suitable mechanism.

Key words: Precipitation reaction; Nanocrystalline CuI; X-ray attenuating nature; interdigitated electrode; Dose-sensitivity plot;

Reference:

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AT-11

SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF SOME NEW THIAZOLE AND PYRAZOLE DERIVATIVES CONTAINING NAPHTHOTHIAZOLE MOIETY

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ABSTRACT

In an endeavour to find a new class of antimicrobial agents, a series of thiazole docked with pyrazole and other related compounds containing naphthothiazole moiety were prepared via the reaction of pyrazole with appropriate chemical reagents. These compounds were screened for their antibacterial activity against gram-positive bacteria (*Staphylococcus aureus* and *Salmonella typimhurium*), gram-negative bacteria (*Pseudomonas aeruginosa* and *Escherichia coli*) and antifungal activity against *Candida* and *Aspergillus vulgaris*. Among the synthesized compounds, thiazole showed equal activity with chloroamphenicol against *S. aureus* (MIC 3.125 microg/mL), while its activity was 50% lower than of chloroamphenicol against *S. typimhurium*. Thiazole and pyrazole were found to exhibit the most potent in vitro antifungal activity with MICs (6.25 microg/mL) against *A. vulgaris* and *C. albicans*. Structures of the newly synthesized compounds were established by elemental analysis and spectral data.

AT-12

CHARACTERIZATION STUDIES ON DYES DOPED KDP CRYSTAL

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ABSTRACT

Potassium dihydrogen orthophosphate (KDP) crystal is a popular non-linear optical inorganic material. In my present investigation, KDP crystal and Lawsoniainermis (Henna) leaves extract doped KDP crystal has been grown by slow evaporation at room temperature growth technique. The grown crystals have been analysis through various viz. Fourier Transform Infrared spectroscopy has been used for spectral analysis of grown crystals. The crystals are subjected into X-ray diffraction for structural analysis. Using Vicker's microhardness test the mechanical properties of KDP crystal and Henna leaves extract doped KDP has been studied. The dielectric properties of the pure and doped crystals are investigated through LCRZ meter.

KEYWORDS: KDP,X-RAY, Henna, Slow evaporation, Dielectric

AT-13

AN EXPERIMENTAL AND THEORETICAL FINDINGS OF STRUCTURAL AND SPECTROSCOPIC PROPERTIES OF SYRINGALDEHYDE

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ABSTRACT

The optimized structural parameters, spectroscopic properties, frontier molecular orbitals (FMO's), mulliken charges, molecular electrostatic potential surfaces (MESP) and thermodynamical parameters of syringaldehyde have been analyzed by experimentally and theoretically. The vibrational and electronic spectra were recorded in the mid IR respectively. All the computational calculations were stimulated by Density Functional Theory (DFT) using B3LYP/6-311++G(d,p) basis set. From the obtained findings, the experimental and theoretical value shows good correlation, thereby to confirm the molecular structure of syringaldehyde.

Keywords

FT-IR, UV-Vis, HOMO-LUMO, MESP, syringaldehyde

AT-14

FTIR, FT-RAMAN SPECTRAL INVESTIGATIONS, NBO ANALYSIS AND STRUCTURAL STUDY, THEPMODYNAMIC FUNCTIONS OF PHENYTION SODIUM

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ABSTRACT

The FTIR and FT-Raman spectra of phenytoin sodium have been recorded and analyzed. Natural bond orbital analysis has been carried out for various intra-molecular interactions that are responsible for the stabilization of the molecule. HOMO-LUMO energy gap has been computed with the help of density functional theory. The statistical thermodynamic functions (heat capacity, entropy, vibrational partition function and Gibbs energy) have been obtained for the range of temperature 100-100 K. The infrared and Raman spectra have been also predicted from the calculated intensities. Comparison of the experimental and theoretical spectra values provides important information about the ability of the associated with each atom have also been reported and mapped molecular electrostatic potential (MEP) surfaces have also been performed with the same leve31 of DET.

Keywords: Vibrational spectra; NBO; HOMO-LUMO; MEP surface, DET.

AT-15

“PRODUCTION OF BIODEGRADABLE PLASTIC BY BACTERIA ISOLATED FROM MARINE ENVIRONMENT”

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ABSTRACT

Life is a beautiful word that holds many information within itself. It can be said that it is a system or object with many characters like self-sustaining and signalling mechanisms which differentiates them from other objects. Those others are called non-living objects or non-living systems. Pollution is a condition in which contaminants are introduced in to the natural environments leading to adverse changes in the environment and human activity is the main cause for the same. Pollutants or contaminants are the components that cause pollution and they may be foreign chemicals, substances or different forms of energy like heat, noise etc. Pollution may be point source or non-point source. Isolation and bacterial isolates from marine water were performed. Screening of different isolates of marine water bacteria for production of bioplastic were performed. Extraction of produced PHB in the potent isolates were performed. Extraction of produced PHB in the potent isolates were performed. Two bacterial isolates such as *Bacillus sp* and *Pseudomonas sp* were isolated from marine water. Bioplastic producing bacteria were confirmed by using sudan B staining and plating method. Phb granules were isolated from these two isolates. And it is used for large amount at world wide.

AT-16

GROWTH, OPTICAL, SPECTRAL AND MECHANICAL STRENGTH OF THE 2-BENZOFURAN-1, 3-DIONE SINGLE CRYSTAL

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ABSTRACT

Optically good transparent 2-Benzofuran-1, 3-dione single crystals were grown by slow evaporation solution growth technique at a room temperature. The grown crystal was characterized by various techniques. Such as single crystals x-ray diffraction, powder x-ray diffraction, FT-IR and FT-Raman, UV- Visible NIR-spectra, Vickers micro hardness test, dielectrics studies and photo luminescence spectra. Kurtz powder method was employed to explore the NLO characteristics of the grown crystal.

Key words:

Organic crystals, single XRD, Powder XRD, di-electronics, Kurtz powder method.

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AT-17

STRUCTURAL PROPERTIES OF 4-METHOXYPHENYLBORONIC ACID

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ABSTRACT

The ¹H & ¹³CNMR chemical shifts were calculated using the Gauge Independent Atomic Orbital (GIAO) method and compared with the experimental data. In addition, the natural bond orbital (NBO) analysis was also performed to have an Intramolecular Charge Transfer (ICT) with the molecule. The geometrical parameters, the NMR and UV-Vis analysis, vibrational analysis of the 4-Methoxyphenylboronic acid (4MPBA) have been performed using the Density Functional Theory (DFT) B3LYP method with 6-311++G(d,p) basis set. The experimental FT-IR and FT-Raman spectra were obtained in the region 4000-400cm⁻¹ and 3500-100cm⁻¹ respectively. The UV-Vis absorption spectra were analyzed in the solvent (DMSO) in the range of 200-400nm Also, the HOMO and LUMO energies and the Thermodynamic function were presented.

KEYWORDS: NMR, HOMO-LUMO, NBO, FT-IR

AT-18

INTRA ORAL X-ray SENSING BEHAVIOUR OF NANOCRYSTALLINE CaWO₄ THICK FILMS

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ABSTRACT

In the present work, CaWO₄ nanocrystals were prepared by double exchange reaction and then thick film of CaWO₄ was deposited on the top of patterned metal electrodes to study their intra oral X-ray sensing behaviour. The X-ray sensing measurement was performed for different exposure times at room temperature up to 3.2 sec. Difference in the photocurrent characteristic of the sample under the illumination of X-ray was recorded using a Keithley 2450 source meter. Prior to the sensing measurement, powder CaWO₄ structural, microstructural, optical properties and stopping power were studied respectively using X-ray diffraction, scanning electron microscope, spectrophotometer and Suniray-2 radiography imaging system. The observed results reveal that, sample exhibits single phase without any other impurities presence and micron sized thick dense films without any crack. The observed linear percentage of sensitivity for different exposure time explores CaWO₄ is a promising material for low dose of X-ray sensor device development.

AT-19

SYNTHESIS OF COPPER OXIDE NANO PARTICLE USING LEAF EXTRACT OF ANTIBACTERIAL APPLICATIONS

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ABSTRACT

Using *Spermacoce hispida* L. extract. First we prepared leaf extract of *Spermacoce hispida* L. in deionised water. This extract added to 1mMol of copper sulfate solution and we observed the change in color of the solution from colorless to colored solution, this indicates that there is a formation of Cu nanoparticles. These bioactive compounds have many applications in antioxidant, anticancer, anti-inflammatory and anti-ulcer properties. These biosynthesized CuO nanoparticles were characterized with the help of X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and the EDX analysis affirms the results obtained from the XRD analysis. It was observed that the leaf extract can reduce copper ions into copper and oxide nanoparticles within 10 to 30 min of reaction time. Thus, this method can be used for rapid and eco friendly biosynthesis of stable copper nanoparticles.

Keywords: Green Synthesis, *Spermacoce hispida*, XRD, FTIR, SEM

AT-20

PLANT MEDIATED GREEN SYNTHESIS OF Ag-NPs USING LEAVES EXTRACT FROM ALLIUM CEPA ASSESSMENT OF THEIR ANTIBACTERIAL ACTIVITIES

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ABSTRACT

Green synthesis of silver nanoparticles (Ag-NPs) was effectively made using *Allium cepa* leaf extract simple, rapid, eco-friendly and this method. In this study, we used *Allium cepa* extract for synthesized AgNPs which reduces silver nitrate into silver ions material. The presence of biosynthesized AgNPs at 438 nm was confirmed by UV-Visible spectroscopy and also nanocrystal of AgNPs confirmed through the XRD analysis, DLS analysis reveals that the size distribution found to be around 54.3nm and good stability for the zeta potential. TEM representation showed poly-dispersed, spherical shape of synthesizes silver nanoparticles (AgNPs) size range from 19-30 nm. The Energy Dispersive X-ray (EDX) confirmed that the present of silver (Ag) content in the synthesized AgNPs. FTIR spectrum was used to confirm the presence of potential bioactive molecules such as alcohols, carbonyl group, alkanes, and primary of proteins act as both reduction and stabilization of nanoparticles. The green synthesized AgNPs exhibited a good antibacterial activity against both Gram positive (*staphylococcus aureus*, *Pseudomonas aeruginosa*) and Gram negative (*Escherichia coli*, *Enterococcus faecalis*) bacteria.

Keywords: *Allium cepa*; AgNPs; UV; XRD; TEM-EDAX; FTIR; Antibacterial activities;

AT-21

SYNTHESIS OF COPPER OXIDE NANOPARTICLES USING FROM BORRERIA HISPIDA LEAF EXTRACT AND ANTIBACTERIAL MICROBIAL ACTIVITY

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ABSTRACT

Synthesized nanoparticles have an incredible application in biomedicine owing to its simplicity eco-friendly properties and low cost. The present study aims to determine the green synthesized copper nanoparticles from Borreria hispida leaf extract. Synthesis conditions were optimized for maximal narrow size range synthesis of copper oxide nanoparticles. The result nanopowder was characterized using various analytical techniques, such as Energy Dispersive X-Ray Spectroscopy (EDX), Fourier Transform Infrared spectroscopy (FTIR), X-Ray Powder Diffraction (XRD), Scanning Electron Microscope (SEM). Hence an easy effective approach for synthesis of copper oxide nanoparticles, with efficient antibacterial microbial activity is reported in the study.

Keywords: Green synthesis, Borreria hispida, FTIR, SEM, EDX, XRD.

AT-22

GREEN SYNTHESIS OF GOLD NANOPARTICLES USING DIFFERENT MEDICINAL PLANTS AND ITS UV-VIS SPECTROSCOPIC ANALYSIS AND ANTIBACTERIAL ACTIVITY

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ABSTRACT

Gold nanoparticles are the most prominent metal nanoparticles and having wide range of applications in drug delivery and much therapeutic potential. In this present investigation we have used some Indian herbal plants for the green synthesis of gold nanoparticles and its antibacterial efficacy was measured. The medicinal plants such as *Alternanthera bettzickiana*, *Gymnema sylvestre* and *Andrographis paniculata* used for the synthesis and characterized using UV-vis spectroscopy. The antibacterial activity of gold nanoparticles such as *Bacillus subtilis*, *Staphylococcus aureus*, *Micrococcus luteus*, *Enterobacter aerogenes*, *Salmonella typhi* and *Pseudomonas aeruginosa*.

Key words: Gold nanoparticles, Medicinal plants, UV-Vis, Antibacterial activity.

AT-23

**AN EXPERIMENTAL AND THEORETICAL EVIDENCE FOR
STRUCTURAL AND SPECTROSCOPIC PROPERTIES OF 2-HYDROXY-
5-METHOXYBENZALDEHYDE**

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ABSTRACT

The optimized structural parameters, spectroscopic properties, frontier molecular orbitals (FMO's), mulliken charges, molecular electrostatic potential surfaces (MESP) and thermodynamical parameters of 2-hydroxy-5-methoxybenzaldehyde have been analyzed by experimentally and theoretically. The vibrational and electronic spectra were recorded in the mid IR and UV-Vis region, respectively. All the computational calculations were stimulated by Density Functional Theory (DFT) using B3LYP/6-311++G(d,p) basis set. From the obtained findings, the experimental and theoretical value shows good correlation, thereby to confirm the molecular structure of 2-hydroxy-5-methoxybenzaldehyde.

Keywords

FT-IR, UV-Vis, HOMO-LUMO, MESP, 2-hydroxy-5-methoxybenzaldehyde

AT-24**MECHANICAL PROPERTIES OF ADP DOPED CRYSTAL****E.Parimala^a, S.Rajeshkumar^{a*}**

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Ammonium Dihydrogen phosphate (ADP) crystals are one of the most popular crystals used for Non-linear optical (NLO) applications. Pure and dye (Allura Red) doped ADP crystals were grown by slow evaporation technique at room temperature. Grown crystals have been characterized using power X-ray diffraction and Fourier Transform Infrared Spectroscopy (FTIR). The presences of dyes were confirmed by FTIR and UV-visible spectra. Dye molecules possess π electron similar to conjugated polymers, but the molecules themselves are not very big. Their energy level structure shows the presence of bands containing many closely spaced levels corresponding to vibrational and rotational states. The analysis of single crystal XRD spectra conforms that the doped sample has the perfect crystal properties. Their energy level structure shows the presence of bands containing many closely spaced levels corresponding to vibrational and rotational states. A variety of dyes for many laser operating wavelengths were employed in the past. The NLO reports of the samples are having high energy level comparing with pure ADP. The Vicker's hardness studies carried out for the Pure and doped crystals from the crystallographic planes. It shows that an increased hardness of the doped crystals with comparison of pure ADP. A variety of dyes for many laser operating wavelengths were employed in the past. Dye embedded in ADP crystal and dye doped crystal were also reported as useful non-linear optical media.

KEYWORDS:ADP crystal, FTIR, UV-visible,NLO

AT-25

STRUCTURAL ANALYSIS AND CONFIRMATION OF CARBON ATOMS OF GABAPENTIN

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ABSTRACT

The optimized molecular geometry, chemical shifts of gabapentin were simulated using Density Functional Theory (DFT) employed with B3LYP/6-311++G(d,p) basis set, and results were comprehensively discussed. The experimental FT-IR and FT-Raman spectra were recorded in the mid IR region. The experimental NMR spectra were recorded at base frequency of 400 MHz for ^1H and 100 MHz for ^{13}C nuclei. The vibrational spectra in the range of $1345\text{--}1180\text{ cm}^{-1}$ have been used to confirm the presence of carbon atoms in the gabapentin and results were discussed. The obtained experimental and theoretical results show an excellent correlation, thereby to confirm the molecular structure of gabapentin. And also to determine the antibacterial activity of non antibiotic gabapentin against gram positive and gram negative bacteria.

Keywords

Carbon confirmation, FT-IR, FT-Raman, NMR, DFT, Gabapentin

AT-26

DISORDER DETECTION OF EGGPLANT USING IOT AND MACHINE LEARNING

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ABSTRACT

India is an agricultural country and this sector accounts for 18 percent of India's GDP. This sector is the backbone of the country and focuses on better yield by using pesticides and fertilizers to prevent plant disorders which directly affect the yield. The primary method adopted for detecting disorders is through visual observation and other methods are quite expensive. Many authors have proposed solutions to this problem such as IoT for grapes, or system designed for accurate disorder detection using machine learning with limited scope. This paper showcases a prototype that uses multi-modal analysis through sensor data, computer vision. The main objective of this system is to accurately detect disorders in eggplant using IoT, Machine Learning, Cloud Computing, and Image Processing.

Keywords

Plant Disorders, IoT, Machine Learning

AT-27

THE GROWTH AND OPTICAL PROPERTIES OF 4 -NITROPHENOL AND L-CITRULLINE NLO SINGLE CRYSTAL

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ABSTRACT

Single crystals of 4-Nitrophenol and L-Citrulline(4NPLC) have been grown by the slow evaporation technique at room temperature using aqueous solution. The single crystal XRD study confirms monoclinic system for the grown crystal. The functional groups present in the grown crystal have been identified by FTIR spectral studies. Lower cut-off and optical band gap were determined from the UV-vis spectral studies using solid crystal sample. Further, the thermal resistance was observed by using TG/DSC analysis. The photoluminescence spectrum of 4NPLC was recorded. In order to determine mechanical strength of 4NPLC crystal for various loads using Vickers micro hardness tester. The Dielectric behaviour of the crystal has been determined in the frequency range from 50 Hz to 5 MHz at various temperatures.

Keywords: Optical materials, Crystal growth, X-ray diffraction, Optical properties.

AT-28

**ASSESSMENT OF NATURAL RADIOACTIVITY MEASUREMENT IN
SEDIMENT SAMPLES ALONG THE ENNORE PORT AREA, EAST
COAST OF TAMIL NADU, INDIA BY USING HPGe GAMMA RAY
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Viridhachalam, Tamilnadu – 606001*³*PG and Research Department of Physics, Government Arts College, Tiruvannamalai, Tamilnadu – 606603***ABSTRACT**

Natural radionuclides have been the components of the earth since its existence. It is widely spread in earth's environment and exists in soil, sediment, water, plants and air. There are many naturally occurring radionuclides in environment, containing uranium and thorium series radioisotopes and natural ⁴⁰K. The prime objectives of the present work is (i) to determine the activity concentrations of ²³⁸U, ²³²Th, and ⁴⁰K in sediment samples collected from study area, (ii) Absorbed dose rate (DR) and (iii) Activity utilization index (AUI). 26 sediment samples were collected from Ennore Port area of East cost of Tamilnadu, India using Peterson grab sampler during the pre-monsoon period. Using HPGe detector based on high-resolution gamma spectrometry system, the activity of samples is counted. The activity concentrations range and mean values (in properties brackets) of the activities for ²³⁸U, ²³²Th and ⁴⁰K are 4.37 – 56.00 (18.28), 8.06 – 317.00 (65.83) and 216.00 - 508.00 (397.58) Bqkg⁻¹, respectively. Measured activities of the radionuclides differed widely, as activity levels in the marine environment depend on their physical, chemical and geo-chemical and the environment. From the results it is clear that the mean activity of ²³⁸U is lower while ²³²Th and ⁴⁰K are greater when compared with worldwide average value.

Keywords

Radioactivity, Activity concentrations of ²³⁸U, ²³²Th, and ⁴⁰K, Ennore Port area and HP-Ge detector.

AT-29

IDENTIFICATION AND DETERMINATION OF BIOACTIVE PHYTOCHEMICAL CONSTITUENTS FROM THE ETHANOLIC EXTRACT OF *ACHYRANTHES ASPERA* BY GC-MS ANALYSIS

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ABSTRACT

In this study, the use of *ACHYRANTHES ASPERA* commonly known as chaff-flower or prickly chaff flower (family of amaranthaceae) has much more medicinal benefits and is used as a remedy for treatment of hemorrhoids, indigestion, cough, asthma, anemia, jaundice and snakebite. Although widely used for dyeing purpose of preparation of local ink, and dyeing cotton fabrics. This dye is used as antiadhesive for various colours and making the colour brighter. It was tried to characterize chaff-flower leaves by Soxhlet extraction technique in ethanol as a solvent used. The phytochemical analysis of extract, secondary metabolites present in the medicine plant, the GC-MS analysis identified the bioactive chemical compounds. The compounds were predicted from Pass online biological activity.

Keywords: GC-MS, Soxhlet, Pass online, *Achyranthes aspera*

AT-30

**STRUCTURAL, OPTICAL AND ELECTRIC PROPERTIES OF CuO THIN FILM
PREPARED BY JNS PYROLYSIS TECHNIQUES FOR PHOTODETECTOR
APPLICATION**

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ABSTRACT

CuO thin films were prepared at different substrate temperatures such as 300, 400, 500 and 600°C using JNS pyrolysis technique. The XRD results reveal the polycrystalline nature with monoclinic phase and it shows that the obtained crystallite size varies with the substrate temperature. The EDS results displayed the presence of Cu and O. UV-Visible spectrophotometer has been used to record the CuO transmittance spectrum. The Tauc's relation is used to calculate the bandgap of CuO and the bandgap is found to depend on substrate temperature. The SEM image indicates the golf ball-like structure and particles are agglomerated together. The electrical conductivity depends on substrate temperature. The CuO was formed on the n-Si substrate using jet nebulizer spray pyrolysis technique in order to fabricate the diode. The diode parameters have been evaluated in darkness and in the presence of different light sources such as Halogen and Metal halide lamps for the fabricated p-CuO/n-Si diode.

Keywords: JNS pyrolysis, monoclinic phase, golf ball-like structure, electrical conductivity.

AT-31

ESTIMATION OF GAMMA RADIATION DOSE INDICES AT PRIMARY SCHOOLS IN NORTHERN REGION OF VELLORE DISTRICT

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ABSTRACT

Background: Indoor and outdoor gamma radiation exposure levels were measured in a total of 23 primary schools selected dwellings categorized as local, semi modern, modern buildings across Tamilnadu, Vellore city to determine the annual effective doses.

Materials and Methods: All radiation measurements were taken using a calibrated PG Geiger Muller detector and a GPS for geographical coordinates of sample points. Equal number sample point measurements were carried out for indoor and outdoor measurements. Measurements at each location point were performed holding at survey meter 1m above ground surface or floor to avoid unwanted effects of radiation from soil or building floor. The detector was also held at least six to seven meters away from the buildings in order to avoid unwanted effects of building materials on outdoor measurements. Each measurement was repeated four to five times and the average was taken to represent the value for a sample point.

Results: The average outdoor and indoor effective dose rates were determined as (363691.03 ± 71230.50), (407164.80 ± 62712.79), (449913.60 ± 40225.35), (443466.24 ± 31334.46), (624237.60 ± 142654.55) respectively. The highest contribution to the total indoor dose was from the local buildings contributed the least dose. The average annual effective dose for five schools was calculated as (0.36 ± 0.07), (0.41 ± 0.06), (0.45 ± 0.04), (0.44 ± 0.33), (0.62 ± 0.14), which is higher than the world average value.

Conclusion: In view of the potential radiation resulting from building materials, comprehensive assessment of natural radiations in such materials is required.

AT-32

MOLECULAR STRUCTURAL CONFIRMATION AND MATRIX REPRESENTATION OF C_{2v} AND T_d POINT GROUP SYMMETRIES

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ABSTRACT

C_{2v} is low point group symmetry and T_d is the high point group symmetry. Molecules belong to these symmetries are described based on both geometry and operations which it performs in the Cartesian coordinate system. The displacement coordinates for each atom and molecule are gets displaced based on the symmetry operation which it performs. These displacement coordinates in each atom are expressed in matrix form. Each individual matrix is called a representative of the corresponding symmetry operation and the complete set of matrices is called a matrix representation of the group. NH_2 molecule belongs to C_{2v} point group and P_4 molecule belongs to T_d point group. Based on these operations the structure of molecule is confirmed. Each symmetry operation in a molecule is expressed in a matrix form. The change in displacement coordinate in NH_2 and P_4 molecule of C_{2v} and T_d point group symmetries are expressed in matrix representations.

Keywords: Matrix representation; Coordinate displacement; C_{2v} and T_d .

AT-33

FERROMAGNETIC PROPERTIES OF MICROWAVE SINTERED $\text{LaFe}_{1-x}\text{Ti}_x\text{O}_3$

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ABSTRACT

Perovskite orthorhombic structure LaFeO_3 and $\text{LaFe}_{1-x}\text{Ti}_x\text{O}_3$ nanoparticles were prepared by microwave techniques. The prepared samples LaFeO_3 and $\text{LaFe}_{1-x}\text{Ti}_x\text{O}_3$ nanoparticles were characterized by X-ray diffraction (XRD) analysis for phase formation. Personalized surface morphology analyzed using scanning electron microscopy (SEM), The ferroelectric property was elucidated by means of polarization against applied electric field loop at ambient temperature. The M-H loop of the pure sample is paramagnetic, while the doped samples tend to be ferromagnetic with increasing Ti content. The magnetization, retentivity, squareness and coercive field of the Ti-doped sample with $x = 0.6$ is enhanced compared to that of pure LaFeO_3 and thus the doping of Ti would enhances the quality of device applications.

Keywords: Microwave sintered, XRD, SEM, PE LOOP and VSM.

AT-34

ON DIFFERENT TYPES OF FUZZY CONTINUOUS FUNCTIONS

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ABSTRACT:

In this paper, the concepts of different types of fuzzy continuous functions like somewhat fuzzy continuous function, somewhere fuzzy continuous function and fuzzy Baire continuous functions between fuzzy topological spaces are introduced and studied few applications in different branches of Mathematics and Physics theory. For example fuzzy topological spaces can be applied in the modeling of spatial objects such as rivers, roads, trees and buildings. Since fuzzy topology forms an extension of general topology and our results can be applied in modern physics and GIS problems.

Kew Words:

Fuzzy set, fuzzy Baire set, fuzzy dense set, fuzzy Baire dense set, fuzzy resolvable function, fuzzy Baire space, Fuzzy irresolvable space.

AT-35

**MOLECULAR SYMMETRY AND MATRIX REPRESENTATION ON THE
STRUCTURE OF SOME SIMPLE MOLECULES****D. Sowmiya^{1,*}, S.Saranyadevi¹, E.Balumahindran¹, S. Kumaresan¹, S.Selvaraj²**

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ABSTRACT

The aim of our project is to represent the behaviours of the linear and non linear molecule such as rotation, reflection and identity in the form of matrix. We will analyse these behaviours by introducing Cartesian 3 dimensional coordinates. All atoms continuously vibrates with respect to mean position. We will describe the position of each atoms by introducing coordinates: h_1 , h_2 and, etc. Each coordinate is corresponds to single degrees of freedom. When molecules vibrates, displacement takes place and the position of each atom during vibration can described by position coordinates h_1 , h_2 and h_3 and each single atom is described by 3 degrees of freedom. With the help of symmetry operations, we will describe rotation, reflection and identity operations for three selected molecules such as Br_2 (diatomic molecule), F_2O (triatomic molecule) and HCHO (tetraatomic molecule) in the form of matrix.

Key words: Degrees of freedom, Matrix rpresentation, Cartesian coordinates, Symmetry operations

AT-37

**ACETONE SENSING BEHAVIOUR OF OPTICAL FIBER CLAD
MODIFIED WITH γ -CuBr NANOCRYSTALS****T. Subashini^a, B. Renganathan^b, A. Stephen^c and T. Prakash^{a,*}**

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ABSTRACT

Measurement of volatile organic compounds (VOCs) in human exhaled breath is a non-invasive promising tool for medical diagnosis of metabolic changes or pathological disorders. A single human breath consists of 500 different VOCs which are typically in the range of parts per billion, parts per million and parts per trillion. Those are biomarkers to indicate several diseases, among other VOCs acetone is a biomarker of diabetic coma. For healthy people, exhaled acetone is usually in the range of 0.2-1.8 ppm and it can increase in the range of 1.25-2.5 ppm for people with diabetes. There was not any suitable device to detect acetone in exhaled breath. This work focus on the detection of acetone using clad-modified optical fiber coated with γ -CuBr. Nanocrystalline copper bromide (γ -CuBr) was prepared by hydrothermal method. The as-synthesized sample was characterized for its structural and microstructural properties using XRD, TEM, and EDS. The surface characteristics and optical properties of the sample were further studied with spectroscopy techniques such as FTIR, Raman, diffuse reflectance and fluorescence. Then, γ -CuBr nanocrystals was used as a gas sensing material in clad-modified optical fiber gas sensing system to explore its sensing behaviour for acetone (C_3H_6O) was shown superior sensor response about 5.9% to acetone gas.

Key words: Copper bromide nanocrystals; Hydrothermal; acetone; clad-modified optical fiber

AT-38

STRUCTURAL, OPTICAL AND ANTI CANCER ACTIVITY ON METAL OXIDE NANO PARTICLES

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ABSTRACT

The Nobel metal oxide like cerium oxide and Titanium has an excellent progress in the Nano field and this work provides the structural and biological behaviour of a metal oxide Nano particle. This covers the fundamental science, synthesis, characterization, physicochemical properties and an application of oxide nanomaterial explains fundamental aspects that determine the growth and behaviour of these systems. The Cerium with Titanium were synthesized by microwave method and analysed the presence of oxide, the crystal sized of **5 nm** was determined by *XRD*, *FTIR* for functional groups, band gap by *UV*, *SEM*, Optical studies on Photo luminescence and biological studies on anti-cancer on **MDA MB 231** by *MTT* assay for human breast cancer was analysed.

Keywords: Nano structure, Microwave method, Microbial activity, Anti-cancer.

AT-39

**SPECTROSCOPIC ANALYSIS OF ISONICOTINIC ACID:
EXPERIMENTAL AND THEORETICAL APPROACH**

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ABSTRACT

A study of vibrational and structural properties of pyridine-4-carboxylic acid chemical compound (molecular formula $C_5H_4NO_2$) is reported and characterized with aid of various spectroscopic techniques viz, 1H & ^{13}C , FT-IR, UV-visible, Raman etc. The correlation of experimental and theoretical data of structural and vibrational studies of compound has also been explored by DFT. Approach using B3LYP and HF/6-31 G (d,p) basis sets. The experimental spectroscopic data has been found to be in good agreement with the calculated results. The Mulliken population analysis on atomic charges, electric dipole moment, polarizability, natural bond orbital analysis, thermodynamic properties like heat, capacity, entropy and Zero vibrational energy have been analysed.

Keywords: DFT, B3LYP, Raman, NBO, FT-IR, UV-visible.

AT-40

ANTIHYPERGLYCEMIC AND ANTIOXIDANT EFFECT OF *ALLIUM SATIVUM* AQUEOUS BULB EXTRACT AGAINST ALLOXAN-INDUCED DIABETIC MALE *ALBINO* RATS

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ABSTRACT

Herbal drugs play an important role in health programs worldwide and there is a resurgence of interest in herbal medicines for the treatment of various ailments including diabetes mellitus. In both insulin-dependent (Type 1) and non-insulin-dependent diabetes (Type 2), an increased oxidative stress has been notified. In the present study, the folklore medicinal plant *Allium sativum* was selected to evaluate its antihyperglycemic and antioxidant effect against alloxan-induced diabetic male albino rats. The biochemical parameters such as blood glucose, insulin, and lipid profile (cholesterol, triglycerides, high-density lipoprotein, low-density lipoprotein (LDL) and very LDL, urea, uric acid, and creatinine) were analyzed. Finally, the antioxidant parameters such as superoxide dismutase, catalase, glutathione peroxide, and glutathione S-transferase also analyzed. The aqueous extract shows very good antidiabetic activity confirmed by biochemical parameters and histopathological analysis.

KEY WORDS: *Allium sativum*, Alloxan, antioxidant, Diabetes

AT-41

SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES FROM ETHANOL LEAVES EXTRACTS OF PERSEA AMERICANA AND ITS ANTIMICROBIAL EFFECTS IN HUMAN PATHOGENS

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ABSTRACT

This research was aimed to Synthesis and characterization of nanoparticles from the extract of *Persea americana* leaves. **Method:** The *Persea americana* leaves extract was obtained via the soxhlet extraction method using ethanol 96%. The ethanol extract of *Persea americana* leaves was turned into nanoparticles. The complete reduction of silver ions was observed after 12 hrs of reaction at 40° C under shaking condition. The color changes in reaction mixture (pale yellow to dark brown color) was observed during the incubation period. Then the extract were dried in hotair oven at 40-45°C. The dried power were milled with ball milling equipment to obtain a powder in nanometer scale. The synthesized silver nanoparticles were characterized by using various instrumental techniques such as Ultra Violet -Visible spectroscopy, (UV-Vis) Fourier Transform Infra-Red (FT-IR) spectroscopy analysis and Scanning electron microscopy (SEM). **Result:** The ethanol extract of avocado leaf is optimum for the synthesis of silver nanoparticles and it is also known to have the ability to inhibit the growth of various pathogenic microorganisms (*Lactobacillus sp*, *Streptococcus mutans*, *Streptococcus aureus*, *A. niger*, *Fusearium* and *A. flaves*).

Key words: Nanoparticles, *Persea Americana*, antimicrobial activity Disc diffusion method

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AT-42

GREEN ROUTE FOR THE SYNTHESIS AND CHARACTERIZATION OF Ag-NPs FROM *ABUTILON INDICUM* LEAF EXTRACT

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ABSTRACT

Silver nanoparticles (AgNPs) were synthesized using *Abutilon indicum* leaf extract with silver nitrate as initiating material. Synthesized nanoparticles shows the Ultra Violet – Visible (UV–Vis) Spectroscopy absorption peak at 450 nm which is one of the distinct features of AgNPs. Fourier Transform Infrared (FTIR) Spectrum implies that the role of aliphatic amines, alkyl halides and carboxylic acids were responsible for the synthesis of AgNPs and its stability. X- Ray Diffraction (XRD) spectrum confirmed that the synthesized silver particles were in the form of nanocrystals. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) images showed spherical shapes of synthesized silver nanoparticles size ranges between 23 – 38 nm. The Energy Dispersive X-Ray Analysis (EDAX) confirmed that the presence of silver content in the synthesized silver nanoparticles and it asserts that the process of biosynthesis of nanoparticles was carried out in accordance.

Keywords: Ag-NPs; *Abutilon indicum*; UV; FTIR; XRD; SEM; TEM-EDAX;

AT-42

SYNTHESIS OF COPPER OXIDE NANOPARTICLES USING FROM BOERHAVIA DIFFUSA LEAF EXTRACT AND ANTIBACTERIAL MICROBIAL ACTIVITY

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ABSTRACT

Synthesized nanoparticles have an incredible application in biomedicine owing to its simplicity eco-friendly properties and low cost. The present study aims to determine the green synthesized copper nanoparticles from Boerhavia diffusa leaf extract. Synthesis conditions were optimized for maximal narrow size range synthesis of copper oxide nanoparticles. The result nanopowder was characterized using various analytical techniques, such as Fourier Transform Infrared spectroscopy (FTIR), X-Ray Powder Diffraction (XRD), Scanning Electron Microscope (SEM). Hence an easy effective approach for synthesis of copper oxide nanoparticles, with efficient antibacterial microbial activity is reported in the study.

Keywords: Green synthesis, Boerhavia diffusa, FTIR, SEM, XRD.

AT-43

**ISOLATION AND CHARACTERIZATION OF DROUGHT STRESS
TOLERANT PLANT GROWTH PROMOTING RHIZOBACTER FROM
CHILI CROP**

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ABSTRACT

Chili is one of the important vegetable crops in India. Its area under production is limited by water scarcity. Microbes can promote plant growth by the regulating nutritional and hormonal balance, producing plant growth regulators, solubilizing nutrients (like phosphate) and including resistance against plant pathogen, these are collectively known as Plant Growth Promoting Rhizobacter (PGPR). In present study deals with, isolation and characterization of drought stress tolerant plant growth promoting bacteria (PGPR) from chili crop (*Capsicum annuum* L). The drought tolerant and plant growth promoting activity were screened by their biochemical activity like exo-polysaccharide, phosphate solubilization and indole acetic acid production. Totally 12 bacterial isolates were isolated from rhizosphere soil of chili plant. Among the twelve isolates, seven showed strong plant growth promoting activity like phosphate solubilization activity, exo-polysaccharide production and all isolate produced indole acetic acid (IAA).

Key words: PGPR, IAA, Exo-polysaccharide, Po₄ Solubilization, etc.,

AT-44

DIELECTRIC PROPERTIES OF THIOUREA DOPED CRYSTALS FOR LASER APPLICATIONS

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ABSTRACT

The technology strength of the nation the key to reach this developed status in fluency of doping the Xylenol orange in Thiourea crystals grown by slow evaporation room temperature method has been investigated. The concentration of metal dopants in the mother solution with xylenol orange for Thiourea solution were obtained with well-defined morphology, structural characterization of the grown crystals were carried out by single crystal XRD analysis. The FT-IR spectra study reveals the presence of ruinous functional groups and confirms the slight distortion of the structure of the crystal due to doping. The UV-visible spectra study was carried out to analysis the optical transmittance of the obvious regions for both pure and doped crystals. The dielectric loss and dielectric constant are analyzed by dielectric studies. The hardness of the pure and doped crystals is studies by using Vicker's tester.

Keywords

Thiourea Crystal, XRD analysis, FTIR studies, Dielectric Studies

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AT-45

SPECTROSCOPIC INVESTIGATION, VIBRATIONAL ASSIGNMENTS, HOMO-LUMO, MEP AND MOLECULAR DOCKING EVALUATION CALCONCARBOXYLIC ACIDE

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ABSTARCT

The experimental FT-IR and FT-Raman spectra of Calconcarboxylic acide have been recorded. Quantum chemical calculations of geometry and Vibrational wave numbers of the title compound are carried out theoretically and were compared with the experimental results. NBO analysis, HOMO-LUMO, hardness, softness, first hyperpolarizability and molecular electrostatic potential results are also reported. The negative regions of the MEP are related to electrophonic reactivity and the positive regions to nucleophilic reactivity, as shown in the MEP plot and the title compound has several possible sites. Natural bonding orbital (NBO) assessment was completed with a reason to clarify charge transfer, inter hybridization and delocalization of electron density within the molecule. The study is extended to calculate the binding energy of the title compound with suitable protein by Autodesk software. The RDG scatter graphs and the RDG gradient isosurface further illustrate that the interactions between 5CMF belong to the Vander Waals interactions

KEYWORDS:MEP, NBO,HOMO-LUMO, 5CMF

AT-46

SELF-CONSISTENT GW CALCULATION ON METALLIC SYSTEM CrNiO₄

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ABSTRACT

Electronic band structure and density of states calculations were performed on CrNiO₄ by using DFT methods such as LDA (local density approximation), GGA (generalized gradient approximation) and self-consistent GW (Green Wave) methods with and without spin orbital coupling. The band properties were discussed with respect to the calculations. The results obtained on the basis local density approximation/generalized gradient approximation (LDA/GGA) were been optimized at different k-points on the basis of Hohenberg and Kohn-Sham total energies. The spin natures on density of states (DOS) and partial density of states (PDOS) were mainly discussed based on the results obtained by GW method.

AT-47

SYNTHESIS OF MAGNESIUM OXIDE NANOPARTICLES USING FROM ACHYRANTHES ASPERA LEAF EXTRACT AND ANTIBACTERIAL MICROBIAL ACTIVITY

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ABSTRACT

Synthesized nanoparticles have an incredible application in biomedicine owing to its simplicity eco-friendly properties and low cost. The present study aims to determine the green synthesized Magnesium nanoparticles from Achyranthes Aspera leaf extract. Synthesis conditions were optimized for maximal narrow size range synthesis of Magnesium oxide nanoparticles. The result nanopowder was characterized using various analytical techniques, such as UV Spectroscopy, X-Ray Powder Diffraction (XRD). Hence an easy effective approach for synthesis of Magnesium oxide nanoparticles, with efficient antibacterial microbial activity is reported in the study.

Keywords: Green synthesis, Achyranthes Aspera, UV Spectroscopy, XRD.



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