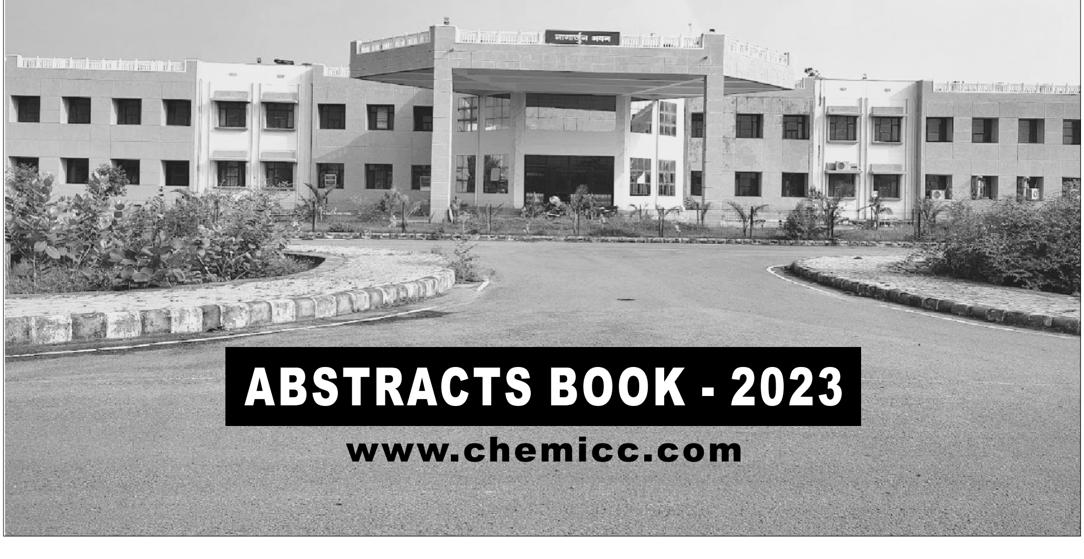
XXXXII
ANNUAL CONFERENCE
INDIAN
COUNCIL OF CHEMISTS
20th - 22nd DECEMBER, 2023

DEPARTMENT OF PURE & APPLIED CHEMISTRY
UNIVERSITY OF KOTA
KOTA - 324 005 (RAJASTHAN)



ABSTRACTS BOOK - 2023

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INTERNATIONAL SYMPOSIUM ON "MATERIALS FOR HEALTH, ENVIRONMENT AND SUSTAINABLE DEVELOPMENT"

Dr.. Neelu Chouhan
Department of Pure and Applied Chemistry
University of Kota-324010 (Rajasthan)

INDIAN COUNCIL
OF
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ABSTRACTS BOOK

Department of Pure & Applied Chemistry
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Kota - 324 005 (Rajasthan)

20th - 22nd DECEMBER, 2023

Editor : Prof. R.K.S. Dhakarey

Welcome

Dear Fellow Researchers & Scientists

On behalf of the Indian Council of Chemists, it is my pleasure and honour to welcome you all to the XXXXII Annual Conference of ICC from 20th - 22nd December, 2023 at Department of Pure & Applied Chemistry, University of Kota, Kota-324005 (Rajasthan).

The leading researchers and key opinion leaders in Chemistry have been invited to facilitate sessions and deliver lectures at XXXXII National Conference of ICC.

There will be vast range of learning opportunities at invited talks, oral, poster presentations and symposium session. Participants can also look forward to expanding their network at various networking events such as conference lunch, dinner and cultural programme. Apart from the scientific programme, there are many tourist attractions in and around Kota (Rajasthan). You can enjoy there too.

Thank you for your participation.

Prof. R.K.S. Dhakarey
Secretary, ICC

PROVISIONAL PROGRAMME

Wednesday, December 20th, 2023

Venue : Nagarjun Bhawan, Kota University, Kota

08.00 to 09.30 am	Registration and breakfast
09.30 to 01:00 pm	Inauguration function and keynote address
01:00 to 02:00 pm	Lunch
02:00 to 05:30 pm	International Symposium on "Materials for Health, Environment and Sustainable Development"
05:30 to 06:00 pm	Tea break
06:00 to 06:30 pm	ICC Executive Committee meeting (to be attended by EC members only)
06:30 to 08.30 pm	Cultural programme
08:30 pm onwards	Dinner

Thursday, December 21st, 2023

Venue : Vachaspati Bhawan, University of Kota, Kota

08:00 to 9:00 am	Breakfast
09:00 to 9:30 am	Sectional President Address in respective Technical sections
09:30 to 1:00 pm	Invited talk & paper presentation in respective Technical sections
01.00 to 02.00 pm	Lunch
02:00 to 05:00 pm	Invited talks & paper presentations in respective Technical sections
05:00 to 05:15 pm	Tea break
05:15 to 06:30 pm	Poster presentations and ICC General Body Meeting
06:30 to 08:30 pm	Kota City Night Tourism
08:45 pm onwards	Dinner

Friday, December 22nd, 2023

Venue : Vachaspati Bhawan, University of Kota, Kota

08:00 to 9:00 am	Breakfast
09:00 to 1:00 pm	Invited talks & paper presentations in respective Technical sections
01.00 to 02.00 pm	Lunch
02:00 to 03:00 pm	Poster Sessions
03:00 to 05:00 pm	Valedictory Function

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Kota - 324 005 (Rajasthan)

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Instructions for the Preparation of Poster Presentation

Your poster should be displayed as per the poster board number given in the abstract book. Posters will be displayed during the Poster Sessions and must be mounted from the start of sessions and removed upon conclusion of sessions on the scheduled day. Authors are requested to stand next to their poster boards during the Poster Sessions.

- You should be printing and bringing your poster to the conference.
- The dimensions of poster **should NOT exceed 90 cm wide × 120 cm high.**
- Please prepare your poster to fit the dimensions specified. It is recommended that poster be prepared on one sheet. Alternatively presenters may display their material on several smaller sheets.
- Allocate the top of the poster for the title and authors as stated on the submitted abstract.
- The text, illustrations, etc. should be bold enough to be read from a distance of two meters.
- Double sided tape and technical equipment will be available for the mounting of posters. Staff will also be available to assist you.
- DO NOT write or paint on the poster boards. DO NOT use nails, push pins, screws, or any tools that will puncture the poster boards.
- Please use the board that displays the same number assigned to you.

For any help kindly contact the concerned **Sectional President** or **Prof. Ajay Taneja**, Joint Secretary-ICC.

Acknowledgements

The Indian Council of Chemists is going to hold its XXXXII Annual Conference at Kota (Raj.) on 20th - 22nd December, 2023 and the abstract book containing the abstracts of papers selected for presentation in the Conference is in your hands. The Council justifiably feels proud of its achievements during the past 42 years of its existence.

The Council is grateful to Prof. Neelima Singh, Dr. Neelu Chouhan, Dr. Bhawani Singh, Staff Members and Students of School of Chemistry, Department of Pure & Applied Chemistry, University of Kota, Kota-324005 (Rajasthan) for their utmost cooperation in organizing the Conference.

The Council on its own behalf and on behalf of the Organizing Committee thanks all those who have helped in preparing and publishing this Abstract Book. The assistance given by Dr. Manoj Rawat, Dr. S.C. Goyal and Prof. Ajay Taneja is gratefully acknowledged.

Some of the abstracts have been edited by Sectional Presidents, due to paucity of funds and also on account of pressing limitations on the space available, a few others have also been condensed and as such some inadvertant omissions might have occurred for which ICC offers its apologies.

Prof. R.K.S. Dhakarey

Editor

CONTENTS

ABBREVIATIONS

AIL - Analytical Invited Lecture
AO - Analytical Oral
AP - Analytical Poster
IIL - Inorganic Invited Lecture
IO - Inorganic Oral
IP - Inorganic Poster
OIL - Organic Invited Lecture
OO - Organic Oral
OP - Organic Poster
PIL - Physical Invited Lecture
PO - Physical Oral
PP - Physical Poster
CYSA - Contestent for Young Scientist Award
MHESD-SP - Symposium

SECTIONAL PRESIDENTS

Dr. Neelu Chouhan
Symposium on
"Materials for Health, Environment and Sustainable Development"

Prof. G. S. Gugale
Inorganic Chemistry Section

Prof. Kishore Chikhalia
Organic Chemistry Section

Prof. Pradeep K. Sharma
Physical Chemistry Section

Prof. Jaya Dwivedi
Analytical and Environmental
Chemistry Section

AWARDEE 2023

Dr. G.C. Saxena
Life Time Achievement Awardee

Prof. Hitesh D. Patel
Prof. S.T. Nandibewoor Awardee

Dr. Prabhakar Chetti
Dr. Arvind Kumar Memorial Awardee

Prof. J. Manjanna
Dr. P.N. Sharma Memorial Awardee

Prof. P. Shyamala
Prof. Kaza Somsekhara Rao Awardee

Prof. Ramesh L. Gardas
Dr. S.P. Hiremath Memorial Awardee

Prof. Rengaraj Selvaraj
Prof. W.U. Malik Memorial Awardee

Prof. Sangita Sharma
Dr. S.M.L. Gupta Memorial Awardee

Prof. Suresh C. Ameta
Key Note Speaker

Key Note Speaker Lecture

Photocatalysis : An Emerging Green Pathway

Suresh C. Ameta

Professor of Eminence, Department of Chemistry, Faculty of Science, PAHER University, Udaipur-313024 (Raj.)
E-mail : ameta_sc@yahoo.com

The whole world is facing two major problems these days. These are: (i) Rapidly increasing water and air pollution and (ii) Shortage of conventional energy resources. Advanced Oxidation Processes are eco-friendly pathways and out of them, photocatalysis is one of the promising processes, which can provide a simultaneous solution to both these burning issues. Hydrogen has been long advocated as a fuel of future, which can be produced photocatalytically from photosplitting of water. Global warming is another existing challenge of concern, and the carbon dioxide has been predicted as the main culprit. Carbon dioxide can also be reduced photocatalytically to some value added fuels. The major limitation of photocatalyst in most of the cases is their limited activity due to little or no absorption in visible range and also to control recombination of electron- hole pairs. Efforts are being made to combat against both these limitations by increasing the photocatalytic activity through modifying semiconductors by metal or non-metal doping, sensitization, use of cocatalysts, composite formation, Z-scheme, S-Scheme, etc. All this will be discussed along with other interesting applications of photocatalysis.

To be presented in
Inaugural Section

Prof. W.U.Malik Memorial Awardee Lecture

2D-g-C_3N_4 Nanosheets : An Effective Materials for the Separation of Oil from Water and Wastewater

Rengaraj Selvaraj

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One of the most common methods used for the treatment of oily contaminated water is the filtration method by modified surfaces. In our laboratory, we have developed g-C_3N_4 via thermal condensation method. These materials were characterized by using various advanced chemical and structural techniques including XRD, XPS, UV-DRS, FTIR, SEM, and EDX. In order to separate oil from water, stainless-steel meshes were modified and coated with the prepared g-C_3N_4 Nano sheets to be used for the separation of oil and water mixture. The nanomaterials coated mesh were functionalized with hydrophobic agents. Different tests were performed to investigate the nature of the coated meshes and their stability and efficiency. After many separation tests, it was found that the most efficient coating among all the modified meshes was g-C_3N_4, which was functionalized using HDTMS. The separation efficiency of this coated mesh reached nearly 75% and it resulted to fast separation, which happened in a few seconds. In addition, the modified mesh can be used for many cycles and still gives good separation efficiency. These results suggest that the 2D nanostructured coated meshes will be the promising method for the oil spill problem and it will help to remove the oil from the oily contaminated water. Also, our research group applied these materials for the effective removal and degradation of pharmaceuticals, VOC's, EDC's and other contaminants present in water and wastewater.

To be presented in Symposium

Prof. S.P. Hiremath Awardee Lecture

Ionic Liquids as Benign Solvents for Chemical and Technological Applications

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A novel class of molten salts referred to as ionic liquids possess the unique combination of particular properties, unlike molecular liquids, namely negligible vapor pressure (~ 10^{-11} to 10^{-10} bar at room temperature), wide thermal window (~ -50 °C to +250 °C), wide electrochemical window (~ ±3 Volt vs. NHE), non-flammability, high ionic conductivity and a highly solvating capacity for organic, inorganic and organometallic compounds. This unique combination of particular properties allows them to be exploited as "alternatives to organic solvents" and gives them increasing attention in academic and industrial research. The research areas on ionic liquids are growing very rapidly, and the potential applications are numerous, mainly because simple changes in the cation and anion combinations or the nature of the moieties attached to each ion allow the physical properties of ionic liquids such as hydrophobicity, viscosity, density, coordinating ability, ion selectivity, and chemical and electrochemical stability to be tailored for specific applications. The proposed talk will briefly introduce ionic liquids and understand the unique thermophysical properties of novel ionic liquids for metal ion extraction, CO_2 capture, desulphurization of fuels, and aqueous biphasic systems for the extraction of value-added products. Further, the effects of thermophysical properties of ionic liquids on these applications and current research trends on ionic liquids as solvents for the chemical industry will be discussed.

To be presented in
Physical Chemistry Section

Dr. Arvind Kumar Memorial Awardee Lecture

Optoelectronic Properties of Organic Materials : A Molecular Modeling Approach

Prabhakar Chetti

Department of Chemistry, National Institute of Technology (NIT), Kurukshetra-136119

Organic molecules possessing linear and star-shaped structures have been demonstrated to be effective optoelectronic materials due to their enhanced stability to air degradation and superior charge transport abilities. Acene, Furan, Thiophene, Selenophene based linear and star shaped organic materials possess diverse uses in organic photovoltaics (OPV), organic field-effect transistors (OFET), dye-sensitized solar cells (DSSC), light-emitting diodes (LED), organic light-emitting diodes (OLED), nonlinear optical materials (NLOs), and lasers (LASERs). The study employs density functional theory to evaluate the structural impact of the linear and star-shaped organic thiophene-based molecules on the optical and charge transport characteristics. The frontier molecular orbitals (FMOs), highest occupied molecular orbital, lowest unoccupied molecular orbital and HOMO-LUMO energy gap are assisted in the determination of suitable energy levels for electron transfer. The required photovoltaic parameters like J_{SC}, “G_{reg}, “G_{inj}, LHE and other associated parameters are calculated. The investigated compounds have exhibited minor disparities in the respective hole and electron reorganization energies and photovoltaic parameters. Consequently, these substances can be employed in organic electrical devices.

To be presented in
Organic Chemistry Section

Prof. Kaza Somsekhara Rao Awardee Lecture

Kinetics and Mechanism of Electron TransferReactions in the Presence of Reverse Micelles

P. Shyamala

Department of Chemistry, Andhra University, Visakhapatnam (A.P.)

Micelles can be classified into two types, normal micelles and reverse micelles. Normal micelles are good models for understanding observed rate enhancements; specificities and to mimic enzymes. Reverse micelles formed from surfactant aggregates in non-polar solvents, are better and a more effective medium for approximating the effects of selective substrate partitioning ,changes in the effective micro environment of the reactants and impressive rate enhancements. Water is solubilised in the core forming a *water pool* and its physical properties are different from those of bulk water. Some of the physical properties of water pools are: (1) The water pool has lower micropolarity and dielectric constant than the conventional aqueous medium. (2) The water has high nucleophilicity and low activity. Its concentration is small and comparable to that of reactant concentrations. (3) The water pool has high ionic strength (ionic strength is equal to counter ion concentration of the surfactant in the case of ionic surfactants). (4) If the reactants are water soluble then there will be substantial concentration effect because the volume of solubilised water is small. (5) The pseudo phases of the reverse micelle viz., the water pool and organic phase have far different solubilising properties.

Though various physico-chemical properties have been extensively studied in reverse micelles, kinetic studies in reverse micelles are only slightly explored. Therefore, we have carried out a kinetic study of different kinds of reactions, unimolecular, bimolecular and complex reactions in the presence of two types of reverse micelles, AOT/Heptane (anionic) and CTAB/$CHCl_3$/Hexane (cationic). The experience gained from these kinetic studies and the catalytic effect of reverse micelles on rates of reactions will be presented in the talk.

To be presented in
Physical Chemistry Section

Prof. S. T. Nandibewoor Awardee Lecture

Therapeutic and Diagnostic Agents Development for Microorganism (MTB) Through Computational Chemistry

Hitesh D. Patel

Drashti Darji, Kinjal Patel, Neelam Prajapati, Mayuri Borad, Mahesh Vasava, Manoj Bhoi, Dhanji Rajania Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, INDIA aTuberculosis Research Centre, Surat, Gujarat

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AMR is a global health and development threat. It requires urgent multisectoral action to achieve the SDGs. Computational chemistry is the smartest tool for new drug development. Computational study of existing drugs and other potent molecules from the literature. Based on our previous study we had lead molecule. We have optimized the lead molecule and found better results during the computational study. Now synthesis of the newly designed molecules and their characterization. All newly synthesised molecules will be screened against the Microorganism (MTB) strains. The cell line toxicity study of the active compounds was performed. Then the study will be carried out in the animal for the potency of the compounds, toxicity and pK-pD. We will complete the phase – 0 (Preclinical). This work will give the best molecules for the Clinical phase which will work as the Microorganism (MTB) agents. With the therapeutic development, the diagnosis of the microorganisms is equally important. Because early diagnosis can save lives better than later treatment.

To be presented in
Organic Chemistry Section

Dr. S.M.L. Gupta Memorial Awardee Lecture

Computational Quantum Chemical Study, in Silico ADMET and Molecular Docking Analysis, in Vitro Biological Evaluation of Some Flavanoids as Potential Neuroprotectants

Sangita Sharma

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Neuroprotectants are well known for treating dementia which directly affects the brain and involves the failure of nerve cells. Since in every 3 seconds a person on this planet develops dementia and drugs available for these treatment are limited. Ayurveda therapy, Generic Medicine therapy and Homeopathy therapy are only ways to treat dementia. Numerous studies support that herbal medicines are amongst the most commonly used group of treatments among Complementary and alternative medicine(CAM) for dimentia. The study on interactions of components of herbal medicines in comparison to conventional medications, is limited and insufficient data concerning the possible hazards of herbal consumption is available. Drug likeness assessment of selected flavanoids as active ingredients and ADMET pharmacological model is tested here because herbal extracts are notably used for dementia. A Computational quantum chemical study and molecular docking analysis, in vitro biological evaluation of some flavanoids present in herbal formulations as potential Neuroprotectants in prediction Of enantioselectivity of flavanoids against proteins responsible for dementia is discussed here.

To be presented in
Organic Chemistry Section

Dr. P. N. Sharma Memorial Awardee Lecture

(Nano) Materials for Energy Devices and Environmental Remediation

J. Manjanna

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The development of sustainable energy systems is among the most pivotal challenges of the 21st century. Nanostructured materials are critical for developing novel and highly efficient devices. They offer huge surface to volume ratios, favorable transport properties, altered physical/chemical properties, and confinement effects resulting from the nanoscale dimensions. In this presentation, the (nano)materials to be used as electrolytes in solid oxide fuel cells (SOFC) are discussed. Recent report from our group on rare-earth metal doped ceria and transition metal doped titania as oxide-ion conductors have encouraged their potential applications for intermediate temperature SOFC. Also, we have studied on the dilute magnetic semiconductors (e.g., Fe/Co/Ni doped ZnO, In_2O_3 etc) towards spintronic devices.

For environmental remediation of nuclear and conventional water pollutants such as hexavalent chromium and dye molecules [10], we have investigated on the use of different metal oxides and modified clay minerals. Alteration of clay minerals relevant to geological disposal of high-level liquid waste (HLW) relevant to nuclear industry is presented. Basic properties of Fe-montmorillonite towards sorption and diffusion of radionuclides are studied. The importance of Mo removal from simulated HLW is accounted.

To be presented in Analytical and Environmental Chemistry Section

INTERNATIONAL SYMPOSIUM ON "MATERIALS FOR HEALTH ENVIRONMENT AND SUSTAINABLE DEVELOPMENT"

Convenor's Address

Defect Story of S-type Heterojunction S-doped g-C_3N_4 / g-C_3N_4 for Enhanced Photocatalytic Water Splitting

Neelu Chouhan
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Energy is the axis of life on earth and green / clean energy is the need of the time. Hydrogen generated from breaking of water is the green and sustainable solution of clean energy production. The S-type sulfer-doped g-C_3N_4@ g-C_3N_4 heterosystem was fabricated by using in-situ calcination method, using different precursors (urea, thiourea, melamine, and urea-thiourea). As formed systems were examined for water splitting for hydrogen generation in 20% CH_3OH under 300W light source. It was noticed that the system made by urea and thiourea (1:1) exhibits the maximum hydrogen generation rate via water split, i.e., 485.51 µmolg^{-1} h^{-1} (apparent quantum efficiency~ 1.75%) which is 1.37 and 1.29 times higher than native g-C_3N_4 system made by urea. 353.77 µmolg^{-1} h^{-1} and thiourea 376.07 ìmolg^{-1} h^{-1}. The improved hydrogen evolution rate is observed because of compatible S-type heterojunction between S-doped g-C_3N_4 and g-C_3N_4, effective reduction sites, improved charge separation and higher redox ability of the system . Based on advanced analysis techniques (XRD, UV-Vis, SEM, EDX, PLE, ESR, XPS, SPV, etc.) photocatalytic electron transfer mechanism was also proposed for the studied system.

MHESD-SIT-01 : Performance Improvement Mechanism of Lead-Free Perovskite Solar Cells Revealed by Electron Spin Resonance

Kazuhiro Marumoto

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Perovskite solar cells (PSCs) are expected to be one of the next-generation solar cells owing to their advantages such as low cost, flexibility, and high efficiency. However, traditional lead-based PSCs face a serious problem related to lead toxicity. Therefore, lead-free tin-based perovskite materials have been suggested as alternative materials to solve this problem. Unfortunately, the power conversion efficiency and stability of tin-based PSCs are still lower than those of lead-based PSCs owing to the problems such as easy oxidation of Sn(II). To suppress the oxidation of tin and to improve the efficiency and stability, introducing large organic cations to form Ruddlesden-Popper phase tin-based perovskite has been reported to be a practical method. In this talk, we present the charge states and charge transfer at the interface between a transport layer (PEDOT:PSS) and the tin-based perovskite layer under dark condition using electron spin resonance (ESR). Under simulated solar irradiation, there is a correlation between a performance improvement and an ESR increase, which can be ascribed to an enhanced electron barrier at the PEDOT:PSS/perovskite due to the reverse electron transfer from perovskite to PEDOT:PSS. These results are important to improve the efficiency and stability of the tin-based PSCs.

MHESD-SIT-02 : Cow Urine : A Treasure of Medicines

Ramesh Chandra Agarwal

Director, Universal Chemicals, F191 Idrprasth Ind. Area, Kota

The medicinal utility of cow urine has been mentioned in many ayurvedic texts - *Charka Samhita, Sushruta Samhita, Bhav Prakash, Ashtang Hridayam*, etc. In India, consumption of cow urine is practiced for thousand of years. It's analytical reports shows that the cow urine is not a toxic waste discharge by the body but it contains many minerals, vitamins, enzymes, hormones and the substances, which are beneficial against the oxidative stress of the body. Cow urine contains the substances which are also present in the human body and its consumption maintains the balance of these substances to cure many diseases. We herewith, developed a commercial methodology to make cow urine palatable by deodorizing, flavourizing and preserving that includes its treatment with some carboxylic acids and monoterpenoids containing essential oils. The enzymes in cow urine improve the digestive system and build -up a robust immune system. There is a need to fit this ancient treasure of drugs into modern therapeutic system.

MHESD-SIT-03 : Purpose-Built Molecules and Molecular Assemblies for Therapeutic Applications

Amitava Das

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Multimodal phototherapy has been utilized in the last decade for antimicrobial applications. Very recently photocatalytic therapy based on inorganic materials is also being utilized against new drug-resistant emerging bacterial infections.1·2 However, advances and insights achieved in utilizing the optoelectronic properties of inorganic materials, especially halide perovskites, are mostly focused on energy research. Literature reports on the utilization of photoinduced electron/energy transfer processes of perovskite-based materials in photocatalytic therapy for treating bacterial infections or other therapy applications are scarce. A water-stable perovskite halide-based multi-heterojunction with aligned band-edges and effective exciton dynamics between multisite heterojunction is derived from $Cs_3Bi_2Br_9$ perovskite as core, covered with TiO_2 surface functionalized with Ru-based photosensitizer. Our strategy allows the injection of two simultaneous one-electron into the conduction band of TiO_2 to be utilised for photocatalysis, leaving behind the exciton hole in bismuth perovskite and Ru(III) photosensitizer oxidant. These eventually induce a multimode photo redox catalytic cycle and generate a cascade redox process via reactive oxygen species and reactive nitrogen species. The scope of this hybrid photo-active material in treating certain bacterial stains will be discussed.

MHESD-SIT-04 : Waste-to-Wealth : Spent Lithium Ion Battery-Derived Ni^{3+}-Enriched β-$Ni(OH)_2$ for Ultrafast Electrocatalytic Oxygen Evolution Reaction

Joyee Mitra

CSIR-Central Salt & Marine Chemicals Research Institute, G. B. Marg, Bhavnagar, Gujarat 364002
Academy of Scientific and Innovative Research (AcSIR), AcSIR Headquarters, CSIR-HRDC Campus, Sector-19, Kamla Nehru Nagar, Ghaziabad 201002, U.P.

Urban mining of e-waste, especially end-of-lifelithium ion batteries

(LIBs), is gaining momentum as a potential secondary source for valuable metals considering the limited abundance of these metals in India, and due to the environmental impact associated with their disposal. Utilization of these metals in renewable energy-related applications could cater to the realization of a circular economy by re-using industrial waste for sustainable applications. In this regard, the selective extraction of Ni from spent LIBs, and its use as a precursorto form Ni^{3+}-enriched β-$Ni(OH)_2$is discussed.The LIB-derived β-$Ni(OH)_2$wasexplored as an electrocatalyst for water splitting to generate dioxygen gas (Oxygen evolution reaction, OER). As-synthesized β-$Ni(OH)_2$ required a minimal overpotential of 300 mV to reach a current density of 50 mA cm^{-2} with a low Tafel slope of 42.7 mV dec^{-1}. The usual sluggish kinetics of the OER was mitigated due to the strategic presence of a small amount of NiOOH, and surface oxygen vacancies. In situ impedance analysis strongly supported the improved OER performance of Ni^{3+}-rich β-$Ni(OH)_2$ due to facile OH* adsorption followed by rapid charge transfer at the electrode–electrolyte interface. The combined effect was manifested in ultrafast OER with mass activity 1044 mA mg^{-1} and TOF 257.2 s^{-1}, which are exceptional for Ni-based systems. The structural integrity of the catalyst was validated with post-OER characterization experiments, delineating the applicability of e-waste-derived materials for renewable energy applications.

MHESD-SIT-05 : Computational Studies, with Density Functional Theory (DFT), of Small Molecule Activation by Main Group Compounds

Kumar Vanka

Physical and Materials Chemistry Division, National Chemical Laboratory (CSIR-NCL), Pune

An important area of research that has seen rapid development in recent years is the determination of routes to small molecule activation that can be alternatives to transition metal based processes. Several interesting routes involving main group compounds have therefore gained prominence. My talk will focus on three stories from my group that highlight three different main group processes, where computational studies that we performed with density functional theory (DFT) led to a greater insight and understanding on how these systems actually functioned. These are (i) the use of low valent aluminum compounds to activate sigma bonds, where we showed that aromatic solvents play an important role, (ii) DFT studies that showed that there are many reactions where $B(C_6F_5)_3$ actually acts as an initiator more than as a catalyst, and (iii) computational studies that shed light on the triune nature of hydroborating and cyanosilylating agents in solvent and external catalyst free chemistry.

MHESD-SP-01 : Bio Inspired Synthesis of Biologically Active Cobalt Nanoparticles using Camelus Dromedarius Urine

Viquar S. Shaikh[1], Kailas M. Doke[1], Yaseen I. Shaikh[1],
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Physiologically processed bio-molecules present in camel excreta can be used to reduce metal ions into metal nanoparticles in a single step by novel synthetic routes. This biogenic reduction of metal ion to base metal is quite rapid and easily scaled up. These NPs exhibit excellent catalytic activities for studied organic reactions. X-ray diffraction pattern of reaction product confirmed the formation of Cobalt nanoparticles. The synthesized CoNPs shows potential activity for organic transformation. Antimicrobial activity of nanoparticles determines biogenic potential of the nanoparticles against different microorganisms and antioxidant activity determined the potential of free radicals. Both of the antimicrobial and antioxidant activity helps in study application of nanoparticles in medical and veterinary sciences.

MHESD-SP-02 : Phytochemical Study and Biosynthesis of ZnO NPS of Carica Papaya (ZnO bCA NPs) Leaf Extract and its Stabilization Mechanism with Microbial Efficacy

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Carica Papaya is a herbaceous whose fruits, leaves, seeds and latex are used medicinally. Extracts of Carica Papaya leaf are wide and traditionally use in many diseases especially in dengue fever in recent time. This work presents the phytochemical study of leaf extract of Carica Papaya and identify the chemical constitution by specific chemical test. In this work, biosynthesis method was adopted for the synthesis of zinc oxide nanoparticles with the leaf extract of Carica Papaya (ZnO bCA NPs) was utilized for biosynthesis scheme. In antimicrobial efficacy, the improved antibacterial responses of the biosynthesized variants were obtained due to the higher rate of stabilization mechanism of the nanoparticles by the organic chemicals (terpenoids, Phenolic and steroids) present in the Carica Papaya leaf extract.

MHESD-SP-03 : Antibacterial Potential: Synthesis, Characterization And Applications of Silver Nanoparticles

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In recent years, scientists have come up with ways to make nanoparticles that are inexpensive and good for the environment. It is a detailed overview of the synthesis of silver nanoparticles (AgNPs) exist in different forms such as size, shape, and surface that the specific form of silver nanoparticles can significantly influence their physical, chemical, and optical properties. These particles have high reactivity and antibacterial activity against microorganisms like bacteria, and fungal activity etc. they characterized some specific technique UV-Vis. Spectroscopy (to find absorption peaks of synthesized AgNPs), SEM (Scanning Electron Microscopy), and TEM (Transmision Electron Microscope) to define their morphology. It indicate that AgNPs were obtained the spherical in shape and have an average size of 48nm. Additionally, spectrophotometer analysis were use to determine an antibacterial and fungal activity of the synthesized AgNPs.

MHESD-SP-04 : Tailored Calcinative Impulses for The Modification of Fly Ash and Its Catalytic Applicability

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Herein, we are reporting the green and efficient synthesis of some pharmacologically important azomethine derivatives of isoniazide (INH) using Modified Fly Ash (MFA) as an excellent zeotic solid acid catalyst. The catalyst, by virtue of its terminal hydroxyl groups, forms hydrogen bonds with carbonyl compounds, which activates these reactants for condensation. The MFA was assessed for various aspects like crystallinity, porosity, elemental composition, linkages and also for its stability, which were confirmed with the help of some physical spectral analyses like XRD, BET, EDS, FTIR and TGA. An effective MFA synthesis was achieved by the calcination of an aqueous mixture of fly ash with ferric chloride, successfully incorporating the iron to generate a slightly acidic crystalline zeotic material, which served as an energy efficient catalyst by allowing access to the reaction at room temperature.

MHESD-SP-05 : Carbon Nitride–Graphene Oxide (g-C_3N_4@GO) Nanocomposites for Photocatalytic Hydrogen Production by Water Splitting

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We report to prepare the graphene oxide/ reduced graphene oxide and g-C_3N_4 was prepared separately by modified Hummer's method and calcination method (using precursors urea and thiourea) respectively. Thereafter, the composite of GO@g-C_3N_4 and reduced graphene oxide (reduced by ascorbic acid and $NaBH_4$) with g-C_3N_4 were fabricated using ultrasonication process. As prepared samples were tested for water splitting for hydrogen generation in 20% CH_3OH solution under 300W Xe light source after laode with 1.5% Pt as cocatalyst. It was found that the nanocomposite rGO(AA)@g-C_3N_4 exhibited the maximum rate for hydrogen generation 0.3091 $mmolh^{-1}g^{-1}$ (with 1.24% apparent quantum efficiency), which is 3.4,1.6,5.6, 3.4, and 1.4 times higher than the, pristine GO 0.0908 $mmolh^{-1}g^{-1}$, C_3N_4@GO 0.1908, $mmolh^{-1}g^{-1}$, rGO(AA) 0.0545$mmolh^{-1}g^{-1}$, rGO($NaBH_4$) 0.0908 $mmolh^{-1}g^{-1}$ and g-C_3N_4@rGO(AA) 0.2182 $mmolh^{-1}g^{-1}$ respectively via water splitting . Based on the advance analyses techniques (XRD, FT-IR, UV-Vis, PLE, etc) photocatalytic electron transfer mechanism was also traced for the studied system.

MHESD-SP-06 : Copper Catalyzed Intermolecular Heteroannulation Reaction between O-Acyl Oximes and 4-Thiazolidinones for the Synthesis of 2H-Pyrrolo[2,3-d]thiazole

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An intermolecular copper catalyzed heteroannulation reaction using Csp^3-Csp^3 radical coupling approach has been accomplished to synthesize 2H-pyrrolo[2,3-d]thiazole. C-C coupling between 4-thiazolidinones and O-acyl oximes under Cu catalyst further cyclizes to the target molecule "Thiazolidine-Fused Nucleus.". This unified method offers access to novel fused heterocycles with pyrimidines bearing 4-thiazolidinone in moderate to higher yields. The optimization study includes various copper catalysts, oxidants, bases, and solvents at different temperatures.

MHESD-SP-07 : Phosphomolybdic Acid Loaded Zeolite based Catalyst : Synthesis and its Application in Conversion of Carbohydrates

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In the recent scenario, heterogenous catalysts have been enormously explored for the sustainable development in green chemistry and catalysis. Synthesis of industrial based chemicals, biofuels and new bio-based materials has received much attention through conversion of biomass feedstock. In this research, carbohydrates (glucose and fructose) have been used as sustainable reactants. Natural zeolite has excellent catalytic performance as they are highly stable, microporous, resistant towards high temperature. This research highlights about the synthesis of natural zeolite based phosphotungstic acid loaded catalyst and its use in conversion of carbohydrates. Synthesized catalysts found efficient and 5-HMF is obtained as product which is an important industrial chemical. .

MHESD-SP-08 : Green Synthesis of Au-Nanoparticles using Allium Cepa L. and Evaluation of Their Biological Activities

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Green technology is currently in high demand, making it crucial to synthesize gold nanoparticles. These nano-sized particles have gained attention for their excellent optical properties, including shape and size, as well as their stability, low cost, environmental friendliness, and use of less hazardous chemicals. In this study, the goal was to use onion peel extract to synthesize gold nanoparticles. The extract contains various bioactive compounds, such as flavonoids, nucleotides, dipeptides, enzymes, and glycosides, which are believed to act as reducing agents in the synthesis process. The resulting Au-NPs showed promising anticancer properties against DLA cells. The formation of Au-NPs was confirmed by a color change from green to dark brown and validated through UV-Vis spectrophotometry (show an absorption peak), FTIR (to identify functional groups on the Au-NPs), SEM, and TEM (to analyze the spherical morphology of the Au-NPs). Zeta potential was also used to assess their stability. The biosynthesized Au-NPs demonstrated antimicrobial activity against various bacterial pathogens, including Escherichia coli, Klebsiella pneumoniae, and Staphylococcus aureus. This study successfully highlights the green and biocompatible synthesis of Au-NPs and their potential for applications such as anticancer, antimitotic, and radical-scavenging.

MHESD-SP-9 : Construction of a -NH_2 functionalized Metal Organic Framework (UiO-66-NH_2) for efficient removal of aquatic pollutants

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NH_2-functionalized metal-organic frameworks (UiO-66-NH_2) were prepared using a simple hydrothermal process. X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDAX) and transmission electron microscopy (TEM) were used to characterize the as-prepared materials. The adsorption and visible light photocatalytic studies were carried out on Rhodamine B (RhB), a model organic pollutant. Compared to pure MOF (UiO-66), UiO-66-NH_2 exhibits superior photocatalytic activity and adsorption. A synergistic approach of photocatalysis and adsorption eliminates RhB up to 99%. UiO-66-NH_2 has a greater adsorption capacity due to its unique micropore structure and its more negative zeta potential resulting from charge balancing for the protonation of -NH_2. The prepared material would serve as a low-cost, environmentally friendly and efficient photocatalyst for the sequential removal of aquatic pollutants.

MHESD-SP-10 : A Novel Polyelectrolyte Complex Nanocomposite of Modified Chitosan and Guar Gum for Co-delivery of Cisplatin and 5-fluorouracil in Cancer Therapy

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Platinum-based drugs are widely used in cancer therapy, but are reported to exhibit toxic side effects and resistance. Combinational drug delivery represents an effective chemotherapeutic strategy

wherein the negative effects of a drug can be compensated by co-delivery. In the present work, we developed a novel polyelectrolyte complex nanocomposite of modified polysaccharides namely, chitosan and guar gum for co-delivery of cisplatin (Cp) and 5-fluorouracil (5-Fu) in combination chemotherapy. The experimental conditions for the formation of the polyelectrolyte complex (PEC) of trimethyl chitosan (TMC) and carboxymethyl guar gum(CMGG) nanocomposite have been optimized. FTIR, ^{1}H-NMR, FE-SEM, P-XRD, HR-TEM, and TGA techniques were employed for the physical, chemical characteristics of nanocomposite material. The swelling study indicated the pH responsiveness of the polyelectrolyte complexes with higher swelling in a solution of pH 7.4 compared to that in pH 1.2. The swelling capacity of nanocomposite increased with an increase in Ag content. Hence the composite with 5% Ag was selected for the drug release study. Cp and 5-Fu were successfully loaded using the swelling method. The dual drug loaded PEC nanocomposite was evaluated for its drug release behavior. The results indicated the release of 98% of Cp and 93% of 5-Fu in the medium of pH 7.4 during 24 h. The study indicated that PEC nanocomposite is a promising material for the development of dual drug delivery in cancer treatment.

MHESD-SP-11 : Electroless Plating Loaded CoP on GO for Enhanced Photocatalytic Water Splitting

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Hydrogen is the cleanest fuel ever-known and can be produced by water splitting without producing any green-house gas. But it requires photocatalytic material and Graphene as a 2D material with various unique properties such as non-toxicity, low cost, thinness, strongness with high surface area and good conductivity (electricity and heat), is a good candidate for water splitting. We here in used the 3% CoP Co-catalyst modified graphene oxide (GO) by using two step electroless plating method. As-synthesised materials shows 10 folds increment in photocatalytic H_2 production rate of GO/CoP (454.385 ìmolg^{-1}h^{-1}) in comparison to the pristine GO (45.437 μmolg^{-1}h^{-1}) in 20% CH_3OH under 300W Xe light source. The apparent quantum efficiency of the studied systems (GO unused, GO used, GO/CoP unused, and GO/CoP used) were calculated i.e. 0.16%, 0.098%, 1.64% and 1.37%. Based on advance analyses techniques photocatalytic electron transfer mechanism is proposed CoP accelerated the separation of photo e^-- h^+ pair to relay the photo e^- via CoP particles to H_2O that improves the photocatalytic water splitting of pristine GO.

MHESD-SP-12 : Photocatalytic Degradation of Toluidine Blue using Bismuth Vanadate Composites : A Comparative Study with Green Route

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A comparative study for the photcatalytic degradation of Toluidine Blue dye (TB) in aqueous solution has been studied with using independent $BiVO_4$, Tungsten doped $BiVO_4$, and $BiVO_4$ with a adsorbent MWCNTs in the presence of natural light. The progress of the degradation was monitored sepctrophotometically. As synthesized composites were characterized using techniques such as FESEM, EDX and XRD. Different operational parameters were varied to optimize the reaction conditions to achieve highest rate constant such as: pH (8.0 and 9.0), concentration of dye (4.0×10^{-5} M and 6.5×10^{-5} M), Amount of photocatalyst (0.08 and 0.06 g), and Light Intensity (60.0 $mWcm^{-2}$). On the basis of observations, a suitable mechanism for the photocatalytic degradation of toluidine blue has been proposed. From the observations it is also observed that this is an eco-friendly method for the treatment of polluted water. The reusability of the catalyst was also established.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

Sectional President's Address

Development of Efficient Catalysts and Strategies for the Synthesis of Heterocycles

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Heterocyclic compounds have been phenomenal in exhibiting wide array of applications particularly as pharmaceuticals, agrochemicals, veterinary, lubricant, antioxidants, corrosion inhibitors, copolymers, dye stuff etc, The conventional methods of synthesis of these heterocycles are frequently associated with some limitations viz. less selectivity, low yield, requires high temperature, longer duration, generation of impurities etc.

To address these issues, greener and sustainable approaches have emerged as reliable tools that have facilitated the desired selective organic transformations with higher selectivity, low energy, reduced use of toxic solvent and affords high product yield in mild condition as compared to conventional synthetic methods. Of note, the transition metal catalysis, one pot domino approach, microwave assisted reactions provide an expeditious synthesis of heterocyclics.

In this context, our group is consistently making efforts to develop mild, efficient and eco-friendly greener synthetic protocols to afford medicinally important heterocyclic scaffolds particularly nitrogen-containing heterocycles. The developed catalysts and strategies have facilitated the synthesis of bioactive hybrids for varied applications under mild conditions with high selectivity, atom economy and yields.

AEIL-01 : Nanomaterials based Sensors for Environmental Monitoring : Air, Water, Soil

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Sensors play a crucial role in modern electronics. Different sensors such as energy sensors, flow sensors, humidity sensors, gas sensors, weather prediction sensors, light sensors, temperature sensors, bio-sensors etc. are an integral part of our life. For the development of these sensors, the use of nanonmaterials is inevitable in view of expected miniaturization, fast response, high sensitivity, long durability, cost effectiveness etc. Variety of nano-materials such as ceramics, oxides, sulfide, metallic nanoparticles, quantum dots, carbon nanotubes, graphene, organic/conducting polymers and polymer/inorganic hybrid materials have been extensively investigated and used as a sensing material to fabricate sensors for different applications. Moreover, the development in Internet of Things (IoT) has also added a new perspective in the sensing technology.

The development of nanomaterials-based sensors with IoT have enabled the efficient environmental monitoring with respect to essential life elements viz air, soil and water. This talk covers the overview of recent advancement in sensing technology and the development of nanomaterials-based sensors at C-MET in these areas.

AEIL-02 : Functionalized Metal Nanoparticles and their Analytical Applications for Removal of Metal Ions

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The magnetic Fe_3O_4 nanoparticles were functionalized with glycine at pH 6. The glycine functionalized magnetic nanoparticles (GFMNPS) were then entrapped into alginate polymer as beads and used as adsorbent for the removal of Pb(II) ions. The developed adsorbents were characterized by fourier transform infrared spectroscopy, vibrating sample magnetometer and scanning electron microscopic analysis. The surface of beads contains amino and carboxylate groups which make them effective adsorbent for the removal of Pb(II) ions. The adsorption of Pb(II) ions from aqueous solution was found to be highly pH dependent. The kinetic data fitted well with pseudo second order model and the equilibrium reached in 100 min with 99.8% removal of Pb(II) ions from aqueous solution. The adsorption isotherm strictly followed Langmuir model with the maximum adsorption capacity of 555.5 mg/g of the adsorbent. The thermodynamic study confirmed that the adsorption was spontaneous and endothermic in nature. The adsorbent could be regenerated four times simply by 0.2 M HNO_3 retaining 90% of the adsorption capacity. The synthesized adsorbent was found to be eco-friendly, cost effective, efficient and superior over other polymer based adsorbents for removal of Pb(II) ions from aqueous solution.

AEIL-03 : Functionalisation of PVDF based Membrane Incorporated with Fly Ash for Fuel-Cell Applications

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Direct methanol fuel cells (DMFC) are promising devices for small-scale portable applications. These are characterized by their high energy density that have been claimed to be ten times higher than that of the lithium ion batteries. Hence, they have the potential to be prosperous alternatives to replace secondary batteries. However, their performance is restricted due to Methanol Cross-Over (MCO) through the electrolyte membranes especially at high methanol concentration. This stimulates the idea to tailor a new membrane to minimize MCO; this may result a crucial improvement towards the commercialization of DMFC. In order to develop low cost and high efficient polymer electrolyte membrane (PEM), the fly ash has been incorporated within the structure of S-PVDF using common solvent DMF via, solution cast technique followed by ultrasonication and subsequently sulfonation by using chlorosulfonic acid. Furthermore, the PEM were subjected to different structural and physicochemical characterization such as FTIR, XRD, AFM, TEM, WU, IEC, DSC and TGA. The samples containing 2- 7% w/w fly ash have been tested. At optimum value, the membrane characteristics in terms of WU value is about 18.8%, corresponding to IEC of 0.48 meqg^{-1} vis-à-vis Nafion-117. The selectivity of composite membrane was observed to be nearly one and half fold greater as compare to Nafion-117. The composite membrane shows supress fuel crossover of the order 10^{-7} , which is 10-fold less than the Nafion-117. Further, the AFM, SEM and EDS studies shows the strong interaction between host material and dopant, which are correlated with the water uptake, ion exchange capacity, proton conductivity as well as selectivity of the composite membrane. The DSC and TGA curve confirm the thermal stability of membrane.

AEIL-04 : Application of Doped Nanomaterials and Nanocomposites for the Removal of Organic Contaminants

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The rapidly increasing population, depleting water resources, and climate change resulting in prolonged droughts and floods have rendered drinking water a competitive resource in many parts of the world. The development of cost-effective and stable materials and methods for providing the fresh water in adequate amounts is the need of the water industry. Traditional water/wastewater treatment technologies remain ineffective for providing adequate safe water due to increasing demand of water coupled with stringent health guidelines and emerging contaminants. Nanotechnology-based multifunctional and highly efficient processes are providing affordable solutions to water/wastewater treatments that do not rely on large infrastructures or centralized systems. The aim of the present study is to review the possible applications of the nanoparticles/fibers for the removal of pollutants from water/wastewater. The paper will briefly overview the availability and practice of different nanomaterials (particles or fibers) for removal of viruses, inorganic solutes, heavy metals, metal ions, complex organic compounds, natural organic matter, nitrate, and other pollutants present in surface water, ground water, and/or industrial water. Finally, recommendations are made based on the current practices of nanotechnology applications in water industry for a stand-alone water purification unit for removing all types of contaminants from wastewater.

AEIL-05 : Green Synthesis of Silver Nano Particles and its use Photocatalytic Degradation of Textile Dye

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Nanoparticle synthesis from the parts of plants is a great achievement over the synthesis of nano-catalyst using physical and chemical method. The present study reported green method for the synthesis of nano particles of silver by using Coriandrum sativum leaf extract which act as reducing and stabilising agent. The photo-catalytic activity of the silver particles observed for the degradation and the removal of the harmful dye Acid black 24. The green synthesis of silver nano particles was firstly observed by the UV-Vis spectral analysis, which give the maximum absorption peak at the range of 410-420 nm it revealed the formation of nano particles in colloidal solution. SEM-EDX, XRD conducted for the confirmation of the shape, elemental analysis of the catalyst, crystalline nature respectively and the formation of the particles at nano scale. Effect of Various parameters affecting the photo-catalytic degradation of the Acid Black 24 like initial catalyst loading, dye concentration and Ph observed. This approach of synthesis of silver nano-particles by using the leaf extract is a very environmental benign method and effective for the removal and degradation of textile dyes and efficient for the treatment of textile dye effluents released from textile industries.

AEIL-06 : Air Quality Determinants and their Importance in Health Risk Assessment Indoors

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Pollution is regarded as one of the great existential challenges of the Anthropocene epoch causing the largest category of welfare damage. Nine out of 10 people in the world breathe polluted air, causing more than 7 million premature deaths every year — double the number of people dying from HIV, malaria and tick-borne encephalitis combined.. The study of Indoor air quality can be henceforth regarded as a dome in lieu of merely a discipline as the researcher's approach initially begins with addressing the concern related questions latterly followed by identification of suitable tools/ techniques needed for solving the related 'purpose'. The effects of indoor air pollutants range from short term effects including eye and throat irritation to respiratory diseases and cancer abiding in the fullness of time. In this work, a selection of datasets of studies done on indoor air quality at North Central part of India (Agra) region in homes and buildings located in different microenvironments during last fifteen years is presented Chemical Sampling composition of PM including metals and ions were identified. Source apportionment through PCA explained 76-88% of source contribution. Recent studies undergone elaborated the issue of size fractionated chemical composition of PM including ultrafine particles collected through deployment of impactors. Bioavailability index further calculated showed the importance of smaller size particles in simulated lung environment that further varied with element and size elucidating increase in aerosol enrichment to finest particle. The work too includes the emerging issue with and future scenarios of the current pollution status in Indian context. It concludes with various remediation strategies and policy abatement by different governmental agencies in pollution control methods and technologies. The mainstay of control is henceforth trusted upon the education and awareness of the masses to pollution free 'cleaner' indoor environment.

AEO-CYSA-01 : A Geochemical Assessment and Evaluation of Groundwater Suitability for Irrigation in Vidisha District Madhya Pradesh, India

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The groundwater quality is of far most important for irrigation purposes, especially in the Vidisha district, which is highly dependent on groundwater. In the present work, we investigated the groundwater quality and compared it with the hydrogeochemistry of the Vidisha district of Madhya Pradesh, India. Vidisha has hard rocks (basalt, sandstone, shale etc.), but water-rock interaction, especially after increased rainfall, changes groundwater quality. Also, the use of high amounts of fertilizers and pesticides and their interaction with surface water ultimately affect groundwater quality. We collected over 180 water samples and conducted comprehensive physicochemical analysis for about 20 parameters and their comparison with BIS as well as whom permissible limit has done. The appropriateness of groundwater for irrigation was evaluated using multiple indices. From the estimated indices, the groundwater sample analysis data were plotted using the Gibbs, Piper, USSL, Wilcox, and Chadha plots and determined the irrigation water quality index (IWQI). Maximum samples have been found to suit for irrigation purposes, though some were found unsuitable due to dissolution of high mineral amounts.

AEO-CYSA-02 : In@CdS Sensitized TiO_2 Nano-Rod for Photocatalytic and Photoelectrochemical Water Splitting under Sunlight

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A one-step hydrothermal method for synthesis of titanium dioxide

(TiO_2) nanorods was used, followed by cadmium sulphide (CdS) and Indium (In) doped CdS quantum dots (QDs) sensitized on the surface of TiO_2 nano-rod by using successive ionic layer adsorption and reaction (SILAR) method. Characterization of this material is carried out using XRD, XPS, FE-SEM, EDX, Raman, UV-DRS, PL. The XRD pattern confirmed that the preferential orientation of TiO2 grains is along the (101) plane perpendicular to the FTO substrate. The XRD pattern also attributed the sensitization of CdS QDs in form of hexagonal CdS QDs and doping of In into CdS QDs. FE-SEM analysis showed the TiO_2 nano-rod are uniform, thick and grown vertically on the FTO substrate. The decrease in band gap energy as doping of In in CdS/TiO_2 nano-rod is observed by UV-DRS studies. The photoelectrochemical and photocatalytic performance of In doped CdS QDs embellished on the surface of TiO_2 nano-rod photoanode was studied by varying the concentration of In. The photo electrochemical (PEC) and photocatalytic H2 generation performance under natural sunlight of the as prepared photoanode was investigated in terms of photocurrent density and amount of H2 production. Among all the synthesized materials, the 2% In-CdS/TiO_2/Pt/FTO nano-rod showed highest photocurrent density of 4.78 (mA/cm^2) and 22.12 ml/h/g of hydrogen production.

AEO-CYSA-03 : Synthesis of $K_2W_7O_{22}$ for Room Temperature Acetone Sensing

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Herein, we report, synthesis of $K_2W_7O_{22}$ by hydrothermal method using oxalic acid as a surfactant. The as synthesized $K_2W_7O_{22}$ was characterized using XRD, Particle size analysis, RAMAN, UV-Visible spectroscopy, FESEM, FETEM and FTIR analysis. The XRD analysis of the $K_2W_7O_{22}$ revealed the hexagonal crystal structure. The FESEM analysis shows the rectangular Nano blocks like structure. The dimensions of rectangular shaped nanoparticles are 30 nm in width and ~ 100 nm in length. The synthesized $K_2W_7O_{22}$ was tested for acetone gas sensing at ambient room temperature. The acetone concentration was varied from 10 ppm to 100 ppm. The $K_2W_7O_{22}$ has shown highest sensitivity towards acetone gas with minimum cross

sensitivity towards other gases and organic vapors. The sensitivity obtained is around 70% with response time of 11 s and recovery time of 40 s respectively.

AEO-CYSA-04 : White Fluorescent Carbon Dots-Cadmium Sulfide Quantum Dots Nanocomposite Probe for Sensitive and Selective Detection of Chromium (VI) Ions

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Carbon dots are 0D spherical nanoparticles having size less than 10 nm which are good candidate for fluorescence sensing due to its good optical and electrical properties. Similar to carbon dots, CdS quantum dots are also well known due to their size confinement, large surface area and narrow band gap which are also quite useful in sensing. This work involves novel fluorescent probe which is composed of carbon dots (CD) and cadmium sulfide quantum dots (CdS QD) for the sensitive and selective fluorescence detection of Cr (VI) ions. The blue fluorescent CD and orange fluorescent CdS QD are synthesized by hydrothermal method. The CD are synthesized from natural precursor apricot which is not reported before. The carbon dots- cadmium sulfide quantum dots (CD-CdS QD) nanocomposite was synthesized and characterized using different characterization techniques which shows white fluorescence under UV light. The white fluorescence is quenched selectively in the presence of Cr (VI) ions and linear decrease in the fluorescence was observed in the concentration range 5-90 µM of chromium (VI) ions with the limit of detection 2.73 µM. This is novel probe for sensitive, selective and rapid detection of chromium (VI) ions.

AEO-CYSA-05 : Electrochemical Sensing of Carcinogenic p-Dimethylamino Antipyrine Using Sensor Comprised of Eco-Friendly MoS_2 Nanosheets Encapsulated by PVA Capped Mn doped ZnS Nanoparticle

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p-Dimethylamino Antipyrine (p-DAAP) is a carcinogen that causes agranulocytosis and is found as an addition in cocaine samples. It is necessary to use a sensitive analytical approach capable of identifying trace quantities. In this work, we used a voltammetric technique to build an electrochemical sensor for p-DAAP trace level monitoring. Synthesized PVA capped Mn doped ZnS encapsulated by synthesised MoS_2 nanosheets drop casted on glassy carbon electrode (Mn:ZnS/ MoS_2@GCE) was used as an electrode for p-DAAP investigation. XRD, SEM-EDX, and FTIR were used to characterise the surface. The material's performance was investigated using electrochemical impedance spectroscopy (EIS). To evaluate p-DAAP, cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used. Under various phosphate buffer solutions, the p-DAAP displays an oxidation peak and a reduction peak between 0 - 0.8 V capabilities, with pH 6.0 giving the best result. The effect of numerous parameters on electrochemical characteristics was studied, indicating diffusion as a regulator of the electrode process. The DPV is used to calculate the quantitative value of p-DAAP. The linearity field was determined to range between 0.2 M to 16M. The LOD and LOQ were 1.08×10^{-8} M and 3.60×10^{-8} M, respectively, and outperformed previous techniques. Furthermore, the innovative approach was used to assess p-DAAP concentrations in biological and water samples.

AEO-CYSA-06 : Facile Solvothermal Synthesis of Ternary $Ni_3Bi_2Se_2$ Chalcogenides and their MWCNT Composites as Bifunctional Photo-eElectrocatalysts for Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER)

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Clean and sustainable energy is an illuminative field of research for the scientific community to avoid contagious emissions from burning fossil fuels. Photo-electrochemical (PEC) water splitting holds strong potential to generate clean energy fuel by modern-day renewable energy devices. Regarding large-scale hydrogen production by water electrolysis, achieving the bifunctional photo-electrocatalyst with high efficiency and stability at high current densities is significant but remains a grand challenge. To address this issue, herein, one unique hybrid ternary nickel (Ni)-bismuth (Bi)-selenide (Se) nanosheet arrays and their MWCNT composites were synthesized via a one-pot solvothermal reaction. Material characterization was undertaken with X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDX), and UV-visible spectroscopy. A dual-functional ternary ($Ni_3Bi_2Se_2$@MWCNT) heterostructure is designed for PEC water-splitting properties exhibiting an overpotential (285 mV & 181mV) at a current density of 10 mA/cm^2 and a low Tafel slope (68 mV dec^{-1} and 48 mV dec^{-1}) in presence of light environment for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Upon injecting the light, the as-prepared ($Ni_3Bi_2Se_2$@MWCNT) exhibits remarkably improved efficiency of 24% and 19% for HER and OER, respectively. A long-term durability test of ($Ni_3Bi_2Se_2$@MWCNT) for 12 h at 10 mA /cm^{-2} current density suggests it may be a suitable substitute for noble-metal-based electrocatalysts for water oxidation in alkaline media.

AEO-CYSA-07 : Facile Synthesis of Graphene/La Supported Activated Carbon for Scavenged of Fluoride from Water

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Human health can be seriously affected by drinking water resources with high concentrations of fluoride (>1.5 ppm). The addition of the fluoride ion to drinking water is a widespread procedure because of its utility in treating osteoporosis and promoting better dental health. To improve fluoride removal efficiency from aqueous solutions, graphene was modified with lanthanum ions and activated carbon. In present study graphene was synthesis using liquid phase exfoliation method, La_2O_3 NPs was synthesis using precipitation method. We use Acetamide as fuel, CTAB as Surfactant and water as solvent in precipitation method. After that G/La supported activated carbon was synthesised by impregnation evaporation technique. FT-IR, XRD, FE-SEM, EDS, and N_2 adsorption- desorption study (BET) was used to evaluate the modified G/La supported activated carbon composite. Analysis of fluoride adsorption on G/La supported activated carbon was carried out using batch systems, adsorption isotherms, and kinetic studies. FE-SEM image shown that after La_2O_3 and AC modification, the composite layer thickened and several tiny particles were discovered on the graphene surface. Importantly, the Langmuir isotherm model and pseudo second order kinetics model fitted the adsorption data well, and the highest adsorption capacity of G/La supported activated carbon was 50.10 mg/g in the Langmuir model at a dosage of 2.0 g/ L. The experimental results show that the G/La supported activated

carbon composite could be a highly effective material for the removal of fluoride from water.

AEO-CYSA-08 : Selective Colourimetric and Fluorimetric Sensing of Capped Silver Nanoparticles for the Detection of Metal Ion, Its Review Study

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The applications of nanoparticles have increased a lot in recent years owing to their distinctive physical and chemical detection properties. AgNPs based sensors have fascinated a lot, due to their SPR bands and tuneable optical properties and also, they have proved to be suitable for their selective and sensitive colorimetric and fluorometric probe. The present work focusses on the synthesis of AgNP and its physical, chemical, and biological detecting ability of metal ions, in various aqueous solution and in the environment.

AEO-CYSA-09 : Spatial and Temporal Variation in Metals Associated with School Settled Dust and their Risk Assessment in School Children of Agra (India)

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Re-suspension of school settled dust can be an important source of exposure to metals and can develop detrimental health effects in children. The present study was carried out from December 2021 to November 2022 to examine variation in metals concentration with season and associated health risk from school dust of Agra, India. Dust samples collected from schools representing varied microenvironment were analysed for metals concentration by ICP-AES. Pollution indexes viz. Geo-accumulation (Igeo), pollution (PI), integrated pollution (IPI) and pollution load (PLI) were employed to determine metals contamination while multivariate static were employed for source apportionment. Further, USEPA health risk assessment models were utilized to assess the health risks in children. The results concluded that in all seasons roadside schools settled dust had higher accumulation of metals as compared to residential schools except semi urban schools in post monsoon season. The PLI values

of settled dust of all schools were ranged from <1 to >1 indicates pollution levels by metals in all four seasons. Meanwhile, from the Igeo values revealed that school dusts were moderately and heavily contaminated by Cd in all seasons. The assessment of health risk specifies ingestion as the main exposure route while Hazard Index (HI) value for all examined metals was lower than safer limit of one. The findings suggest that more investigations are required on Pb, Cd and Cr in schools of Agra.

AEO-CYSA-10 : Dual Application of High-Performance Flexible (Cu@RGO/CF) Textile Fabric in Supercapacitors and Antimicrobial Applications

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High-performance textile electrodes are multifunctional (wearable, stretchable, washable, hydrophobic, antifungal and antibacterial) materials with sensing, heating, and supercapacitive properties. All these functionalities are integrated into a one-layered fabric that can be used as a portable intelligent electronic textile for potential application in healthcare monitoring, smart sportswear, and energy storage devices. Herein, dual- functional novel fabric electrode consisting of copper nanoparticles (Cu) decorated on reduced graphene oxide (RGO) based cotton fabric (Cu@RGO/CF) was fabricated by a simple, efficient, environment friendly, and low-cost chemical reduction method along with a screen-printing technique. The resulting superior (Cu@RGO/CF) textile material was confirmed by various characterization techniques including X-ray diffraction (XRD), Fourier transform infrared (FTIR), UV-visible spectroscopy and Photoluminescence (PL). Utilizing cotton fabric as its textile foundation, RGO offers double electric layer capacitors, which aid in establishing a high-speed conductive pathway by connecting cotton fibers in a series. Moreover, the inclusion of Cu nanoparticles amplifies the catalytic effectiveness of RGO/CF. This (Cu@RGO/CF) is employed as an electrode in supercapacitor application, resulting in a specific capacity of 217.5 F/g with a notable 93.6 % retention capacity after 1000th cycles. It also shows effective antibacterial and antifungal properties that play an important role in healthcare sector. These promising outcomes from electrochemical and biological properties indicate that the (Cu@RGO/CF) textile fabric developed holds significant potential for a wide range of applications in wearable textiles.

AEO-CYSA-11 : Electrochemical Synthesis of ZnO Decorated with Carbon Dots for Efficient Photoelectrochemical Water-Splitting under Visible-Light Irradiation

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Photoelectrochemical (PEC) water splitting is considered as one of the most cost-effective and desirable methods for meeting ever-growing energy demands. However, the low photoconversion efficiency limits the practical applicability of PEC water splitting. ZnO is synthesized vertically on fluorine-doped tin oxide (FTO) through a simple electrochemical deposition technique to develop an efficient photoelectrode. For then the ZnO nanosheets was sensitised by carbon dots through the dip-coating method. As synthesized ZnO/Carbon Dots photoanode is characterized by field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray (EDX), diffuse reflectance spectroscopy (UV-DRS), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR) and photoluminescence (PL) techniques. Photoelectrochemical (PEC) performance was investigated using linear sweep voltammetry (LSV), chronoamperometry (CA), and electrochemical impedance spectroscopy (EIS). The ZnO nanosheet-based photoanode exhibits superior photoresponse and PEC capability. Furthermore, the ZnO photoanode sensitized by carbon dots (CDs) can further enhance PEC performance due to the narrower bandgap of CDs and the improved efficiency of photogenerated electrons transfer from CDs to ZnO nanostructures.

AEO-CYSA-12 : Estimation of Human Airway Deposition of Size-Segregated Particulate in the Semi-Urban Region of Northern India : Age-Specific Variations

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Real-time monitoring of size-segregated Particulate Matter by means of 32 bins aerosol spectrometer (Grimm model 1.109) was done at a traffic-prone residential site near a national highway in the semi-urban location of Tundla city during the monsoon period in 2023. From the outcome, it was concluded that the mass concentrations of, PM_{10}, $PM_{2.5}$ and PM_1 were 113.70 ±64.81μgm^{-3}, 64.44 ±37.46

μgm^{-3} and 44.69±27.96 μgm^{-3} respectively, which exceeded the WHO, and NAAQS, prescribed limits. A computational model Multiple-Path Particle Dosimetry Model (MPPD) was used to evaluate the deposition of $PM_{2.5}$ in the airways of infants, children, and adults. From the deposition model, it was concluded that the total deposition of $PM_{2.5}$ fraction in the entire human airways was highest for adults (63%) followed by children (61%), and infants (59%) while it was predominantly deposited in the head followed by tracheal bronchial and pulmonary region for infants, child, and adults. The highest deposition was in the head (58.8%) in adults whereas the lowest was in Pulmonary (31%) for infants. Mass Visualization by the Age-Specific 5 Lobe model also revealed that the maximum deposition of $PM_{2.5}$ mass concentration was in adults (0.26140mg) followed by children(0.2065mg) and then infants(0.0143mg).

AEO-CYSA-13 : Atmospheric Aerosol Chemistry: Microscopic Advances and Open Question on the Physiochemical Properties of Aerosols

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In the realm of atmospheric science, this study delves into the intricate dynamics of aerosol chemistry over the Indo-Gangetic Plain. Employing cutting-edge spectroscopic and microscopic advancements, the research illuminates the physiochemical intricacies of aerosols, unraveling a profound understanding of their composition and behavior. Aerosol size distribution, composition, and elemental content were investigated using extensive air quality monitoring and modern analytical techniques like FESEM-EDX.The study explores the elemental and morphological dimensions of aerosol particles. These findings contribute to an enhanced comprehension of the sources, transformations, and fate of aerosols in this vital geographical region. As the Indo-Gangetic Plain stands as a crucible of complex atmospheric interactions, the study ventures into open questions surrounding the physiochemical properties of aerosols. It addresses the multifaceted influences of natural and anthropogenic factors on aerosol composition, examining their role in radiative forcing, air quality, and climate implications. The integration of advanced analytical tools with field measurements facilitates a comprehensive exploration of aerosol characteristics, paving the way for informed strategies in air quality management and climate mitigation.

AEO-01 : Synthesis and Photocatalytic Activity of $ZnFe_2O_3$/$BiVO_4$/ g-C_3N_4 in Real Wastewater

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The current study based on the synthesis and characterization of Z-scheme $ZnFe_2O_3$ /$BiVO_4$/ g-C_3N_4 ternary heterojunction photocatalyst. To prepare g-C_3N_4 nanosheets, a chemical method is followed. The chemical co-precipitation method is used to synthesize Zinc spinel Nano ferrites and $BiVO_4$ yellow plate like crystals are prepared by a hydrothermal process. These materials are structurally characterized by powder PXRD, FTIR, SEM-EDAX, UV-Visible, DRS. The result of X-ray diffraction show the successful establishment of heterojunction between g-C_3N_4, $ZnFe_2O_3$ and $BiVO_4$ and their energy band structure are also analyzed. Other characterizations reveal particle size range, optical absorption property, crystallinity and electronic structural features confirmed from UV-Visible DRS, PXRD and FTIR. The application of the ternary composite ($ZnFe_2O_3$ /$BiVO_4$/ g-C_3N_4) is photocatalytic degradation of organic pollutants from waste water and industrial effluent. This sample performed better activity as compare to its counter parts. Recyclability and reusability of catalyst is analyzed. The probable mechanism of degradation pathway is measured.

AEO-02 : Physico-Chemical Cheristrestics of Soil and Ground Water in Rewa District of Madhya Pradesh, India

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Rewa also Spelled Rewah or Rewa City north eastern Madhya Pradesh State, Central India. Rewa lays between 24'18 and 25'12 north latitudes and 81' and 82'18 east longitudes in the north-eastof the Rewa division. The District is bounded on the north and east by the state of Utter Pradesh in the west with Amarpatan and Raghurajnagar Tahsils of Satna district.The Study Was carried out by Collecting ground water & Soil Samples from different sampling station in Rewa District. The water Samples were analyzed for different physico-chemical parameter like temperature, PH, Turbidity DO, BOD, COD, nitrate, nitrite, Chloride and Sulphate concentration were observed below the recommended prescribed limit of WHO standard (1984). Soil quality Parameters, (i.e. temperature, PH, EC, Organic Carbon) and heavy Metal (i.e. Manganese, Iron, Zinc Cobalt Copper) has been examinedin thesoil samples of Rewa District. Zn and Mn content were found in all the samples are below then the (SQGL) recommended values.

AEO-03 : Impact of Particulate Matter Sources at Highways Toll Plazas in India

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Air pollution: one of the greatest "Environment evil" One of our era's greatest scourges is air pollution, on account not only of its impact on climate change but also its impact on public and individual health due to increasing morbidity and mortality. There are many pollutants that are major factors in disease in humans. Among them, Particulate Matter (PM), particles of variable but very small diameter, penetrate the respiratory system via inhalation, causing respiratory and cardiovascular diseases. Impact of air pollution is that, it is polluting the environment and people are breathing in polluted air. Approach to the problem is without any doubt, the global environmental pollution is considered an international public health issue with multiple facets. Social, economic, and legislative concerns and lifestyle habits are related to this major problem. Highways and roads carry a lot of traffic since they are used for local and long-distance passenger and freight transportation. In India, there hasn't been much research done on particle monitoring and its related toxicity at toll booths and plazas. To limit exposure to this pollutant, study, and investigation must be done at toll plazas. Highway toll station workers exposed to vehicle emissions during their working time could induce excessive polluting species generation and lead to significant health effects. The vehicular traffic is one of the major sources of air pollution affecting the urban population in northern India. Almost all air pollutants have some physiological impacts on human beings, mostly, but not limited, to the cardiovascular and respiratory systems. Pollution is an example of a negative externality Short-term exposure to air pollution can also cause headaches, nausea, and dizziness. Environment impact of air pollution is harming not only human health but also the environment Thus a global prevention policy should be designed in order to combat anthropogenic air pollution as a complement to the correct handling of the adverse health effects associated with air pollution. Sustainable development practices should be applied, together with information coming from research in order to handle the problem effectively.

AEO-04 : Conventional Wastewater Treatment Technology

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Water demand technology gradually increasing with rapid development of social economy, due to this water pollution problem also increasing and it became more severe, to overcome this, technology of sewage treatment is developing rapidly, but it is with various problems .For advanced technology, energy consumption is more, carbon neutrality cost is very high so it is again dangerous, so it is todays need to develop low carbon sewage treatment technology which may consume less energy and less pollution release in environment. Hence it is todays need to focus on conventional sewage treatment technology and low carbon sewage treatment. It is expected to give theoretical basis for practical engineering application LCST (low carbon sewage treatment) which may reach the carbon neutrality goal by comparison and analysis of LCST. The human population explosion has also put a stress for the need of food, clothing and shelter. Shelter requires more land which is the biggest problem in the cities.

AEO-05 : β-Cyclodextrin based Magnetic Ternary Nanocomposite for Wastewater Treatment

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In this work, ternary metal oxide composite $CuO/Fe_2O_3/ZnO$ is synthesized through sol-gel method and further modified with β-cyclodextrin (β-CD) to form a novel and effective β-CD-$CuO/Fe_2O_3/ZnO$ catalyst for organic pollutants adsorption and degradation. Both catalysts are characterized by P-XRD, SEM, EDX, DRS, PL, DTA/TGA and FT-IR. The adsorption and photocatalytic activity of the above synthesized catalyst are carried out at neutral pH and 1g/L catalysts dosage for the degradation of different types of water pollutants and for. β-CD-$CuO/Fe_2O_3/ZnO$ achieved degradation efficiency is 89.3% in 160min (RhB), 93.2% in 160min (Gunner 500), 84.1% in 200min (Cefixime), and 81.5% in 180min (p-NP). It is also observed that presence of β-CD enhanced the degradation efficiency. Kinetics results followed to the pseudo first order (PSO) with the k_1 values as $10.40\times10^{-3}min^{-1}$, $0.17\times10^{-3}min^{-1}$, $4.94\times10^{-3}min^{-1}$ and $1.83\times10^{-3}min^{-1}$ for RhB, Gunner 500, Cefixime and p-NP respectively. These photocatalysts exhibit high efficiency in a short reaction time, and good reusability.

AEO-06 : Correlation of Mechanical Properties and IR Frequency of Carbamate Links in Surface Functionalized Fly Ash Reinforced Polyurethane Composites : A Study

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The interaction of fly ash filler with polyether polyol, cross-linking agent, and curing agent in a particular ratio led to the synthesis of polyurethane composite. The results of the research article reveals that the hydroxyl moieties of surface functionalized fly ash adhered physically or chemically bonded decrease the mechanical properties of polyurethane composite. The research article also correlates the mechanical properties of polyurethane composites with the carbonyl stretching frequency of carbamate link in surface functionalized fly ash reinforced polyurethane composites . The insight at microphasic level pertaining to the proximity and segregation of hard and soft segment in composite which determine their mechanical properties can be analyzed in depth by the trends of carbonyl stretching frequencies of carbamate links , an inverse correlation was noticed for the carbonyl stretching frequencies of carbamate links and the mechanical properties of the composites. Thermally activated fly ash reinforced polyurethane composite with minimum carbonyl stretching frequency (1734cm^{-1}) exhibits high mechanical properties while lesser mechanical properties were shown by uncalcined fly ash reinforced polyurethane composites with maximum carbonyl stretching frequency (1798cm^{-1}) .the experiments were performed at higher index ratio (IR; 1.64) to compensate the excess of hydroxyl group contribution attributed by OH loaded fly ash which too was revealed by NCO peak (2240 -2280 cm^{-1}) intensity in IR spectra of composite

AEO-07 : Analysis of Groundwater Quality of Agra District with Special Reference to Fluoride Concentration

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Water is a vital resource for human survival. Safe drinking water is a basic need for good health, and it is also a basic right of humans. Analysis of groundwater samples for fluoride from twelve sampling

stations of Agra district for a period of one year during different seasons has been carried out. The analysis of different parameters namely- temperature, pH, total alkalinity, electrical conductivity, total hardness, chloride and fluoride were carried out as per standard methods. The results were compared with the values stipulated by Indian standards for drinking water. It was found that the fluoride content of all the water samples obtained were well above the permissible limits set by WHO (2004) and BIS (10500: 1991). The results reveals that the water quality of most of the sites of Agra district is not suitable for drinking purpose which recommends the use of indigenous technologies, to make water fit for drinking purpose.

AEO-08 : An Application on Tb^{3+} Rare Metal Complex with Benzoxazole Derivative

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The combination of some rare metal ions with an important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide (BSPA) ligand to form coordination compounds is an important area of current research. Less explored biologically important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide ligand is allowed to react with solution of some rare metal perchlorates and attempt has been made to synthesize solid 2-(1,3-benzoxazole -2-yl- sulfanyl)-N-phenyl acetamide complexes. These 2-(1,3-benzoxazole-2-yl-sulfanyl)-N-phenyl acetamide complexes are subjected to antimicrobial activity of these complexes has been evaluated by standard methods and attempts have been made to correlate structural characteristics with properties of these 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide complexes.

AEO-09 : Adsorption Kinetics of Disperse Orange 37 onto Activated Carbon Prepared from Jackfruit-PPI-1 Waste

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In the present study, the rind and pulp of Jackfruit-PPI-1 waste was impregnated in K_2CO_3 then carbonized at 600^0C and named as JC_{600}. Characterization of the prepared activated carbon was done by SEM, BET, TGA, and TPD analyses. Batch mode adsorption studies were conducted to know the adsorption capacity of the prepared

activated carbon for the removal of Disperse Orange 37 (DO37). Freundlich, Langmuir, Temkin, and Dubinin Radushkevich equilibrium isotherm equations were used to describe experimental adsorption. In the adsorption process of selected dye, fitting of the kinetic data demonstrates that the dynamics of sorption could be better described by pseudo-second-order model indicating a chemisorptive rate-limiting.

AEO-10 : Evaluating the Mutagenic Potential of Airborne Particles, Identifying PM_1-Associated Polycyclic Aromatic Hydrocarbons (PAHs) in Urban Air, and Considering their Health Implications.

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The health of the human population faces significant risks from atmospheric particulate matter (PM), which exacerbates air quality issues and has adverse effects on respiratory and cardiovascular health. In this research, we assessed the mass concentrations, chemical compositions, and seasonal variations of PM_1 in an urban area within the city of Taj, Agra, India. Our sampling method involved the use of an APM 577 high-volume sampler and sampling was done from December 2021 to November 2022. To analyse the contents of PM_1, for polycyclic aromatic hydrocarbons (PAHs) Gas Chromatograph Mass Spectrometry (GC-MS) was used. The annual mean PM_1 concentration was found to be 109.4±75.4 ìg/m3, which is roughly twenty-two times higher than the recommended safe limit set by the WHO (5 ìg/m3). The annual average concentration of 16 USEPA PAHs was measured at 373.94±17.21 ng/m^3.Also calculated the excess life time cancer risk linked to PAHs. An Ames test was conducted using TA98 and TA100 strains of Salmonella typhimurium, both with and without metabolic fraction S9. This test revealed instances of frameshift mutations and base pair substitutions during the winter and post-monsoon seasons. This comprehensive characterization provides readers with a clear and in-depth understanding of PM_1. Consequently, it underscores the importance of considering chemically characterized properties when assessing carcinogenic risk. The study lays the groundwork for essential measures to address local emission sources and draws the attention of local authorities to enhance air quality in rapidly developing urban areas.

AEO-11 : Efficient Microwave Synthesis of Imidazolium-Based Ionic Liquids for Unprecedented Mild Steel Corrosion Inhibition in 0.5 M H_2SO_4 Solution : An Electrochemical and Theoretical Analysis

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The inhibition potential of newly synthesized imidazolium-based ionic liquids on mild steel corrosion in a 0.5 M H_2SO_4 solution was investigated using gravimetric analysis, potentiodynamic polarization, and electrochemical impedance spectroscopy at various temperatures. This study focuses on the microwave-assisted synthesis and characterization of imidazolium cation-based ionic liquids. The Density Functional Theory using the B3LYP method revealed that the alkyl chain length at the N-3 position in imidazolium cation-based ionic liquids significantly influences their inhibition potential. Notably, IL-2, with a longer alkyl chain, exhibited higher inhibition efficiency (92.51% at 303 K) compared to IL-1 (88.71% at 303 K). Additionally, Gravimetric analysis indicated that the adsorption of imidazolium-based ionic liquid inhibitors followed the Langmuir adsorption isotherm. Potentiodynamic polarization results suggested a mixed-type behavior of the inhibitors, impacting both anodic and cathodic slopes. Surface morphological analyses revealed the corrosion inhibition potential of the IL-1 and IL-2, confirming the formation of a protective film on the mild steel surfaces. The mechanism suggests that these ionic liquids obstruct both anodic and cathodic sites, thereby effectively inhibiting the corrosion process in a 0.5 M H_2SO_4 solution.

AEO-12 : Method Development and Validation for Residue Analysis of 76 Multiclass Pesticides in Water Employing Tandem Gas Chromatography Mass Spectroscopy

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A miniaturized, QuEChERS based, liquid–liquid extraction method followed by tandem gas chromatography–mass spectrometry determination was developed and validated for 76 pesticide residues

determination in water using SANTE/11312/2021 guideline. The accuracy, precision, specificity, linearity, recovery, repeatability, reproducibility, robustness, LOD and LOQ of the method were evaluated. Each Pesticide was optimized in terms of different MS parameters and chromatographic conditions by GC-MS/MS using MRM mode. Samples were quantified by matrix-matched calibration with internal standards. All pesticides showed good linearity in the respective range, both with values of $R^2>0.99$. The average recoveries of the pesticides spiked samples ranged from 70.0% to 120.0%. The method performance complied with the regulatory requirements, and thus, can be implemented. LOD and LOQ of the pesticides were found at 10µg/kg and 30µg/kg respectively and recovery studies were carried out by spiking mixture in water at 1LOQ, 5LOQ, 10LOQ levels. The method provided a high throughput analysis of multi-class pesticides with satisfactory selectivity, sensitivity, accuracy, and precision.

AEO-13 : 4-Acyl Pyrazolone Modified Silica as a New Sorbent for Selective Solid-Liquid Extraction of Pb (II)

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A Schiff base reaction was used to create a newly constructed silica hybrid material (SiNP-L_3) by functionalizing (4-chlorophenyl) [5-hydroxy-3-methyl-1-(4-methylphenyl)-1H-pyrazol-4-yl] methanone over modified silica. To show the successful addition of Schiff base groups, scanning electron microscopy, the Fourier transformation of infrared spectroscopy, elemental examination, BET surface measurement, Barrett-Joyner-Halenda pore dimension, solid-state ^{13}C-NMR, powder XRD, and thermogravimetry measurements were done on the prepared sorbent, which was used to remove lead in the aqueous media selectively. Batch studies were used to examine the effects of interaction duration, starting concentration, pH levels, and sorbent dosage on the degree of sorption of lead (mg/g). Langmuir adsorption isotherm and Pseudo second order (PSO) kinetic model fit best to the obtained data with R^2 values of 0.98 for both which shows the major possibility of chemisorption. The positive values of $\Delta S°$ and $\Delta H°$ reflect the endothermic behavior of the adsorption technique. In contrast, a downward trend in Gibbs free energy ($\Delta G°$) with rising temperature demonstrates the spontaneous character of the adsorption process. Additionally, the newly created material stimulates easy recycling up to five times in sequence without compromising the extraction

percentage and shows high selectivity for Pb (II) having an adsorption capacity of 16.8 mg g^{-1}.

AEO-14 : Fabrication of Nanocomposite Membrane Composed of Sulfonated PVDF and Thermo-mechanically Modified Fly Ash for Application in Direct Methanol Fuel Cells

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The present work deals with the fabrication of cost-efficient nanocomposite proton exchange membrane (PEM), prepared by incorporation of nanoparticles of Fly Ash (FA) collected from M/s Bina thermal power plant Madhya Pradesh India; within the host PVDF [poly(vinylidene fluoride)] polymer matrix. Subsequently, the nanocomposite membranes are treated with the well-known sulfonating agent chlorosulfonic acid at 60ºC for 1.5 hours. The successful incorporation of FA nanoparticles within the host polymer structure along with the sulfonation of the nanocomposite membranes was confirmed by using FTIR, XRD, FESEM-EDX, and AFM studies. The ion exchange capacity (IEC) and proton conductivity (PC) of nanocomposite membranes are observed to be 0.58 meq g^{-1} and 3.30×10^{-2} S cm^{-1} respectively. Further, it was interesting to note that the fabricated membranes exhibited enhanced water uptake capacity up to 19.6% with supressed methanol crossover ($1.7 \times 10^{-7} cm^2/s$). Among all the fabricated membranes, the membrane SPF-5 (containing 5% w/w FA), exhibited significantly high membrane selectivity 1.94×10^5 $Scm^{-3}s$ over corresponding Nafion-117 (2.47×10^4 $Scm^{-3}s$), which clearly indicates its potency towards an alternative to costly Nafion-117 for DMFCs application.

AEO-15 : A Greener Approach for the One Pot Synthesis of Substituted Thiazolidinones using Ionic Liquid

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Environmental pollution caused by chemical and pharmaceutical industries has been regularly increasing for last several decades. Hence, there is a social expectation that scientists and chemists should try to design sustainable chemical processes, which generate less hazardous materials and more environmentally friendly sources of energy production. The roles of ionic liquid based solvent systems have been proposed as an alternative for conventional organic solvents. A conventional protocol for the synthesis of 2,3-diarythiazolidin-4-one has been synthesized by one pot condensation of aryl or heteroaryl amine, aryl aldehyde and 2-mercaptopropionic acid in 3-butyl-1-methyl-1H-imidazol-3-iumtrifloroacetate as ionic liquid [BMIM][TFA]. This green solvent can be easily synthesized, recycled and reused three times. The structures of all synthesized compounds were elucidated by their spectral studies.

AEO-16 : Levels, Sources, and Health Risks Associated with Particle-bound PAHs at an Urban Site in Historic City of Taj

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Air pollution in densely populated areas has escalated globally in recent decades, primarily due to industrialization and inadequate urban planning. In India, numerous studies have investigated Polycyclic Aromatic Hydrocarbon (PAH) levels within various sizes of particulate matter (PM). Among the diverse constituents of organic particles, the presence of trace PAH compounds in the ambient environment raises concerns about their persistence and detrimental health effects. This study focused on assessing the concentration and associated health risks of PAHs adhering to PM in two distinct fractions: Total Suspended Particulate (TSP) and PM_1 at an urban site in Agra. Measurements conducted showed seasonal variation in PAH concentrations. Notably, PAH levels were higher during winter (683.2±256.4 ng m^{-3}) than in summer (91.8±49.6 ng m^{-3}) for TSP and also higher in winter (203.1±20.1 ng m^{-3}) compared to summer (78.1±20.1 ng m^{-3}) for PM_1. The diagnostic ratio pointed to pyrogenic sources, such as coal, wood, biomass burning, and traffic emissions, as the primary contributors to PAHs in TSP and PM_1, especially during winter. Conversely, petrogenic sources played a more significant role during summer. Cancer risk, assessed using Total Carcinogenic Potency (TCP), revealed an average TCP of 4.4 ng m^{-3} in the summer and 14.4 ng m^{-3} in the winter for PM_1. For TSP, the TCP values were 5.9 ng m^{-3} in the summer and 21.0 ng m^{-3} in the winter. The Incremental Lifetime Cancer Risk (ILCR) was evaluated for two age groups: children (5–19 years) and adults (20–70 years). Both summer and winter posed a moderate cancer risk (between 10^{-6} to 10^{-4}) for adults and children primarily through dermal exposure followed by ingestion. However, the ILCR value for adults and children via inhalation remained below the

permissible maximum limit for cancer risk (1×10^{-6}). These findings offer valuable insights for future strategies aimed at mitigating PAH sources and improving the urban population's quality of life.

AEO-17 : Study on Combustion Kinetics of Hydrogen Gas over Freshly Prepared Supported Platinum Catalyst

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Combustion of hydrogen releases energy but in many applications catalytic combustion of hydrogen may prove advantageous over direct combustion. The main advantage of catalytic combustion of hydrogen is that heat can be obtained at lower temperatures as well. We prepared nano-structured alumina supported platinum catalyst using wet impregnation technique. This catalyst has active metal component on the surface of a nano-structured support, a highly porous, thermo stable material and hence the catalyst life. The activity of our prepared catalyst for combustion of lean mixtures (< 2%) of hydrogen was studied in the present work and the kinetics of catalytic combustion of hydrogen has been established. The combustion of hydrogen on alumina supported platinum catalyst starts at 323K and it is observed that conversion becomes almost constant after 400 K. It is likely that reaction have become external film mass transfer controlled above 400 K. Two reaction models have been investigated for possible mechanism of the reaction. The kinetics follows Hougan-Watson model where both hydrogen and oxygen adsorb on same site; hydrogen undergoes dissociative chemisorption and surface reaction being the slowest step. However, a simplified power law type rate equation was also established which adequately fits the experimental data for temperature between 373 & 673 K.

AEO-18 : Preparation and Characterization of Polyamide Metal Oxide Nanocomposites

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Bio-based polyamides (PAs) can be synthesized by using castor oil and vegetable oil. This polymer possesses significance importance on the basis of ecological and economic point of view and these are used in macromolecular chemistry and modern industry. We have discussed various synthesis and properties of PAs, the properties of PAs can be enhanced by using metal oxide nanocomposites and these properties includes magnetic, mechanical, interfacial, glass transition temperature electrical and thermal properties. Nanocomposites are suitable for applications as high-performance composites, where good dispersion of the filler can be attained and the properties of the nanofiller are substantially different or better than those of the matrix. At the end we have discussed applications of the polymer nanocomposite in the areas of flame retardant, packaging, textile, biomedical and automotive parts and focus on ecofriendly sustainability of polyamides nanocomposites.

AEO-19 : Human Health Risk Assessment of Heavy Metals Present in Groundwater of Agra and Firozabad Districts (UP) India

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Heavy metals (HMs) in groundwater are an environmental problem that has been increasing in the past few years. The purpose of this study was to investigate the current status of HMs concentration in groundwater of 18 different block areas of Agra and Firozabad districts. Groundwater plays an important role in this region, and thus, it is imperative for us to improve our understanding of the heavy metals present in the groundwater of these areas. Sample were collected over two consecutive seasons pre-monsoon and post-monsoon of year 2021. Each groundwater sample was analysed for 10 heavy metals Pb, As, Cd, Cr, Cu, Fe, Mn, Ni, Zn and Hg. Human health risk assessment was conducted where carcinogenic risks and hazard quotients (HQs) were evaluated separately. The concentration of the studied HMs in most samples was higher than the permissible limit for drinking water. The heavy metal evaluation index (HEI) and heavy metal pollution index (HPI) values of samples were higher than the permissible limit of drinking water.

AEO-20 : Synthesis of 2 and 3D Inorganic Semiconductors use for Photocatalytic Application

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The inorganic (ZnO) semiconductor were synthesized using a

hydrothermal technique. The prepared ZnO nanostructures were characterized with different spectroscopic and microscopic techniques. The XRD indicates the formation of the hexagonal phase of ZnO in all the prepared samples. The UV-visible absorbance spectrum depicts the absorption peak at 380 nm corresponding to the band gap of 3.27 eV. The photoluminescence spectra show band edge emission at 390 nm and a small hump at 470 nm. The FESEM confirms the formation of hexagonal shaped plate like ZnO nanostructures having size in the range of 50 to 100 nm with the thickness of 10-15 nm, at 2 h reaction time. Further increase in the reaction time leads to increase in thickness of hexagonal ZnO plates resulting in formation of three dimensional (3D) distorted spherical structures with facets. The TEM validates the formation of highly crystalline hexagonal shaped ZnO plates having size in the range of 0 to 150 nm.

The organic semiconductor 6, 13 - Pentacenequinone (PQ) was synthesis with previous reported method. PQ/ZnO nanocomposite prepared with different weight ratio. The photocatalytic activities of prepared ZnO composite were investigated by following degradation of 100 mL, 10 ppm methylene blue (MB) dye.

AEO-21 : Green Synthesis and Characterization of Imidazolium-based Ionic Liquids and their Application as Corrosion Inhibitor for Mild Steel in Acidic Medium

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Synthesis and characterization of two imidazolium-based ionic liquids namely 1-Heptyl-3-methyl imidazolium bromide [HMImBr] and 1-Benzyl-3-methyl imidazolium bromide [BzMImBr] was performed using microwave irradiation and spectroscopic techniques respectively. Their corrosion inhibition performance towards mild steel in 0.5 M sulphuric acid at different temperature was investigated using gravimetric method, Potentiodynamic polarization, electrochemical impedance spectroscopy, Scanning electron microscopy and Atomic force microscopy AFM. As per the outcomes, [BzMImBr] is a potent inhibitor with an inhibitory efficacy of 95.49 percent at 1000 ppm for a 36-hour immersion period. The results obtained from the PDP studies revealed that both the anodic and cathodic slopes were affected in the presence of both ionic liquids which marks them as mixed type inhibitors. The adsorption of these ionic liquids on the mild steel surface obeys Langmuir adsorption isotherm. The kinetic and thermodynamic parameters at different temperature for MS corrosion and inhibitor adsorption were determined and discussed. The value of ÄG$_{ads}$ is suggestive of physical and chemical adsorption of ImILs on the surface of mild steel. Surface roughness in presence of inhibitor was investigated and measured through EDS, AFM and SEM techniques.

AEO-22 : Airborne Microbial Endotoxin Enumeration and Characterization of Particulate Matter in Agra, A Semi-Arid Region of India

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LPS components (lipopolysaccharide) also called endotoxins, cause dangerous contamination, and can cause inflammations or septicemia in animals and tissue cultures. Endotoxin can combine with dust particles, resulting in symptoms such as fever, shivering, arthralgia, influenza-like symptoms (malaise), blood leukocytosis, neutrophilic airway inflammation, asthma symptoms such as dry cough, dyspnea, and chest tightness, bronchial obstruction, dose-dependent lung function impairment, and decreased lung diffusion capacity. The present study highlights the concentration of PM$_{10}$, PM$_1$, endotoxin concentration, and bacterial and fungi in Agra, a semiarid region in India from July 2022 to November 2022.

The mean concentration of PM$_{10}$ is 372 ìg m^{-3} and ranges from 158.3 ìg m^{-3} to 691. 5 ìg m^{-3} and the mean concentration of PM$_1$ is 74.126 ìg m^{-3} and ranges from 20.83 ìg m^{-3} to 138 ìg m^{-3}. The average endotoxin concentration was found to be 18.8 EU m^{-3}. The growth of bacteria increases with the concentration of deposition in samples; the mean value of bacterial growth in Petri dishes is 480 CFU/milliliter, and characterization between gram-positive and gram-negative bacteria is done by using gram staining. The growth of bacteria increases with the concentration of deposition in samples; the mean value of bacterial growth in Petri dishes is 480 CFU/milliliter, and characterization between gram-positive and gram-negative bacteria is done by using gram staining. In all samples, the mean concentration of endotoxin was 2–20 EUm^{-3}. This indicates a lower concentration of endotoxin in the samples, which is not toxic to human health.

AEO-23 : Study of Bioavailability of Major Elemental Content using In Vitro Method and Protein concentration in Fish Samples from Polluted Water

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In the present study % bioavailability of major elements in fish sample were estimated using In-Vitro method in which sample was subjected gastric and gastrointestinal digestion. The processed fish sample was treated with digestive enzymes (pancreatin, pepsin, a-amylase) and bile salts. It is observed that the total elemental concentrations of Ca, K, Na and Mg were 128.99, 331.1, 101.35 and 21.75 ppm in the sample respectively. Fairly good amount of Ca, K, Na and Mg was found in the fish sample. During gastric digestion, the % bioavailability of Na is found to be higher than K, Na and Mg and is in the order Na > K > Ca > Mg. The percent bioavailability of Ca, K, Na and Mg during gastro – intestinal digestion was found to be higher than gastric digestion. The concentration of protein in fish sample determined from calibration curve was found to be 0.51 ppm.

AEO-24 : Health impacts of Size Segregated Particulate Matter and Black Carbon in Industrial Area of Firozabad (UP) India

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Particulates are ubiquitous in the air environment and cause serious threats to human beings such as lung cancer, COPD, and Asthma. Particulates mainly arise from industrial effluent, vehicular emission, and other anthropogenic activities. In the glass industrial city Firozabad, real-time monitoring (mass as well as number) of size segregated Particulate Matter (PM) and black carbon was done by Aerosol Black Carbon Detector (ABCD) and GRIMM portable aerosol Spectrometer at two different sites in which one site is urban and another is a rural. The average mass concentration of size segregated PM during the study period (March & April, 2022) was recorded as PM_{10} (223.73 mg/m^{-3}), $PM_{5.0}$ (44.955 mg/m^{-3}), $PM_{2.5}$ (59.275 mg/m^{-3}),

$PM_{1.0}$ (33.02 mg/m^{-3}), $PM_{0.5}$ (2.05 mg/m^{-3}), and $PM_{0.25}$ (2.99 mg/m^{-3}). In number mode, PM concentration was found as PM_{10} (27.46mg/m^{-3}), $PM_{5.0}$(233.48mg/m^{-3}), $PM_{2.5}$ (646.61mg/m^{-3}), $PM_{1.0}$ (1134.94 mg/m^{-3}), $PM_{0.5}$ (14056.04g/m^{-3}), and $PM_{0.25}$ (182906.4 mg/m^{-3}). The highest concentration of BC was found in Urban due to the emissions from diesel engines, and wood burningwhile NO_2 was highest at the rural sites. The concentrations of PM_{10}, $PM_{2.5}$ exceeded the NAAQS and WHO guidelines. The sensitive exposed population may be at risk of developing health-related problems from exposure to size-segregated PM and BC. They will be discussed during presentation.

AEO-25 : Wetland Studies of District Mainpuri (U.P.)

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Wetlands are among the most threatened habitats globally, and it is estimated that since 1900 more than half of the world's wetlands have been destroyed and lost to other land uses. Wetlands are among the most threatened habitats globally, and it is estimated that since 1900 more than half of the world's wetlands have been destroyed and lost to other land uses.

In district Mainpuri wetlands and agricultered fields contributes to the healthy population of Sarus and other wetland birds. A large number of wetlands are situated in Mainpuri and many others emerges during Mansoon season.The present study was carried out to estimate the Physiochemical parameters of five wetlands study sites viz- Site-I(Markandeshwar), Site-II (Bhamwat Canal), Site-III (Saman), Site IV(Sauj) and Site-V(Kirithua). Physiochemical studies of wetlands of Mainpuri was conducted six times in an year, to evaluate the pollution level of water of wetlands at Mainpuri.In this paper we discuss Colour, Cadmium, Carbon-di-oxide, Chloride, Fluoride Phosphate, Turbidity and Mercury contents in water. The conservation of wetlands will help in conservation of the State bird of U.P. (Sarus Crane) and other local and migratory birds inhabiting the wetlands and maintaining the ecological balance. The future of Indian Sarus crane. Grus antigone antigone and other migratory and resident water birds is closely tied to the quality of these wetlands in Mainpuri which serves of their habitat. It is suggested that Site I, II and V should also be given important status like IBAs.

AEP-CYSA-01 : Photocatalytic Degradation of Methylene Blue Dye under Natural Sunlight By Bi_2O_3/ G-C_3N_4 Nanocomposite

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This study investigates the photocatalytic degradation of Methylene Blue (MB) dye using a Bi_2O_3/g-C_3N_4 nanocomposite under natural sunlight irradiation. The nanocomposite is synthesized through a facile and cost-effective method, combining bismuth oxide (Bi_2O_3) and graphitic carbon nitride (g-C_3N_4) to harness the synergistic effects of these materials in enhancing photocatalytic performance. These all fabricated materials were precisely characterized by characterization techniques such as SEM, EDAX and XRD techniques. The bare g-C_3N_4 and Bi_2O_3 along with modified Bi_2O_3/ g-C_3N_4 catalyst were employed for photocatalytic degradation of cationic dye MB dye. The modified Bi_2O_3/ g-C_3N_4 found to be excellent over degradation efficiency of MB with almost 98% of dye degradation.

AEP-CYSA-02 : Evaluation of Drinking Water Quality of Vidisha District Madhya Pradesh, India

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Water is one of the five elements described in "SHASTRA" to form life. Groundwater quality is one of the most important aspects in water resource studies. Vidisha district is located in the middle of the state of Madhya Pradesh, India. The area is lies on the Plateau off the main Vindhyachal Range. There present highly mineral-rich, hard rocks like basalt, sandstone, and shale. The main occupation of the district is agriculture. Due to the high dependency of residents of Vidisha on groundwater, monitoring water quality is essential. We collected around 180 water samples and analyzed 20 different physicochemical parameters. The in-situ parameters were analyzed on the sample spot. TDS, EC, salinity, ORP, and DO of the samples were determined by using portable multi-parameter. Statistical tools were applied like the WQI, PCA, and CA. Maximum samples have been found to be suitable for drinking purposes, though some were found unsuitable due to the dissolution of high mineral amounts. The major issue was observed with nitrate ion concentration and with total hardness. 25-29% of samples were found to have nitrate ion

concentration above the specified BIS limit (45 ppm). While only 20-43% of samples have water hardness under the specified BIS limit (200 ppm).

AEP-CYSA-03 : Unlocking the Potential of Functionalized GO in Environmental Clean-up : Trapping Lead and Cadmium for a Cleaner World

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Contamination of natural water sources by heavy metals poses a persistent environmental challenge, necessitating advancements in purification technologies. This research focuses on the synthesis of a novel thiol-functionalized Graphene Oxide (GO-MBT) for the removal of heavy metals, specifically Pb(II) and Cd(II), from aqueous mediums. The synthesized GO and GO-MBT were comprehensively characterized using various techniques such as HR-TEM, XPS, EDX, FTIR, FE-SEM, TGA, AAS, and XRD. The adsorption kinetics were found to follow the pseudo-second order model, exhibiting high regression coefficients for both Pb(II) and Cd(II). Thiol-functionalized GO-MBT demonstrated remarkable adsorption capacities for Pb(II) at pH 6 and for Cd(II) at pH 7. Density Functional Theory (DFT) calculations provided valuable insights into the structural and energy properties, confirming the stability and reactivity of GO and GO-MBT. The developed GO-MBT emerges as a highly effective adsorbent for the removal of Pb(II) and Cd(II) from contaminated water, offering a promising solution to address the ongoing environmental challenge of heavy metal contamination.

AEP-CYSA-04 : Ni-P and Cr-P Loaded on GO via Electroless Plating for Enhanced Photocatalytic Water Splitting for Hydrogen Production

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Hydrogen, a form of energy that is both clean and renewable, is now being researched and developed as a source of alternative energy. It can be produced by water splitting without producing any green-house gas. But it requires photocatalytic material and Graphene as a 2D material with various unique properties such as non-toxicity, low cost, thinness, strongness with high surface area and good conductivity (electricity and heat), is a good candidate for water splitting. NiP and

CrP have been considered as the active co-catalysts for the enhanced photocatalytic activity of graphene oxide. In this work, a series of graphene oxide samples with 3% NiP and CrP loading have been successfully prepared by using two step electroless plating method. The as-prepared samples have been characterized in detail. The activities of the samples were evaluated by photocatalytic water splitting into 20% CH_3OH under 300W Xenon light source. As-synthesised materials shows 8.99 and 10.8 folds increment in photocatalytic H_2 production rate of GO/NiP (408.947 ìmolg^{-1}h^{-1}) and GO/CrP (400.768 ìmolg^{-1}h^{-1}) in comparison to the pristine GO (45.470 ìmolg^{-1}h^{-1}). The apparent quantum efficiency of the system (GO unused, GO used, GO/NiP unused, GO/NiP used, GO/CrP unused and GO/CrP used) were calculated i.e. 0.16%, 0.098%, 1.64%, 1.49%, 1.60% and 1.37%. Based on advance analyses techniques photocatalytic electron transfer mechanism is proposed metal phosphorus NPs accelerated the separation of photo e^-- h^+ pair to relay the photo e^- via metal phosphorus particles to react with H_2O that improves the photocatalytic water splitting of pristine GO.

AEP-CYSA-05 : Gram-Negative Bacterial Strain as Corrosion Inhibitor

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Corrosion Inhibition Efficiency of Gram-negative bacterial strain on metal plate of various concentration in mild acidic medium was analyzed. Weight loss technique was employed for the determination of corrosion rate and Inhibition efficiency. Scanning Electron Microscope, Fourier Transform Infra-Red spectroscopy, UV visible spectroscopy and X-Ray Diffraction technique were used as to examine the surface of Cu metal after it had been dipped in acidic solution in the absence and presence of inhibitor. For elemental composition, Energy Dispersive X-ray was used. The protective layer developed on the Cu surface was studied using X-ray Photoelectron Spectroscopy. The results obtained showed that as inhibitor concentration is increased, corrosion inhibition efficiency increases. The results were then verified using electrochemical technique- Potentiodynamic Polarization and Electrochemical Impedance Spectroscopy. According to the electrochemical data, metal plate immersed in an acidic solution with inhibitor exhibits higher inhibition efficiency, linear polarization resistance, lower charge transfer resistance, and lower corrosion current density than metal plate immersed in an acidic solution without inhibitor. Adsorption of bacterial strain obeys the Langmuir adsorption isotherm.

AEP-CYSA-06 : Spectrophotometric, Spectral and Binding Studies of Cu(II) Metal Complexes with Different Schiff base Moieties, A Review Study

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The co-ordination ability of Schiff bases to the metal ion especially Cu(II) has become a very important field in the development in chemotherapeutics, as well as monitoring cellular processes in living organism and as molecular probe in recent years. The development of highly selective and sensitive fluorescent probes towards metals have gained more interest. Amongst these fluorescent probes towards Cu (II) metal is very meaningful and challenging work. As the adequate and excessive uptake of copper in biological system can cause oxidation and disorders associated with neurodegenerative diseases like Alzheimer's, Menkes disease and Wilson disease. So, this work represents the binding ability of Cu (II) metal complexes, as well as its different sensing mechanism including ICT, PET, FRET etc and its applicability towards the real-life sensing.

AEP-CYSA-07 : An Electrochemical Sensor for Detecting Aqueous Hydroquinone Built from Thermally Controlled Sheets of $Ce_2(WO_4)_3$@rGO Nanocomposite

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The presence of hydroquinone (HQ) in the environment causes several health issues due to its high toxicity and lack of biodegradation. Therefore, it is crucial to detect it in environmental samples. In this work, we developed an electrochemical sensor using $Ce_2(WO_4)_3$@rGO (CeW@rGO) nanocomposites coated on a glassy carbon electrode (GCE) for the detection of HQ. A novel nano compound was synthesized hydrothermally with different reaction times (2, 6, 12, 24, and 48 h), then mixed with rGO to form CeW@rGO nanocomposites. We modified the GCE using different CeW-X (X = 2, 6, 12, 24, and 48 h), and the CeW-6@rGO nanocomposite showed the best electrochemical behavior. A novel sensor made with CeW-6@rGO nanocomposites exhibits long-term stability and high selectivity. The novel CeW-6@rGO/GCE sensor detects HQ in real-world water samples with a detection limit of 9.6

nM and a linear range of 0.1-115 µM. The innovative sensor could be beneficial in real-world applications.

AEP-01 : Layered Double Hydroxide based Nanocomposites for Water Pollution Mitigation

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Layered Double Hydroxides (LDHs), the materials also denoted as synthetic clays or anionic clays are composed of brucite like positively charged double layers intercalated with exchangeable anions. The amazing capabilities of LDHs to adjust the interlayered distance with selective anoins make them potentially important in the modern research fields like drug-delivery, anion exchange, photo catalysis, fire retardants, nanosorbents, analytical extraction, electronics etc. The biocompatibilities of these materials expand their applications in eco-friendly manner to remove various pollutants. This review article provides an outline on the LDH based nanocomposites and their synthesis methods, characterization techniques, and some recent advancement that has been achieved in pollutant removal, highlighting the areas of water pollutants.

AEP-02 : Purification of Crude Extracts of Moullava Spicata to Isolate Bioactive Phytoconstituents by Different Chromatographic Methods

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Moullava spicata is candy corn plant belong to family Caesalpiniaceae. It is robust climber having potent biological properties. In present investigation fresh plant material was collected, authenticated and then extracted in solvents with their increasing polarity. Extracts were dried under reduced pressure; dried extracts were screened by TLC and HPLC. Extracts were further fractionated in different solvents and their chromatographic analyses was carried out for separation of pure compounds. Simple column chromatography, flash column chromatography, preparative Thin Layer Chromatography (PTLC) was carried out. Pure compounds were isolated and characterized by spectroscopic methods. The conclusion is that, such pure bioactive phytoconstituents were first time reported from the plant M. spicata and methods for purification and isolation of these phytoconstituents were developed. From Ethyl acetate and Methanol extracts of M. spicata Lupeol, Gallic acid, Kaempferol, Vakerin were isolated and characterized by various spectroscopic techniques.

AEP-03 : Synthesis, Characterization and Application of Ionic Liquid as Corrosion Inhibitor for Carbon Steel in Acidic Medium

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The current research monitor the synthesis, characterization and computational study of Ionic liquid as corrosion inhibitor. The experimental section incorporates commonly employed methodologies, such as weight loss analysis,potentiodynamic polarization and impedence spectroscopy, thermodynamic parameteres ,adsorption isotherms. The electrochemical impedence spectroscopy measurements revealed that 1-Ethyl-3benzylimidazolium bromide functions as a corrosion inhibitor. Additionally, polarization dynamic polarization (PDP) results substantiated that it act as mixed type inhibitor.The adsorption phenomenon exhibited by inhibitors is significantly explained by the Langmuir adsorption isotherm. The characterization of surface interactions involving ionic liquid adsorption onto carbon steel was corroborated through an array of analytical techniques, including Scanning Electron Microscopy (SEM). These analyses collectively provide robust evidence supporting the presence and affinity of ionic liquid on the carbon steel surface. It exhibit notable efficiency (95.05% at 1000ppm) in inhibiting metallic corrosion.

AEP-04 : Ambient Air Quality Monitoring of Nandurbar City during a Diwali Festival : A Case Study

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The ambient air quality monitoring was carried out at three different locations in Nandurbar city. Ambient air quality parameters, including particulate matter (PM_{10} and $PM_{2.5}$), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), are monitored at strategically selected locations within Nandurbar City. The study spans the pre-Diwali, Diwali, and post-Diwali periods to capture variations and trends associated with festival-related activities. Real-time monitoring is complemented by meteorological data to understand the influence of weather conditions on pollutant dispersion. The eight and four hour continuous air sampling was done for the collection of RSPM and gas samples at each location respectively. Preliminary findings reveal a noticeable increase in particulate matter and certain gaseous pollutants during the Diwali festival. The concentration levels of PM_{10} and $PM_{2.5}$ exhibit spikes, reflecting the impact of firecracker emissions. Additionally, elevated levels of NO_2 and SO_2 are observed during peak celebration hours. The data is subjected to statistical analysis to discern significant differences between pre-Diwali and post-Diwali periods, providing insights into the extent of pollution attributable to the festival.

AEP-05 : Synthesis and Application of ZrO_2/$BiVO_4$/g-C_3N_4 Nanocomposite

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Photocatalysis has been emerged as a sustainable and promising strategy which is intensively investigated for different applications, including solar fuel production and degradation of environmental pollutants and problems. However, it is still challenging to develop highly active, selective, and durable photocatalyst for practical applications. Photocatalysis can either store solar energy into molecular bonds or use it to degrade pollutants[1]. Due to remarkable stability and activity which is attributed to high specific surface area, robust mechanical structure, and superior electrical conductivity, thin 2D nanomaterials have attracted a lot of attention in the environmental and energy-related research sectors[2]. In this Work, we have synthesized 3 different nanomaterials and after that making ternary $BiVO_4$/ZrO_2/g-C_3N_4 nanocomposite by using hydrothermal method. Final synthesized sample was characterized by different tools. Then this nanocomposite was used in different environmental remediation applications such as treatment with cationic dye and pesticides removal.

AEP-06 : Assessment of Domestic Wastewater Quality with Reference to Physicochemical Parameters at Agra City, UP, India

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Water supplies worldwide are contaminated by pollutants from a wide range of sources, including industrial, domestic, and agricultural waste, which degrades the quality of the water. Similar to this, the scarcity of fresh water in many parts of India is a major issue that necessitates human attention to sustainable water conservation. Greywater and blackwater are the two primary classifications of domestic wastewater. The properties of greywater were the main focus of this investigation. The waste product from all household water use, with the exception of toilet flushing, is called greywater. It is less polluted even though it often comprises the majority of household wastewater. Recycling and reusing treated greywater for non-potable uses may significantly reduce the demand for freshwater. The results of a study on the characteristics of greywater generated by Agra's metropolitan areas are compiled in this article. Therefore, a water quality investigation was carried out in the city of Agra in order to evaluate the present state of physicochemical contaminants and their sources in household wastewater. A variety of characteristics, including conductivity, pH, total hardness, COD, and BOD, were examined. The physicochemical characteristics were found to be outside of the water quality criteria based on the samples.

AEP-07 : The Role of Solar cells in the Current Scenario: An Overview

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As a result of the overuse of natural resources that has led to a dangerous condition known as global warming, solar energy has emerged as a vital source of energy. Scientists and researchers throughout the world are being compelled to look at non-conventional sustainable energy supplies including wind, tidal, hydrogen, and solar energy due to the ongoing population growth and the increase in supply demand. All of them, meanwhile, have significant restrictions related to the local climate and geological makeup. However, solar energy and hydrogen energy are widely available in most places. Similar to this, solar energy may be easily used as an electrical source in warm climates by using various structures including solar cells, concentrating collectors, and flat-plate solar collectors. The addition of Si, another scarce and hazardous mineral, makes Si-solar cells the greatest of all the different types of solar cells, but it also presents a significant drawback. As a result, various solar cells that use environmentally benign materials to gather the most solar energy with the least amount of compromise and damage to the environment–such as pervoskite solar cells, dye-sensitized solar cells, and hybrid-heterojunction solar cells–are garnering a lot of attention.

AEP-08 : Fluoride Mapping of Ground Water Sources of Kota District

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Water is a universal solvent and essential for life system. Water contains so many minerals/ions which are essential for biological system but in limited quantity. Among ions found in water, Fluoride is a highly reactive anion. Its acceptable limit in water is 1.0 ppm and permissible limit is 1.5 ppm. In excessive quantity it is life threatening and causes various disease like teeth decay and skeletal disorder. Contamination of Fluoride in water is major problem in Kota and Bundi Districts of Rajasthan. Fluoride mapping is done by cluster method and points are identified where fluoride is present in excess quantity than permissible limit. Various ground water sources i.e. Tubewells, Handpumps and Single phase motors were detected in which fluoride is present in excess quantity. During mapping of fluoride in Kota District, especially villages of Itawa Block and Sultanpur block are found rich was found fluoride rich. In Kota District fluoride ranges up to 5.0 ppm.

INORGANIC CHEMISTRY SECTION

Sectional President's Address

Synthesis of Organic-Inorganic Semiconductor Photocatalysts and their Composites for Environmental Remediation

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The basic requirements for sustainable development for an increasing population are food, clothing, and shelter. However, providing these necessities to the population pose the significant obstacles, including global health issues, environmental pollution, and energy crises. The investigation of diverse materials, including carbon and metal oxide-based semiconductors, led to the successful synthesis of novel photocatalysts. Key highlights include the controlled fabrication of nano-sized two and three-dimensional ZnO structures, demonstrating exceptional photocatalytic performance in the degradation of methylene blue. Additionally, the study pioneers the synthesis of pentacenequinone (PQ) through a green and innovative solid-state method, showcasing its viability as a visible light-active photocatalyst. The integration of PQ with ZnO yields a remarkable nanocomposite with an impressive degradation efficiency of over 79% within 90 minutes. It not only contributes to the dominion of visible-light-driven photocatalysts but also opens new avenues for future research in the realm of environmental purification. The findings the way for innovative and sustainable solutions, propelling the boundaries of photocatalysis and materials science to address contemporary challenges in water pollution and beyond. It suggest that PQ/ZnO nanocomposites have enhanced photocatalytic activity compared to pure ZnO. The highest activity was observed at 0.5 wt.% PQ loading, indicating an optimum concentration for maximum activity. These synthesized materials are characterized by various spectroscopic and microscopy techniques as FTIR, UV-Visible, SEM, XRD, TEM. Pentacenequinone-based organic semiconductor photocatalysts have excellent photocatalytic properties, making them promising alternatives to traditional inorganic semiconductors.

IIL-01 : Pristine and Tellurium Doped rGO for Molecular Spintronics and Pseudo Capacitor Application

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In recent years, 2D material architecture has captivated attention due to their unique properties. Herein we present studies of spin dynamics in graphene derivatives and their electrochemical properties. We have done synthesis of tellurium (Te) doped reduced graphene oxide (rGO) (0.5-11 w/w) %. These materials are prepared by fabrication via an in situ chemical route. Tellurium (Te) doped rGO system is investigated and compared with its counter parts. The research findings realize the fact that, 1(w/w) % Te-rGO molecule is a pertinent medium for spintronics and electrochemical applications. The study reveals that p-orbital moments of Te contribute, vectorially, to radical electron's spin relaxation process in carbon and, prominently, operative at broken inversion symmetry sites in Te-rGO molecule. Te is selectively chemisorbed in non-sp^2 regime generating the in-plane bond strain of 7% at sp^2 sites and ~ 3% strain/ frustration at disordered zone (sp^3) locally. Presence of Te strengthens the electron-phonon coupling by 13% with respect to its precursor counterpart. In the electrochemical studies, the energy density E_D (Wh/kg), and power density, P_D (W/kg), indicated that, both electrodes were at the interface of battery and electrode double layer capacitor (EDLC) region on Ragone E_D-P_D plane. The ESR studies underline that the diffusion length of the electrons is increased to a large extent, which effectively benefits the migration of electrolytic ions into the multi-layered structures. They possess superior flat cell character, are cost effective and are favourable towards practicality at an industrial scale, as demonstrated on the laboratory bench. Details are presented.

IIL-02 : Synthesis, Crystal Structure and Applications of Metal Complexes Derived from Acyl Pyrazolones and their Structural Analogues

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Acyl pyrazolones and their structural analogues are heterocyclic β-diketones. The importance of the Acylpyrazolones as part of the research field with multi dentisity, expansibility through modifications, more straightforward synthesis and various complex-forming properties for biological (analgesic, protective neurons, anti-infective, anti-pyretic, anti-oxidant, anti-tumour, anti-bacterial, etc.), optical, or electrochemical purposes has been increasing in the last few decades. One of the primary benefits of Acylpyrazolone ligands is their capability to create enduring complexes with a wide range of elements, including main group, transition metals, lanthanides, and actinides, which can be utilized for various purposes. Our laboratory is synthesizing various acyl pyrazolone derivatives and their Schiff bases and characterizing them by various spectroscopic techniques and also by x-ray crystallography. The type of coordination environment, the type of complexation and the coordination number of complexes of these complexes can be established from their spectral analysis. These derivatives along with certain secondary ligands can then be used to prepare metal complexes with transition metals like V(III), Cu(II), Ni(II), Zn(II), etc and inner transition metals like U(VI), Nd(III), Dy(III), Tb(III), etc. The metal complexes also characterized fully by various spectroscopic techniques and finally by x-ray crystallography. DFT and other computational methods are also used to get insight into the structure of these complexes. Theoretical bond properties were also examined by the identification of global index parameters. The Hirshfeld surface analysis is used to study the non-covalent interactions. The attempt have been made to use these complexes in various diverse fields like as anti bacterial and anti tuberculosis activity, DNA binding and DNA cleavage activity, anti cancer activity, as fluorescence sensor, in homogenous and heterogeneous catalysis etc. The present talk is aimed to give highlight of the work going on in my laboratory on the acyl pyrazolones and their structural analogues.

IIL-03 : Green Synthesis of Metals and their Oxides Nanoparticles : Applications for Remediation

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Due to materialistic approach of all the nations in this world pollution is increasing day by day.As a result of this air,water and soil are polluted which are the basic needs of living organisms.Therefore a chemists has to develop synthetic protocols which follow green chemistry approach (Sustainable Chemistry). Catalysts play dominating role in any synthesis and first choice is a bio catalyst in the form of various extracts of different parts of plant such as roots, leaves etc,fungi,enymes even urine cow. In this talk we wish to explore use ofsuch biocatalysts to accompalish synthsis of nanoparticles of some transition mtals and their oxidesn aqueous medium just by stiring technique. This is a sustainable development of chemistry.followed by their application as antimicrobial agent and as a catalyst for various organic reactions.

IIL-04 : Presentation of Reference Measurement Procedure for Uranium Determination in Ores, Concentrates and Other Diverse Matrices in Nuclear Fuel Cycle using Laser Induced Fluorimetry/Led Fluorimetry-a Green Approach

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Application of differential technique in laser-induced fluorimetry/ LED Fluorimetry/ICP-OES for the direct determination of uranium is recommended for routine accurate determination of uranium over a wide range of concentrations in mineralized rocks, ores, concentrates and other diverse matrices in Nuclear Fuel Cycle, which is based on the comparison of the response of the standard with a sample of similar but unknown concentration on the same sample weight basis. By taking advantage of high sensitivity of laser fluorimetry/LED fluorimetry, the interferences from the associated and accompanying elements are eliminated by simple one-step dilution of the sample aliquots using push-button microlitre pipettes, thereby to bring the concentration of uranium within the operational range of the instrument, followed by measurement with differential technique in laser-induced /Pulsed LED fluorimetry using more suitable acidic buffer mixture of H_3PO_4-$NH_4H_2PO_4$ (pH~2, $H_3PO_{4,}$ 1 M and $NH_4H_2PO_{4,}$ 2.17 M) as fluorescence-enhancing reagent. The experiments are designed in such a way that for very diluted sample solutions, prefilter (species absorbing at the laser wavelength, 337 nm, LED wavelength of excitation at 400 nm) and postfilter (species absorbing at the maximum fluorescence wavelengths, 480-560 nm) effects are negligible(verified by spectrophotometry). Differential laser-induced/LED fluorimetry method has been evaluated using standards, SY-2, SY-3, reference uranium ore, BL-2a, low-grade uranium ore-IAEA reference samples, and core samples of diverse matrices.

It fulfills the basic essential requirements of RAPs : Reliability (accuracy and high precision), Applicability (applicable to diverse sample matrices for wide applications in entire nuclear fuel cycle) and Practicability (inherent high sensitivity, high PQ, simple, rapid and direct, easy equipments calibration, method standardization and operation, eco-friendly, cost effective, High sample through put, comparability, and traceability. Over the years, Application of differential technique in Laser-induced fluorimetry/LED-fluorimetry will continue to grow for more reliable measurement of uranium with higher productivity to fulfill the mission and mandate in AMD in entire nuclear fuel cycle.

IIL-05 : Astonishing Chemistry of Ultrathin C and B

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Chemistry of Single layer sp^2 hybrid carbons has emerged as a wonderful universal materials having enormous applications in various fields. Ultrathin 2D nanomaterials possess sheet like structures with the lateral size larger than 100 nm or up to a few micrometers and even the larger but the thickness is only single or a few-atoms thick (typically less than 5 nanometer). The 2D feature is unique and indispensable to access unprecedented physical, electronic, and chemical properties due to electronic confinement in two dimensions. Graphene is an exemplary model due to its unexpected properties including ultrathin room temperature room carrier mobility, high Young modulus, excellent optical transparency and excellent electrical and thermal conductivities. ThD exploration of other graphene like ultrathin 2D nanomaterials are also growing. To name a few transition metal dichalcoginides(TMDs), graphite carbon nitride(g-C_3N_4),layered metal oxides, and layered metal double hydroxides (LDHs) are typical graphene like ultrathin 2D nanomaterials. Promising research on graphene like 2D nanomaterials further enriched the exploration of 2D ultrathin family members, such as M-Xenes, noble metals, metal-organic frame works (MOFs), covalent organic frameworks (COFs), polymers, silicone, antimonene, inorganic perovskites, and organic-inorganic hybrid perovskites. During the present talk the synthesis and applications of such materials with special reference to their application for fluoride removal in the drinking water will be highlighted.

IIL-06 : New Analogues of Bioactive Compounds: Synthesis and Exploring Biological Potentials

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Our exploration was inspired by the incredible biological effects of curcumin and coumarins, motivating us to create a wide range of new thirty analogues using advanced synthetic techniques. These novel analogues were derived from Curcumin and Coumarins. In this report through comprehensive in vitro assays focusing on anti-inflammatory, antioxidant, and cytotoxic properties, we meticulously studied their biological behavior. Our results show that the anti-inflammatory potential of these analogues, surpassing even their natural counterparts. Moreover, they exhibited significant antioxidant capabilities, promising in managing conditions associated with oxidative stress. Additionally, our cytotoxicity assessments carried out using MTT assay revealed selective activity against specific cancer cell lines. Impressively low IC_{50} values of 0.61 and 4.95 µM position these analogues as potential candidates in the development of new anticancer agents. Our investigations into the biological attributes of these newly created analogues highlight their potential as primary compounds in the search for new drugs. Their diverse and promising biological profiles mark a significant step forward in synthesizing therapeutically relevant compounds inspired by nature. The outcomes of this study may contribute to the expanding field of medicinal chemistry as well as in the advancement of these analogues towards future clinical applications.

IO-CYSA-01 : Photovoltaic Study of ZnO/SnO_2 Nanocomposite-based Photoanode for Dye-Sensitized Solar Cell

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A simple hydrothermal process has been used for the synthesis of ZnO and ZnO/SnO_2 nanocomposites. The varied amount of SnO_2 concentration has been incorporated into ZnO to fabricate ZnO/SnO_2 hetero structures. Structural, optical and morphological properties of synthesized materials done by using XRD, UV-Visible analysis, BET, and FESEM characterization techniques. The addition of SnO_2 into ZnO has found to increase the crystallite size with increasing SnO_2 concentration in the nanocomposite structure. Mixed morphologies of nanostructures such as nanoparticles, nanopetals and nanoflakes-like structures observed in FESEM images. Further, synthesized material used to prepare photoanode by using doctor blade technique. The dye sensitized solar cell (DSSC) fabricated using these photoanodes were tested for JV measurements. Results show the enhancement in photovoltaic properties in ZnO/SnO_2 nanocomposites as compared to pristine material. Optimized ZnO/SnO_2 nanocomposite exhibited 275%

higher efficiency than pristine ZnO-based DSSC. The increment in the device efficiency can be attributed to increasing surface area for dye adsorption and reduction in recombination of charge carriers leading to enhance electron life time.

IO-CYSA-02 : Synthesis, Spectrochemical Characterization, DNA Interaction and Antioxidant Screening of a Novel thiazole Schiff Base Ligand and its Cu(II) and Zn(II) Metal Complexes

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Two biologically efficient Schiff base metal (M: Cu(II) and Zn(II)) complexes have been synthesized by condensing the novel thiazole Schiff base ligand 5-(diethylamino)-2-((5-methylthiazol-2-ylimino)methyl)phenol; [4DEA] with respective Copper and Zinc metal salts. The synthesized compounds were spectrochemically characterized by molar conductance, FT-IR, UV-Vis, ^{1}HNMR, Mass spectrometry and Thermal analysis (TGA). The coordination sites of the synthesized ligand are phenolic oxygen, azomethine nitrogen and thiazole nitrogen which makes the ligand monobasic - tridentate. The metal complexes showed distorted octahedral geometry. The DNA binding and cleaving activity of the synthesized compounds was screened against circular plasmid pCAMBIA DNA, which results that the Cu(II) complex gives better DNA binding as well as cleaving activity than the Zn(II) complex and Schiff base ligand(4DEA). Furthermore, testing of the compounds have been done for radical scavenging(antioxidant) potency of the synthesized compounds by using DPPH, which depicts the Cu(II) complex gives better antioxidant activity than the others.

IO-CYSA-03 : Synthesis of Silver Nanoparticles using Plumeria Plant and its Larvicidal Activity against Malaria Vectors

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Malaria is one of the longest known diseases in humans. Malaria is a serious public health problem due to the high cost of living and loss of life. The vaccines are not available for the prevention or treatments on malaria, dengue like diseases. The concept of findings is, to prepare silver nanoparticles (Ag NPs) by using green methodology. We use plant latex for the synthesis of Ag Nps and that material is used to control the mosquito vector. The synthesized Ag NPs are used for larvicidal activity against the malaria vector anopheles stephensi & filariasis vector culex quinquefaciatus. The Ag NPs were characterized by fourier transform infrared spectroscopy (FT-IR), UV spectroscopy, XRD analysis, scanning electron microscopy (FE-SEM). Ag NPs are effectively synthesized from a silver nitrate solution through a simple green route using the plumeria plant latex. It has potential to be used as an ideal ecofriendly approach for the control of the mosquito.

IO-CYSA-04 : Effect of Calcination Temperature on the Structural, Magnetic and Electrochemical Properties of Low Temperature Synthesized Manganese Ferrite

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Manganese ferrite ($MnFe_2O_4$) is a magnetic metal oxide with a mixed spinel structure, whose size, morphology and physicochemical properties depend upon synthesis methods and their operation conditions like pH, precursor concentration, temperature, etc. On account of its unique and tunable properties, $MnFe_2O_4$ is utilized in biomedical applications, catalysis, sensors, heavy metal removal, and as electrode material in Lithium Ion Batteries and supercapacitors. In present study, $MnFe_2O_4$ was synthesized using the co-precipitation method, with a synthesis temperature as low as 80p C. The as-synthesized material was further subjected to higher calcination temperatures of 200p C, 400p C and 600p C to study the effect of increasing calcination temperatures. XRD analysis carried out for structural investigation and phase identification confirmed spinel cubic phase with Fd-3m space group in the uncalcined sample, as well as samples calcined at 200p C and 400p C, without any secondary impurity phase. However, on increasing the calcination temperature to 600p C, secondary phases of α-Fe_2O_3 (hematite) along with oxides of Mn (Mn_2O_3 and MnO) were observed along with $MnFe_2O_4$. Williamson-Hall method was employed to calculate the crystallite size of the synthesized ferrites, and the results show the average crystallite size of the uncalcined sample to be ~34 nm. The formation of pure spinel $MnFe_2O_4$ at low temperatures and subsequent phase transformation at 600p C was also verified using FT-IR and Raman spectroscopy. The magnetic properties were studied using the Vibrating Sample Magnetometer

(VSM) technique, and the data revealed the ferromagnetic nature of as-prepared samples. The uncalcined sample exhibited a high saturation magnetization (M_s) of 40.59 emu/g. However, as the calcination temperature was raised to 600p C, the value of M_s decreased. This decline can be attributed to the formation of antiferromagnetic á-Fe_2O_3 and the partial oxidation of surface Mn^{2+} to Mn^{3+}. The effect of increasing calcination temperatures on electrochemical properties of manganese ferrite was also studied with the help of Electrochemical Impedance Spectroscopy (EIS), DC electrical conductivity and I-V measurements.

IO-CYSA-05 : Graphitic Carbon Nitride Infused with PVA-Mn:ZnS Modified Carbon Sensor for Electrochemical Investigation of Metoclopramide Hydrochloride

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The primary focus is on determining the trace amount of Metoclopramide hydrochloride (MCH) which widely used to treat gastrointestinal disorders such as gastroparesis and acid reflux. The present study involves the development of a novel carbon paste-based sensor modified with Poly vinyl alcohol capped Manganese-doped ZnS nano particles decorated g-C_3N_4 nanocomposite (PVA-Mn:ZnS/g-C_3N_4@CPE), for the detecting and investigation of MCH. Cyclic voltammetry (CV) and square wave voltammetry (SWV) were used to measure the electrochemical performance of MCH. The limit of detection and quantification is found to be 5 nM and 16 nM respectively. Using the SWV technique in pH 7.0 phosphate buffer, the examination of urine and water spiked with MCH was monitored. When PVA-Mn:ZnS/g-C_3N_4 nanocomposite was used as a modifier in electrode-based sensors, results in well-resolved peaks and improved electrochemical current sensitivity. The electrode material was characterized by CV, scanning electron microscopy, atomic force microscopy, and electrochemical impedance spectroscopy. The electro-oxidation of MCH was explored using electro-kinetic characteristics such as heterogeneous rate constant, accumulation time, entropy, enthalpy, Gibbs free energy and other parameters like scan rate and pH. A suitable mechanism was proposed for the number of protons and electrons involved in the electro oxidation of MCH.

IO-CYSA-06 : Tuning the Band Gap of Graphitic Carbon Nitride/TiO_2 Photocatalysts via Phosphorus Doping for Enhanced Hydrogen Production

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The development of heterojunction photocatalyst for efficient solar energy conversion is essential for practical application. In this study, simple and low cost method has been implemented to improve the visible light photocatalytic activity. The graphitic carbon nitride (CN), Phosphorus doped graphitic carbon nitride (PCN) and its composites were successfully characterized by different analytical techniques. The doping of phosphorus in gC_3N_4 changes its optical and textural properties. DRS study clearly depicts increased absorption of visible light in case of PCN as compared to CN. PCN (65 ìmol/g) shows 1.5 times increase in hydrogen evolution capacity as compared to CN (41 ìmol/g). CN and PCN coupling with P25(TiO_2) shows dramatic enhancement in photocatalytic hydrogen evolution activity as compared to bare P25(TiO_2). CN-P25(TiO_2) show twenty-two fold (920 ìmol/g) and PCN- P25(TiO_2) shows nearly forty fold (2531 ìmol/g) increment in hydrogen production as compared to bare P25(TiO_2). The overwhelming enhancement in photocatalytic yield can be attributed to the charge transfer from CN or PCN to P25(TiO_2) thereby reducing the probability of electron-hole recombination. Simple phosphorous doping to CN and then coupling PCN with P25 (TiO_2) has given rise to notable low-cost metal free photocatalyst opening great avenues in the field of energy and environment.

IO-CYSA-07 : Ce doped ZnO Catalyzed Synthesis of Symmetrical Diaryl Disulfides via Cascade Reaction of Aryl Halides and Elemental Sulfur

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Organic disulfides, which belong to an important class of sulfur-containing compounds, have attracted much attention because of their various biological, industrial and synthetic applications. In the current work, bare and Ce doped ZnO nanocrystallites are synthesized by surfactant-assisted hydrothermal method and thoroughly characterized by FTIR, XRD, FE-SEM, BET, PL and UV-visible techniques. XRD showed that the diffraction peaks of all the products were in good agreement with standards. The crystallite size ranging from 32nm -

42nm for Ce ZnO increases with cerium doping. FE-SEM images revealed different morphologies. FTIR study shows the position of different stretching and bending modes present in the sample. PL and UV-Visible spectra show the interesting optical properties of Ce-ZnO. Band gap energy for Ce-ZnO was 3.21eV - 3.26eV. The effective one-pot procedure is developed for the direct synthesis of disulfides from aryl halide and elemental sulfur in DMF by using Ce doped ZnO catalyst. All the disulfide derivatives were thoroughly characterized by IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy. The advantages of the novel and facile protocol are precluding volatile, foul-smelling, and toxic thiols as well as utilizing economically affordable, recyclable, and air-stable catalysts under ligand-free conditions.

IO-01 : Preparation, Characterization and Application of Carboxymethyl Cellouse Stabilized Cobalt Sulfide Nanoparticles

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A biological macromolecule stabilized method for the preparation of cobalt sulfide nanoparticles using carboxymethyl cellouse (CMC) as a stabilizing agent was developed. The formation of cobalt sulfide nanoparticles as a function of different amounts of CMC was done. At 0.05% w/v amount of CMC, the high percentage of cube shaped cobalt sulphide nanoparticles was obtained. The samples obtained from 0.01% w/v and 0.1% w/v amounts of CMC showed random shaped cobalt sulfide nanoparticles and aggregated cobalt sulfide nanostructures, respectively. The obtained cobalt sulfide nanoparticles are stabilized through the interactions of hydroxyl (–OH) and carboxylate (–COO–) functional groups in CMC. The CMC encapsulated cobalt sulfide nanoparticles were shown to have good catalytic activity for chemical reduction of p-nitroaniline in the presence of sodium borohydride.

IO-02 : Synthesis, and Pharmacological Studies of Mixed Ligand Complex of Divalent Nickel with Histidine, 2-Quilnolinecarboxaldehyde Derivatives

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Over the last few decades, the importance of complexes bearing Schiff bases ligands has rapidly increased owing to their application in the biological field. Novel metal complexes have a broad spectrum of biological activities including anticancer, antiviral, and anti-inflammatory, and are widely used as drugs for the treatment of various diseases. New Schiff base (E)-2-((2-phenylhydrazineylidene) methyl) quinoline Schiff base[L] was synthesized as a result of the condensation of phenylhydrazine with 2-Quilnolinecarboxaldehyde [L] in 1:1 molar ratio. A mixed ligand complex was synthesized by a reaction of Ni (II) metal ion with histidine and a newly synthesized ligand. Elemental analysis, ^{1}H NMR, mass spectroscopy, and FTIR have been used to justify their proposed chemical structures. Synthesized compounds have been assayed for their antimicrobial activities against bacterial strains, S. aureus, E. coli, and fungal pathogens, C. albicans were determined.

IO-03 : Development of Novel Heterogeneous Cobalt Acylpyrazolone Catalyst : Synthesis, Characterization and Selective Oxidation of Styrene to Benzaldehyde

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Cobalt acylpyrazolone complex was prepared and characterized using various spectral methods, FT-IR, TGA, UV-visible, DRS, magnetic study, and single crystal XRD. A heterogeneous catalyst consisting of neutral alumina and Cobalt complex was synthesized and characterized using various physicochemical methods and successfully applied to styrene oxidation without a solvent. The effects of the reaction variables (mole proportion of the reactant to hydrogen peroxide and TBHP, quantity of the catalyst, reaction period and reaction temperature) were investigated. No appreciable catalytic activity reduction occurred when the catalyst was utilised again. The catalyst's recycling is verified by infrared and diffuse reflectance spectra confirming that the catalyst was intact and not destroyed following the process. The work's unique feature is its benzaldehyde selectivity under benign reaction circumstances.

IO-04 : Semiconducting Nano Materials Review

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Semiconducting nanomaterials, characterized by their size-dependent properties, are synthesized using techniques like chemical vapor deposition and hydrothermal methods. These materials possess unique electrical, optical, and catalytic properties. In electronics, they enhance transistor performance and sensor sensitivity. In photonics, they enable efficient light-emitting diodes and photodetectors. Semiconducting nanomaterials also serve as catalysts in energy conversion and storage applications such as fuel cells and batteries. Additionally, they find use in healthcare for drug delivery and biosensing. These versatile materials, with tunable properties, continue to drive innovation in diverse domains, promising advances in technology and problem- solving.

IO-05 : Nickel Substituted Calcium Ferrites ($Ca_{1-x}Ni_xFe_2O_4$; x=0.0, 0.2, 0.4, 0.6, 0.8); Natural pn-Heterojunction Material for Photo Catalytic Applications

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The objective of this research is to comprehensively explore the impact of Ni^{2+} ion substitution on the morphology, magnetic properties, and optical characteristics of $CaFe_2O_4$ nanoparticles. The citric acid auto-combustion technique is employed to synthesize ferrite samples characterized by consistent particle size. Calcium Nickel Iron citrate precursors by TG-DTA, revealed the calcination temperature 750 °C. FT-IR spectra confirmed tetrahedral and octahedral stretching bands. The Powder X-ray diffraction (XRD) patterns demonstrated the orthorhombic single-phase formation for x=0.0, 0.2 samples. Further, XRD patterns conclusively verified the presence of Ni^{2+} ions leads to formation of $NiFe_2O_4$ embedded within the lattice structure of $CaFe_2O_4$ owing to formation of natural ($NiFe_2O_4/CaFe_2O_4$) pn-junction hetero composites for $x \geq 0.4$ samples. An observable augmentation in crystallite size is shown by SEM images while, EDX mapping revealed the uniform dispersion of composites. UV-DRS analysis revealed the decreasing trend in band gap energy. Optimizing the loading of Ni^{2+} leads to improved visible light-harvesting capabilities. Analysis of PL demonstrates a prolonged decay time of the composite, accompanied by a decrease in the recombination rate. The Nyquist plots highlighted the excellent separation efficiency and mobility of the charge carriers. Additionally, an assessment of its band edge potentials was conducted using the Mott-Schottky plots, indicating a Z-scheme mode of electron transfer. Hence, the produced composites are deemed appropriate for photo catalytic purposes.

IO-06 : Synthesis and Biological Evaluation of Novel Analogues Inspired by Curcumin and Coumarins

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Inspired by the remarkable bioactivity of curcumin and coumarins, we embarked on a journey to synthesize a diverse array of novel analogues employing advanced synthetic methodologies. Our study includes a thorough exploration of their biological properties through three different series of novel analogues A1 –A10, B1-B10 and C1-C10 synthesized from Curcumin and Coumarins, in vitro assays, including assessments of anti-inflammatory, antioxidant, and cytotoxic effects.

Our results highlight the potent anti-inflammatory potential of these analogues, surpassing the efficacy of their natural counterparts. Additionally, these compounds exhibited significant antioxidant capabilities, showcasing promise for addressing conditions associated with oxidative stress. Furthermore, our cytotoxicity studies demonstrated selective activity against specific cancer cell lines, with IC50 values of 0.61 and 4.95 µM positioning these analogues as prospective candidates in the pursuit of novel anticancer agents. This comprehensive investigation into the biological properties of our newly synthesized analogues underscores their potential as lead compounds in drug discovery endeavours. Their diverse and potential bioactivity profiles indicate a significant advancement in the development of therapeutically relevant compounds inspired by nature. We anticipate that the findings presented in this study will not only contribute to the expanding field of medicinal chemistry but also catalyze further optimization and development of these analogues for future clinical applications.

IO-07 : Synthesis of 2 & 3D inorganic Semi-conductors use for photocatalytic Application

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The inorganic (ZnO) semiconductor were synthesized using a hydrothermal technique. The prepared ZnO nanostructures were characterized with different spectroscopic and microscopic techniques. The XRD indicates the formation of the hexagonal phase of ZnO in all the prepared samples. The UV-visible absorbance spectrum depicts the absorption peak at 380 nm corresponding to the band gap of 3.27 eV. The photoluminescence spectra show band edge emission at 390 nm and a small hump at 470 nm. The FESEM confirms the formation of hexagonal shaped plate like ZnO nanostructures having size in the range of 50 to 100 nm with the thickness of 10-15 nm, at 2 h reaction time. Further increase in the reaction time leads to increase in thickness of hexagonal ZnO plates resulting in formation of three dimensional (3D) distorted spherical structures with facets. The TEM validates the formation of highly crystalline hexagonal shaped ZnO plates having size in the range of 0 to 150 nm.

IO-08 : Biological Potential and Structural Diversity in Organotin(IV) Complexes

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The organic-inorganic hybrid complexes of organotin(IV) complexes shows variable structural patterns and different coordination behaviors. The structural considerations, stereochemical aspects and technological applications of these organotin(IV) complexes provide unprecedented advances. These organic-inorganic hybrid complexes of organotin(IV) complexes show biological relevance and catalytic activity. The presence of organotin(IV) moiety and Sn-N bond may be responsible for the antitumour property and other biological activities of the complexes. The several modifiers like amino acids, pyrazolones, Schiff bases, etc., may be used to modify the stereochemical properties of organotin(IV) complexes. Computational modeling provides in-depth structural insight for the complexes. Optimized topologies, HOMO-LUMO plots, global descriptors, thermochemical properties and MEP map are evaluated by DFT. Theoretical studies also helpful in establishing the structural-activity relationship of complexes.

IO-09 : Synthesis and Antimicrobial Activity of Novel Schiff Bases and its Metal Complexes Derived from 5-Amino Salicylic Acid

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The field of Schiff bas complexes has been first developing on account of the wide variety of possible structures for ligands depending upon the aldehydes and amines. Schiff bases are considered as a very important class of organic compounds, which have wide variety of applications in many fields, including biological, industrial and analytical chemistry. In the field of heterocyclic chemistry, imidazoles are considered as an important pharmacophore in medicinal chemistry encompassing wide spectrum of biological activities such as antibacterial antirheumatoid arthritis, antituberculosis, antiviral, antiepileptic, anti-inflammatory and anticancer activities. Keeping the above literature in view, we prepared new Schiff base of(E)-5-((2-butyl-5-chloro-1H-imidazol-4-yl)methyleneamino)-2-hydroxybenzoic acid (BCIHB) from 2-n-butyl-5-chloroimidazol-4-carbaldehyde (BCI) and 5-amino salicylic acid (AS). Also metal complexes were prepared from chloride salts of Mg (II), Ni (II), Zn (II) and Pd (II) in an alcoholic medium The chemical structures of the Schiff-base ligand and its metal complexes were confirmed by spectroscopic studies like IR, ^{1}H NMR, mass spectra, elemental analysis, molar conductance , thermo gravimetric analysis and also studied their antimicrobial activities.

IO-10 : Smart Nano Sensors

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Smart Nano Sensors, a product of nanotechnology, are set to revolutionize sensing technology. These minuscule sensors operate at the nanoscale, offering unmatched sensitivity and functionality. They can integrate seamlessly into Internet of Things (IoT) systems, collecting real-time data with minimal energy consumption. Utilizing advanced nanomaterials and nanoelectronics, they can detect various parameters, from chemicals to biomarkers and environmental factors. Applications include continuous health monitoring, early disease detection, precise drug delivery in biomedicine, and environmental protection through pollutant detection. Furthermore, their wireless communication capabilities enable remote data collection and control, benefiting agriculture, manufacturing, and other industries. Smart Nano Sensors are paving the way for a smarter, interconnected future.

IO-11 : Ionophore Synthesis and Recent Developments Employing Metal Ion Extraction and Transport

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The dynamic character of host-guest chemistry confers the resulting constructions with fascinating responses. Dipropyleneglycolmonomethyletherbis(acetoacetate) was synthesized as a podand and its capability was analyzed in membrane phase (1,2-dichloroethane, chloroform and carbon tetrachloride) towards the transfer of Na^+, K^+, Li^+, Ca^{2+}, Mg^{2+} as well as coexisting metal (Na^+ and K^+) salts. The experiments were performed to study the selectivity of one metal ion over another. To choose the optimal parameter for a specific cation during extraction and transport, a variety of factors were taken into consideration, including fluctuation in metal concentration, ionophore type, and membrane effect. The results reveal that the concentration and type of ions, membrane type and associated anion alter the transport process from source to receiving phase. External stimuli like as temperature, ion, pH, redox, enzyme, and light also alter the binding affinities of host-guest complexes. Supramolecular chemistry has shown promise as a method for developing sensors to identify environmental and food contaminants as well as catalysts to transform pollutants into recyclable materials as well as in human biology includes designing of host with target species in body for drug delivery to the specific sites.

IO-12 : Synthesis and Characterization of $CuZrO\text{-}_3$ Photocatalyst and its Application as Rose Bengal Dye Degradation

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This article exhibit systematic study of photocatalytic degradation of rose bengal dye under influence of sunlight in aqueous solution by $CuZrO\text{-}_3$ synthesized by mechanochemical solid state synthesis method. The light induced catalyst $CuZrO_3$, synthesized via mechanochemical solid state synthesis method with green chemistry approach. The synthesized catalyst was characterized by various analytical investigative techniques like, Infrared Fourier UV-visible diffused reflectance Spectroscopy, Transform Spectroscopy, X-ray Diffraction, Scanning Electron Microscopy, Tunnelling Electron Microscopy, and BET surface area to carry out structural and microstructural investigation. The frequency bands at 420 cm^{-1} , vibrational frequency range at 730 to 760 cm^{-1} , and 1104 cm^{-1} indicate Zr-O vibrational frequency, The vibrational frequency bands at 509, 518 and 1178 cm^{-1} indicates the presence of the Cu–O. XRD spectrum of $CuZrO_3$, The spectrum well matches with JCPDS data card no- 43-0953. For $CuZrO_3$, the surface area (S BET) is 20.22 m 2 /g, pore volume (V p) is 0.0811 cc/g, and pore diameter (D p) is 30.39 A°.

IO-13 : Nickel Catalysed Heck and Suzuki Reactions using Dissipated Marble Slurry as Solid Support

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Transition metal catalysed coupling reactions such as C-C bond forming Mizoroki-Heck and Suzuki-Miyaura reactions have prevalent and extensively used methods in the synthesis of bioactive molecules, pharmaceutical, agrochemicals, drugs and fine chemicals. In the modern synthetic chemistry, nickel sustain with massive recognition as catalysts in the field of transition metal catalysed C-C cross coupling reaction. Easy access of multiple oxidation states of nickel and facile oxidative addition has facilitated its use as an effective catalyst for many valuable and difficult transformations. However, most of the methods are homogeneously catalyzed reactions in which catalyst is not recyclable and reusable and require costly ligands.

Heterogeneous solid supported catalytic systems are prominent interest in coupling reaction because of their high efficiency and reusability. Herein we report the efficiency of ligand free marble slurry supported Ni catalyst for Mizoroki-Heck and Suzuki-Miyaura cross coupling reactions under an aerobic condition. Marble slurry supported nickel catalyst (Ni@MS) was prepared by wet impregnation method and used for the catalyzing Mizoroki-Heck and Suzuki-Miyaura reactions. The developed method was recyclable upto three cycles with moderate stability of catalyst. Thus, this study paves a way to develop an environmentally friendly method which offer waste to wealth concept.

IO-14 : Synthesis and Biochemically Methods of Some Lanthanide Complexes with Kynurenic Acid

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The compound of lanthanide ions with complexing or chelating biologically important kynurenic acid ligand to form coordination compound is an important area of current research. Less explored biologically important kynurenic acid ligand is allowed to react with solution of lanthanides perchlorates and attempt has been made to synthesize solid kynurenic acid complexes. These complexes are subjected to U.V visible spectroscopy, IR spectroscopy, TGA analysis, Mass Spectroscopy, Elemental analysis and antimicrobial activity of these compounds has been evaluated by standard methods and attempts have been made to correlate structural characteristic with properties of these complexes.

IO-15 : Antimicrobial Activities of Eu^{3+} Rare Metal Complex with Benzoxazole Derivative

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The combination of some rare metal ions with an important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide (BSPA) ligand to form coordination compounds is an important area of current research. Less explored biologically important 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide ligand is allowed to react with solution of some rare metal perchlorates and attempt has been made to synthesize solid 2-(1,3-benzoxazole -2-yl- sulfanyl)-N-phenyl acetamide complexes. These 2-(1,3-benzoxazole-2-yl-sulfanyl)-N-phenyl acetamide complexes are subjected to antimicrobial activity of these complexes has been evaluated by standard methods and attempts have been made to correlate structural characteristics with properties of these 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide complexes.

IO-16 : Silver Compound-Sensitized ZnO as an Efficient Sun Light-driven Photocatalyst for Effective Dye Degradation

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Nanosized silver compound- and silver metal-sensitized ZnO photocatalysts were synthesized, and their photocatalytic activities were evaluated under solar irradiation. The ZnO photocatalyst was synthesized through thermal decomposition of zinc peroxide. The surface-sensitized ZnO photocatalysts were obtained through adsorptive precipitation of silver compounds. The catalysts were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), diffuse reflectance spectra (DRS), FTIR spectroscopy and photoluminescence spectroscopy (PL). The XRD pattern confirmed that the synthesized ZnO is crystalline in nature and has a hexagonal wurtzite structure. SEM images revealed that the grain size and surface morphology of ZnO catalysts is not affected by the loading of sensitizers. The

photocatalytic activities of the catalysts were investigated toward the degradation of the crystal violet dye under solar irradiation. Dye mineralization was confirmed in terms of the chemical oxygen demand (COD). Silver metal- and silver iodide-sensitized ZnO function as efficient photocatalysts for dye degradation.

IO-17 : Marble Slurry Waste Material as Solid Support for Palladium-Catalysed Heck and Suzuki Reactions

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Solid supported catalysis is an excellent substitute to homogenous catalysis which offers many advantages mainly, recovery and recycling of the metal catalyst. As far as sustainability is concerned, solid-supported catalysts are highly recommendable for the demand of modern chemical industry. Marble slurry (MS) waste material from marble processing industries can facilitate cost-effective and environmentally sustainable catalyst support for metal catalyzed organic transformations. It is envisioned to use MS as catalyst support for palladium nanoparticles owing to its excellent adsorption capacity, large surface area and resistant to reaction conditions that can offer a waste-to-wealth concept. Mizoroki-Heck and Suzuki-Miyaura C–C coupling reactions are being very important in organic synthesis due to impressive outcome with high chemoselectivity under mild reaction conditions. Herein, Pd@MS catalyst was prepared by modest wet impregnation method and used for ligand-free palladium nanoparticles catalyzed Mizoroki-Heck and Suzuki-Miyaura coupling reactions. The prepared catalyst is found to be very efficient and facile with maximum TON 4.13×10^2 and TOF 10^2 h^{-1} with good to excellent yields in aerobic conditions. The catalyst was recuperated after each reaction and reused upto five catalytic cycles affording quite satisfactory stability.

IO-18 : Phytochemical Study and Biosynthesis of ZnO NPS of Carica Papaya (ZnO bCA NPs) Leaf Extract and its Stabilization Mechanism with Microbial Efficacy

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Carica Papaya is a herbaceous whose fruits, leaves, seeds and latex are used medicinally. Extracts of Carica Papaya leaf are wide and traditionally use in many diseases especially in dengue fever in recent time. This work presents the phytochemical study of leaf extract of Carica Papaya and identify the chemical constitution by specific chemical test. In this work, biosynthesis method was adopted for the synthesis of zinc oxide nanoparticles with the leaf extract of Carica Papaya (ZnO bCA NPs) was utilized for biosynthesis scheme. In antimicrobial efficacy, the improved antibacterial responses of the biosynthesized variants were obtained due to the higher rate of stabilization mechanism of the nanoparticles by the organic chemicals (terpenoids, Phenolic and steroids) present in the Carica Papaya leaf extract.

IO-19 : Tetrahydro-2-Naphthylamine Based Novel Azo Dye : Synthesis, Spectral Characterizations and Dft Studies

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The present study describes about the synthesis and characterization of a new series of azo dyes produced from 5,6,7,8-tetrahydro-2-naphthylamine. The aforementioned compounds are generated through the conventional diazotization of 5,6,7,8-tetrahydro-2-naphthylamine and coupling reactions with five different coupling components, including α-naphthol, β-naphthol, 6-bromo naphthol,and 8-hydroxy quinoline under suitable experimental conditions. The resulting azo dyes are characterized and confirmed using UV, FTIR, NMR, and mass spectral methods. For the selected azo dye, a latent fingerprint application was carried out. Additionally, computed and summarized DFT investigations of the synthesized azo dyes thereby discussed the NLO properties and its applications.

IO-20 : Facile Synthesis of Functionalized PMMA/TiO_2 Nanocomposites with Enhanced Antioxidant and Antibacterial Activity

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The functionalization of PMMA and the synthesis of its nanocomposites using a simple solution mixing technique are reported in this study. PMMA is functionalized with various amino acid groups and combined with a low amount of TiO_2 nanoparticles to create nanocomposites. The morphology was determined by SEM, average

particle size (50 nm) of TiO_2 nanoparticles was measured by TEM. The pore radius (14.47 A°) and specific surface area (157.89 m^2/g) of TiO_2 nanoparticles were measured by BET analysis. FT-IR and NMR analysis confirms the functionalization of PMMA. The antioxidant activity of functionalized PMMA and its nanocomposites have been analyzed by using 2,2 diphenyl-1-picryhydrazyl assay. The result revealed that functionalized PMMA (PMPA) shows maximum antioxidant activity. The bacterial inhibition against both gram-positive and gram-negative bacteria is effectively enhanced by an increase in TiO_2 nanoparticles concentration. The maximum zone of inhibition (ZOI) was recorded against E. coli ATCC 25922 (30 mm) and S. aureus ATCC 29213 (31 mm) and maximum inhibitory concentration (MIC) over E. coli (64 µg/ml) and S. aureus (32 µg/ml) by PMPA2. Functionalized PMMA nanocomposites that have been synthesised are potentially useful material for biological applications.

IO-21 : Photocatalysis : A Green Approach

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Air and water pollution pose a serious threat to the environment and personal health now a days. Getting a solution of much pollution is not an easy task. Generally, various dyes are found in industrial effluents, which ultimately enter the aquatic ecosystem and can create various environmental hazards. These effluents have very adverse and sometimes irreversible effects on animals and plants as well. The main purpose of waste water treatment is the removal of these toxic substances and colour and to make this water usable for industrial and domestic use. There are various methods like adsorption, osmosis, flocculation, etc. which have been used traditionally to remove these dyes from the water bodies, but these methods suffer from some or the other drawbacks. In recent years, Advanced Oxidation Processes (AOP's) like photocatalysis, photo-Fenton reaction, ozonation, sonolysis, etc. have emerged as successful techniques in combating against the problem of environmental pollution.

Photocatalysis is a promising technique for biodegradation and pollution control. Photocatalysis involves oxidation and reduction reactions with the help of photo-emitted charge pairs under visible light. Photocatalysis is essential as a green technology to clean up water and environmental detoxification via visible light-induced photocatalysis. It has various applications such as CO_2 reduction, organic contaminant degradation, removal of toxic ions and heavy metal ions, water-splitting, antibacterial, self-cleaning, etc. Therefore, design and development of novel semiconductor photocatalysts has received much

attention for these purposes. An electron-hole pair is generated on exposing a semiconductor to light. This hole-electron pair can be used for reducing and oxidising any organic pollutant, respectively. Hydroxyl radicals are generated by abstracting an electron from hydroxyl ion, which are strongest oxidising agent next to fluorine. This can completely mineralize the organic pollutants. The water or air contaminants are degraded to smaller products, which are either less harmful or almost harmless products. This technique can be considered an eco-friendly approach towards treatment of waste water or removing pollutant from air.

For the practical visible light applications of photocatalysis, semiconductors must be modified either by band gap narrowing or by preventing the electron–hole recombination by utilizing a strategy such as the surface and interface design of semiconductors, modulation of energy band configuration of semiconductors, manufacturing of solid-solution photocatalysts with continuous band gaps, and using nanocomposites.

IO-22 : Synthesis, Spectral Characterization and Anti-bacterial Evaluation of Schiff Base and its Metal Complexes

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Novel Schiff base nicotinic acid [1-(3,4-dimethoxy-phenyl)ethylidene]hydrazide was prepared by refluxing 3,4-dimethoxyacetophenone and nicotinic hydrazide in ethanol. And its Co (II), Ni(II), Cu(II) and Fe(III) complexes were prepared. The compounds were physiochemically characterized by infrared, 1H NMR studies, elemental analysis, electronic spectral studies, magnetic studies and XRD. Synthesized Schiff base ligand and its metal complexes were screened against *Staphylococcus aureus and Escherichia coli.*

IO-23 : An Overview of the Plant-based Synthesis of Copper Oxide, Titanium Dioxide and their Antimicrobial Potential

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In recent years, the green synthesis of nanoparticles has gained popularity due to its unique attributes. These approaches are facile, quick, one-step, economically cheaper, non-hazardous, advantageous,

energy efficient and environment-friendly over chemical and physical methods. Plants have natural active biomolecules termed phytochemicals, which act as reducing and stabilizing agents in the formation of nanoparticles. Numerous plant species have been used to synthesize various kinds of nanoparticles. Nanoparticles synthesized by metallic or metal oxides have the highest ranking among all nanoparticles due to their high stability, large surface area to volume ratio, high biocompatibility, and tunable preparation. Nanoparticles have miraculous contributions in the fields of agriculture, environment, medicine, pharmaceuticals, cosmetics, catalysis, electronics, and food. Copper is more effective than expensive metallic antimicrobials, and it has a broad range of antimicrobial activity, including that against bacterial species. Copper oxide has proven to be a good antimicrobial agent. Likewise, titanium dioxide is inexpensive and has good antimicrobial potential. A bulk of studies has been reported in literature regarding the antimicrobial potential of copper oxide and titanium dioxide, which makes these NPs suitable for pharmaceutical purposes such as biomedicine. The present work reviews the plant-based synthesis of copper oxide and titanium dioxide NPs and their antimicrobial potential.

IP-CYSA-01 : Effect of Heat Treatment and Forging on AISI 1028 Steel

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AISI 1028 is a type of medium low carbon steel which is used in widespread general-purpose applications. In the manufacturing of AISI 1028 steel heat treatment is a critical process, and it is essential to understand how it works and benefits it provides. Heat treatment is a process which not only improves the properties of metal but also increases the overall machinability. The present work illustrates study on effect of different types of heat treatment on AISI 1028 grade steel. The change in properties of AISI 1028 steel was studied before and after heat treatment at different temperatures and in different cooling conditions. Mainly annealing, normalizing, forging was carried out on the samples of AISI 1028 steel. The change in the microstructure and hardness after heat treatment were observed. Annealing was carried out @970°C with controlled cooling which resulted in formation of finer equiaxed grains, while the reduction in hardness of about 5.8% was observed. Normalizing the sample was done @915°C, the cooling was done by 2 different methods one sample was cooled by still air and second one was cooled by forced air. Forging process was also done on the steel @920°C and cooled in still air giving an average hardness of 130 BHN. Upto 33% reduction was achieved in forging.

IP-CYSA-02 : Synthesis, Spectro-Physicochemical Characterization, Antioxidant, Antifungal, DNA Cleaving and Binding Potency of Novel Schiff base Ligand and its Ni (II) and Cu (II) Metal Complexes

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Here, two biologically potent Nickel and Copper metal complexes have been synthesized by condensing their metal salts with, a novel Schiff base ligand 2-ethoxy-4-((5-methylthiazol-2-ylimino)methyl)phenol derived from 3-ethoxy-4-hydroxybenzaldehyde and 2-amino- 5-methylthiazol. These compounds were spectrochemically characterized by molar conductance, FT-IR, UV-Vis, mass spectra, 1HNMR, TGA and Electrochemical analysis. The coordination sites of the synthesized ligand are azomethine nitrogen and thiazoline nitrogen. The metal complexes showed distorted octahedral geometry having two chloride molecules. To support the experimental findings theoretical calculations by means of DFT at B3LYP level were incorporated. In addition, HOMO-LUMO energy gap (“E), molecular electrostatic potential (MEP) were also computed at the same level of theory. The radical scavenging potency of the synthesized compounds were analyzed by using DPPH, the Cu (II) complex gives better antioxidant activity than the others. The antifungal activity was tested against two fungal strains Aspergillus niger and Fusarium oxysporum, which depicts that the Cu (II) gives better antifungal activity. The DNA binding as well as cleaving activity was screened against pCAMBIA DNA, which results that the synthesized compounds show intercalative binding mode and the Cu (II) complex gives better DNA binding as well as cleaving ability than the Ni (II) complex and Schiff base ligand.

IP-CYSA-03 : Synthesis and Characterization of Nanoparticle from the Waste for Inhibition of Microbial Growth

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In this study, we delve into the intricate world of aerosol-associated microbial contaminants, embarking on a journey that encompasses the detection of microbial components in aerosol samples, the detailed characterization of bacteria and fungi within respirable suspended particulate matter, and the synthesis of graphene oxide (GO)-based nanoparticles for microbial inhibition. We employ a novel modified Hummers method to convert agricultural waste biomass, specifically coconut shell and pencil waste, into reduced graphene oxide (rGO) under mild operating conditions. The pilot study has been carried out at a suburban site in Agra over Indo-Gangetic basin. The Sub-urban area exhibited dynamic particulate matter fluctuations, reaching PM_{10} and $PM_{2.5}$ levels of 330.4 µg m^{-3} and 249.2 µg m^{-3}. The concentration of respirable suspended particulate matter and fine particulate matter was much higher than WHO, USEPA and NAAQs of India. Microbial analysis revealed varying concentrations, suggesting seasonal influences. The concentration of microbial components in ambient air was in the reported range. Microscopic analysis identified respiratory threats and protozoans in particulate matter. The biomasses yield of rGO with unique characteristics was obtained from the wastes (coconut shell and pencil) through an eco-friendly and cost effective route to produce graphene-based materials. The synthesized rGO was characterized and investigated by advanced techniques such as Field Emission Scanning Electron Microscopy (FE-SEM), EDX, X-ray Diffraction (XRD) and UV-visible spectrophotometer to scrutinize the structural intricacies of the synthesized nanoparticles. The antimicrobial efficacy of these nanoparticles is rigorously assessed through Kirby Bauer tests on clinically relevant strains, providing qualitative insights into their inhibitory potential. Field Emission Scanning Electron Microscopy (FESEM) displayed diverse microbial elements. GO inhibited Coccus by 93.7% and Aspergillus by 100%, while rGO inhibited E. coli by 88% and Brucella by 100%. The antimicrobial efficacy of GO-based nanoparticles is paving the way for innovative strategies in aerosol microbial inhibition across diverse applications.

IP-01 : Synthesis, Physicochemical Characterization, DNA Binding and Antifungal Screening of Novel Bioactive Ligand and its Co(II) and Cu (II) Metal Complexes

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A novel Bioactive ligand 4-chloro-2-(2,5-dimethoxybenzylideneamino)-5-nitrophenol derived from 2,5-dimethoxybenzaldehyde and 2-amino-4-chloro-5-nitrophenol. Its Co (II) and Cu (II) transition metal chelates were synthesized and physicochemically characterized by FT-IR, UV-Vis absorption spectroscopy, electrochemical studies (diffusion-controlled quasi-reversible) and thermogravimetric analysis (TGA). These compounds show moderate to good biological activity and exhibits potent antifungal activity against Aspergillus niger and Fusarium oxysporum. They also give better DNA binding efficacy (against pCAMBIA DNA). The Cu (II) metal complex gives better biological activity than the Co (II) metal complex and parent Bioactive ligand.

IP-02 : Exploration of Pyrazine-Infused Chalcones: Investigating their Synthesis, Electrochemical Characteristics, and Biological Applications

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Six novel substituted Chalcones were synthesized through the utilization of 2-acetylpyrazine and substituted aromatic aldehydes. The compounds underwent comprehensive characterization using Mass Spectrometry, 1H NMR, and FT-IR spectroscopy. Further analysis involved UV-Visible and fluorescence spectroscopy, as well as electrochemical property assessment via cyclic voltammetry. These compounds exhibited promising potential as anti-tubercular agents. Additionally, we investigated the antioxidant properties of select derivatives in the DPPH (2,2-diphenyl-1-picrylhydrazyl) assay, revealing significant scavenging abilities in the substituted derivatives enriched with pyrazine analogs. Furthermore, all compounds underwent evaluation for their antifungal and antibacterial activities.

IP-03 : Synthesis, Spectral Characterization and Antimicrobial Studies of Novel Schiff Base Ligand and its Chelates

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The effective bioactive Schiff base metal complexes were synthesized by condensing the novel Schiff base ligand 6,6'-(((1E,1'E)-1,3-phenylene bis (methaneylylidene))bis(azaneylylidene))bis(3-chloro-5-nitrophenol) with respective metal salts. These compounds were physicochemically characterized by molar conductance, FT-IR, UV-Vis, NMR, and electrochemical studies the coordination sites of the synthesized ligand are phenolic oxygen, and azomethine nitrogen which makes ligand monobasic bidentate. The Azomethine functional group(-CH=N) has been detected at 1656 cm^{-1} in FT- IR which has also been confirmed by NMR spectroscopy. Electronic spectra were also Observed in DMSO. π- π^*, n- π^*, and d-d transition (in Co (II), Ni (II), and Cu (II) metal complexes) confirm the transformation of the molecular environment and chelation of Schiff base ligand. The redox behavior of ligand and their chelates are investigated by cyclic voltammetry. The results indicate that the ligand and their metal complexes possess notable biological properties.

IP-04 : Biocomposite of Chitosan-Supported Ni(II)-Schiff base Complex as a Versatile Heterogeneous Catalyst for the Synthesis of Xanthones

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Xanthones are a unique class of oxygen-containing heterocyclic compounds with dibenzo-γ-pyrone motifs. The biological properties of xanthones can be altered/tuned by introducing different organic groups in different positions in the skeleton. Under this propensity, xanthones are a promising and attractive class of compounds for drug development. So, the development of a new protocol for the synthesis of such type of molecules have fascinated huge devotion.

In recent years, keeping in mind environmental compatibility, there has been a spurt in designing natural polymer-based heterogeneous catalysts for various organic transformations. Naturally occurring polymers are commonly accessible in abundance, economical, and non-toxic. Among various naturally occurring polymers, chitosan(CS) is the second most abundant natural polymer after cellulose.

In this perspective, a new biocomposite of chitosan, chitosan-supported di(pyridine-2-yl)methanone-Ni(II) complex, CS-DPM-Ni, is synthesized for the first time.[4] The biocomposite is thoroughly characterized by various physico-chemical techniques. The potential of developed catalyst was explored in the synthesis of xanthone derivatives. The synthesized xanthones were confirmed by ^{1}H and ^{13}C NMR studies.

IP-05 : Analysis of Inorganic Constituents of Medicinal Plant as Scientific Evidence for the Nutritive Values

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Metal plays an important role to introduce vital dietary nutrition to people. Understanding the availability of these metals is useful for plant physiology, food science and agricultural research. Entada rheedei has various traditional medicinal uses like treatment of jaundice, diarrhea, and musculoskeletal problems. It also showed the pharmacological activities like antioxidant, cytotoxic. Antiulcerogenic and molusccidal activities. The metals like Ca, Na, K & Fe are found to present in the seed kernel of Entada rheedei. These metals may form a complex with other plant proteins and phytochemical to produce metal complexes which has a role in different phytochemical activities and adds pharmacological value to the plant. By considering these ethnobotanical and traditional medicinal uses of this plant, the present research work is carried out to determine the availability of metal elements in this plant and their role in the medicinal property. Extensive research and development work is needed to increase the therapeutic and economic utilization of Entada rheedei.

IP-06 : Needle-shaped α-Ni(OH)$_2$ Nanoparticles Entwined and Embellished on Graphene Oxide : A Heterogeneous Catalyst for the Synthesis of Azines and the α-alkylation of Ketones

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Azines are a vital class of compounds with miscellaneous applications such as ion-selective optical sensors, conductive polymers, scaffolds for drugs, etc. Also, the α-functionalization of carbonyl compounds is one of the imperative methodologies for the C-C bond formation since the α-alkylated carbonyls are key intermediates for synthesizing numerous natural products, pharmaceuticals, and heterocycles. Several compounds containing azines and α-alkylated carbonyl scaffolds are used as antibacterial, anti-cancer, anti-hypertensive, anti-fungal, anti-tumour, anti-spasmodic, anti-diabetic drugs, etc. Therefore, there has been a great deal of interest in the creation of a new protocol for the synthesis of these kinds of molecules.

Graphene Oxide (GO) has served as an ideal support for the synthesis of heterogeneous catalysts due to its low cost, ease of synthesis, large surface area and amenability to surface engineering by chemical modification of various functionalities present on its edges and the surface.

In line with our continued pursuit of synthesising GO-based earth-abundant and cost-effective transition metal catalysts for organic transformations, and encouraged by the active role of α-Ni(OH)$_2$ NPs in hydrogen evolution reactions, and Ni NPs in alkylation of amines with alcohols, we herein report the synthesis of α-Ni(OH)$_2$ NPs adorned on GO, α-Ni(OH)$_2$-GO.

IP-07 : Synthesis, Characterization of Bis-Terpyridyl-Based Molecular Copper Complexes

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Terpyridine ligands are widely used in Chemistry and material sciences owing to their ability to form stable molecular complexes with a various metal ions. A series of different substituted terpyridine (tpy)-based ligands have been synthesized by Kröhnke method. The corresponding ligands were synthesized and fully characterized by elemental analysis, single-crystal X-ray crystallography, mass spectrometry, UV–VIS, ^{1}H NMR, and Fourier Transform Infrared (FT-IR) spectroscopy as well as by cyclic voltammetry (CV). Their binding behaviour was evaluated by complexing them with Cu(II) ion, which resulted in coordination compounds with interesting spectroscopic properties. Molecular modelling was carried out to study the interactions with DNA.

IP-08 : Synthesis, Characterization and Biological Activity of Novel Bioactive Imine Derivative and its Co(II), Ni(II), Cu(II) and Zn(II) Metal Complexes

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A novel imine derivative 6,6'-(((1E,2E)-1,2-Diphenylethane-1,2-diylidene)bis(azaneylylidine)) bis(2,4-dibromophenol) has been synthesized by simple reflux method, further the ligand is allowed to coordinate with Co(II), Ni(II), Cu(II) and Zn(II) metals, which in turn forms stable azomethine chelated metal complexes. Several analytical techniques such as UV-Vis., FT-IR, 1H-NMR, 13C-NMR, Mass spectrometry, electrochemical studies, thermogravimatric analysis etc., are used to analyze the physical and chemical properties of synthesized novel Schiff base ligand and its metal complexes. In addition to it computational studies are also been done to investigate the geometry and shape of the novel ligand and its chelated metal complexes. The synthesized compounds are found to be biologically active compounds as they show good antimicrobial activity against the investigated microbes i.e., Aspergillus niger and Fusarium oxysporum.

IP-09 : Analysis of Metal Ions Present in the Seed Karnel of Entada Rheedei Medicinal Plant

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Various parts of plants of Entada rheedei has various traditional medicinal uses like treatment of jaundice, diarrhea, and musculoskeletal problems. It also showed the pharmacological activities like Antioxidant, Cytotoxic, Antiulcerogenic and Molusccidal activities. The metals like Ca, Na, K & Fe are found to present in the seed kernel of Entada rheedei. These metals may form a complex with other plant proteins and phytochemical to produce metal complexes. These complexes may show different phytochemical activities. By considering these ethnobotanical and traditional medicinal uses of this plant. In the present work we planned to determine the availability of metal ions present in seed kernel of Entada rheedei plant and their role and its medicinal property.

IP-10 : Calcium Content and Wound Healing Property of Tridax Procumbens

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Tridax procumbens is a wild herb distributed through India, Nepal, and Nigeria is used to treat bronchial catarrh, dysentery, diarrhea, and inflammation. This plant was reported in Ayurveda to cure wounds using singly or different formulations. Traditionally the juice from leaves of T. procumbens has been used for healing dermal wound. Wound healing is a complex and highly regulated biological process to repair damaged tissues. Metal elements such as calcium, copper, iron, and zinc serve irreplaceable roles in various regulatory pathways of the human body and directly or indirectly affect the orderly wound repair process. Flame photometric analysis of Tridax procumbens reveals the higher content of Ca and K. Calcium is a key central regulator in wound healing. Calcium plays important role in the normal homeostasis of mammalian skin. Calcium serves as a modulator in keratinocyte proliferation and differentiation. Calcium ions are involved in various mechanisms such as stabilization of cell wall structures, acidic growth, ion exchange properties, and control of the activities of wall enzymes. Rich in calcium in this plant could be the reason for the healing of wound. Systematic investigation of metal-based study provides valuable guidance for future breakthroughs in wound treatment.

IP-11 : Synthesis, IR Spectral Studies and Biological Activities of Some Rare Earth Metal Complexes.

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Biologically active La(III), Sm(III) and Gd(III) Complexes were synthesized by using Furan-2-carboxylic acid (FCA) as ligand and were Characterized by elemental analysis and spectral measurements. Coordination of ligand atoms to the metal ion was deducted by IR spectral data. The in Vitro antibacterial screening of the free acid and its metal Complexes has been carried out against Escherichia Coli, Staphylococcus aureus Antifungal activities of all the synthesized compounds were screened for in vitro growth inhibitory activity against Aspergillus furnirgatus and Aspergillus niger. It is observed that Antimicrobial activities of ligand increase on cordination with metal ion and show more promising activity than the Corresponding free acid.

IP-12 : Synthesis, Characterization and Biological Activity of 3d-Transition Metal Complexes from Pregabalin and Terbutaline Sulphate System

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Terbutaline sulphate and pregabalin as a ligand have been used to create the bivalent metal chelates of manganese, cobalt, nickel, copper, and zinc. Elemental analysis and spectrum methods including molar conductance, IR, UV, magnetic moment, ^{1}H NMR, ^{13}C NMR, and mass studies were used to characterise the compounds. Pregabalin and the ligand terbutaline sulphate coordinate with the metal ion. The geometry of each complex is octahedral. The ligand is crystalline in nature, but all of the complexes are amorphous, according to XRD data. The disc diffusion technique was used to look at the antifungal properties. The complexes of cobalt(II), nickel(II), copper(II), and zinc(II) exhibited favourable activity in comparison to the complex of ligand and manganese(II). The antibacterial properties have been assessed in relation to Escherichia coli and Staphylococcus aureus. Compared to other compounds, the nickel(II) complex exhibited more noticeable action. The chelates of manganese, cobalt, and zinc showed a very good proportion of inhibition over the ligand in their antioxidant activity. When compared to the conventional medication, the findings revealed modest activity. Additionally, nickel(II) complex and ligand molecular docking using CDK2 protein is examined, and it is shown that nickel(II) complex has a higher binding affinity than ligand.

IP-13 : Synthesis, Characterization and Biological Activity studies of Chromium (III) Complexes of a New Schiff Base Ligand

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Schiff bases have been extensively studied for their synthetic flexibility, Selectively, and sensitivity to the central metal atom, their structural similarity to natural biological compounds and the presence of azomethine group (-N =CH-) Which is important in the biological elucidation of transformation and racemization reaction mechanism Schiff bases are an important class of organic compounds which have a wide range of application in the fields of analysis, biology and inorganic chemistry.

In Cr (III) Complex with the new Schiff bases of the type p-HBAT ($C_{10}H_8N_2OS$) and p-HBAMP ($C_{13}H_{12}N_2O$) were prepared by reaction of p-hydroxy benzaldehyde with 2-aminothiazole/2-amino-6-methyl pyridine have been synthesized and characterization with the help of elemental analysis IR, and electronic spectral data. Comparative bacterial behaviour of Schiff bases with their Cr (III) Complexes have also been studied against E coli and S. aureus.

IP-14 : Insights into the Effect of Halide Enriched ZnO Synthesized using Tetrabutylammonium Halides toward Photocatalytic Degradation of R6G

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Photocatalysis, an advance oxidation process (AOP) is a promising technology for the removal/degradation of organic pollutants from wastewater. Anion doping is known to be a superior way to attain high carrier concentration, mobility and it greatly affects the light absorption capability of materials.

In the present work, ZnO and halide (Cl, Br, and I) enriched ZnO samples have been synthesized by polyol method. Halide enriched zinc oxide (ZnO-X) were obtained when synthesis was carried out in the presence of tetrabutylammonium halide ($(C_4H_9)_4N^+X^-$, X=Cl, Br, and I) salts. X-ray results reveal that the halide ions seem to occupy the oxygen vacancy sites as well as interstitial sites of the ZnO lattice increasing the cell volume and strain along the c-axis. Microspheres are observed in the scanning electron micrographs with the size ranging between 170 and 385 nm. Photocatalytic activity of the synthesized samples was tested under UV light irradiation for the decomposition of Rhodamine-6G dye. The halide enriched ZnO samples show higher rate of dye degradation compared to pristine ZnO attributable to their higher bandgap leading to a decrease in the recombination reactions of the electron–hole pair and higher light absorbing ability. ZnO-Br is seen to exhibit the highest rate of degradation due to higher bandgap, light absorbing ability and predominance of (101) facet in the lattice.

IP-15 : An Overview of Lignocellulosic Nano-Adsorbents for Heavy Metal Removal from Industrial Effluents

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This article provides an overview of heavy metal pollutants with description of some most commonly used methods for removing them from variouseffluents of industries; including textiles, paints and pigments, battery manufacturing, metal mining, nuclear power plants, tanneries, paper and pulp, etc. To provide a background of the materials utilised for heavy metal removal from waste water, a literature review of the synthesis of lignocellulosicnano-adsorbents using various approaches such as chemical, biological, and physical methods was done. The study aims to provide a comprehensive overview on relevant published work on adsorption-based heavy metal pollutant removal from industrial waste water, as well as a background and summary of current developments in nano-adsorbents derived from agricultural waste materials.

IP-16 : Aluminium Alkoxides as Unique Synthons for Inorganic Ring Systems

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Increasing interest in the chemistry of metal (hetrometal) alkooxides, perused actively in our laboratories, derives from the accessibility of the soluble forms oligomeric characteristics, interesting structural as well as bonding and ease of hydrolysis with volatile side products, a property that has been frequently exploited not only to utilize them as synthons for mixed ligand, mixed metal species but also for low temperature synthesis of oxide ceramics.

One of the most interesting problem, however, in the application of metal alkoxides for the preparation of ceramics remains the need to maintain the stoichiometry of the heterometallic species during the course of hydrolysis process of during their transition into the gaseous phase. Therefore, our recent research has drawn pointed attention to the synthesis and characterization of heteroleptic derivatives where the labile alkoxy bridging ligands are replaced by ligandswhich are more stable to hydrolysis or thermal treatment such as glycolate, β-diketonates, carboxylates, alkoxyalkanoates or alkanol aminates.

Reaction of aluminum isopropoxide with acetylacetone in 1:1 molar ratio yields a unique derivative $[(acac)_2Al(\mu\text{-}OPr^i)_2Al(OPr^i)_2]$ containing aluminium (III) atoms in 4- and 6- co-ordination states. Further reaction with glycol in 1:2 molar ratio under mild conditions yield derivatives of the type $[(acac)_2Al(\mu\text{-}O\text{-}G\text{-}O)Al(O\text{-}G\text{-}O)]$ [G = $-(CH_2)_2-$,$(-CH_3-CH_2-CH_2-)$, $-(CH_3)CH-CH(CH_3)-$, $-C(CH_3)_2-C(CH_3)_2$, $-C(CH_3)_2-CH_3-CH(CH_3)-$ and $-(CH_2)6-$] containing bridging glycolate rings. All these derivatives are moisture sensitive white shining solids and are soluble in common organic solvents. The spectral (IR,^{1}H,^{13}C and ^{27}Al) studies reveal the presence of 4- and 6- co-ordinated aluminum sites. TGA/DTA and FAB mass analyses indicate interesting variations.

ORGANIC CHEMISTRY SECTION

Sectional President's Address

Synthetic Strategies for the Construction of Building Blocks : C-H Functionalisation

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Construction of bioactive heterocyclic building blocks is in the centre to organic chemistry in past, present and future as well. Numerous methodologies have been established for preparing all kinds of heterocyclic compounds. However, traditional cross couplings require preactivated components such as organo-metallic reagents and organic halides as a starting material. Moreover, the reactions that activate the carbon-halogen bonds of aryl halides generate significant undesired products, creating environmental issues and a major drawback in terms of atom economy, environmental and economic impact. The C-H bond activations with subsequent functionalisation insitu offer an innovative method for introducing functional groups. Theoretically, multistep synthesis can thus, be changed into single-step synthesis, permitting direct access to target assemblies even at late steps of a synthesis and avoiding waste formation. Recently, transition metal-catalyzed cross-dehydrogenative coupling (CDC) reactions have been recognized as one of the most effective approaches for rapidly synthesizing carbon-carbon and carbon-heteroatom bonds. Widespread research into carbon-hydrogen (C-H) bond activation processes through transition metal catalyzes has significantly enhanced our understanding of how to effectively cleave and functionalize inactive C-H bonds. Carbene insertion, CH-NH, CH-X coupling, functionalisation of active methylene of heterocycles followed by annelation of various bioactive entities through decarboxylation, insertion will be discussed.

OIL-01 : Greener Technologies for Pharmaceutical Industries

K. R. Desai

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The demands for green and sustainable synthetic methods in the fields of pharmaceutical industries, healthcare and fine chemicals combined with the pressure to produce these substances expeditiously and in an environmentally benign fashion, pose significant challenges to the synthetic chemical community. Green chemistry protects the environment, not by cleaning it up but by inventing new chemistry and new chemical processes that do not pollute.

In my talk I will mainly focus on Green Brominating technique, Green Diazotization technique, Green Reduction, Oxidation and many others Green methods This may be by changing catalyst, solvent or source of energy, Biocatalyst etc.

Moreover, to overcome the difficulties arising from conventional methods, there is continuous growing research interest to improve the reactions either in basic research or in technology in context to green chemistry. Over the years, there is a tremendous improvement in chemistry to drive the reaction towards green chemistry.

Also focus on increasing selectivity, aiming for 100% atom efficiency and replacing Stoichiometric reagents, with heterogeneous reusable catalyst. The nano-sized particles increase the exposed surface area of the active component of the catalyst, thereby enhancing the contact between reactants and catalyst dramatically and mimicking the homogeneous catalysts.

OIL-02 : Computational Quantum Chemical Study, in Silico ADMET and Molecular Docking Analysis, in Vitro Biological Evaluation of Some Flavanoids as Potential Neuroprotectants

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Neuroprotectants are well known for treating dementia which directly affects the brain and involves the failure of nerve cells. Since in every 3 seconds a person on this planet develops dementia and drugs available for these treatment are limited. Ayurveda therapy, Generic Medicine therapy and Homeopathy therapy are only ways to treat dementia. Numerous studies support that herbal medicines are amongst the most commonly used group of treatments among Complementary and alternative medicine(CAM) for dimentia. The study on interactions of components of herbal medicines in comparison to conventional medications, is limited and insufficient data concerning the possible hazards of herbal consumption is available. Drug likeness assessment of selected flavanoids as active ingredients and ADMET pharmacological model is tested here because herbal extracts are notably used for dementia. A Computational quantum chemical study and molecular docking analysis, in vitro biological evaluation of some flavanoids present in herbal formulations as potential Neuroprotectants in prediction Of enantioselectivity of flavanoids against proteins responsible for dementia is discussed here.

OIL-03 : Preparation and Application of $CoFe_2O_4@SiO_2$-$HClO_4$, as A Novel Heterogeneous Acidic Magnetic Nanocatalyst for the Synthesis of Pyranopyrazoles via MCR's under Solvent Free Condition

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The science and technology of catalysis is of great significance as it affects our daily life. Recently, we have developed a number heterogeneous silica supported catalysts which showed improved efficiency for several important organic reactions. In this work we report the synthesis and identification of $CoFe_2O_4@SiO_2$-$HClO_4$ as a novel and green nanomagnetic solid acid catalyst and its characterization by XRD, FT-IR, TGA, SEM-EDS, Magnetic Hysteresis, TEM and surface area measurements. Moreover, an easy method of its preparation and magnetic recovery of nanoparticles follows the green chemistry principle. Furthermore, we have reported an efficient and eco-friendly three-components protocol for the synthesis of pyrano[2,3-c] pyrazoles via tandem reaction of aldehyde, malononitrile and 5-methyl-2,4-dihydro-3H-pyrazol-3one using $CoFe_2O_4@SiO_2$-$HClO_4$ as a magnetically recoverable nano-catalyst under solvent-free condition and microwave irradiation, which added more value to a greener approach. The product distribution pattern with the variation of different reaction conditions such as reaction temperature, reaction solvent, mole ratio, effect of non-conventional energy source, concentration of catalyst and reaction time. The $CoFe_2O_4@SiO_2$-$HClO_4$ nano-catalyst brought notable organic transformations by its ability to enhance rates of organic reactions, high catalytic activity, magnetic recovery and reusability of the catalyst, which makes the present protocol an attractive. Some important features of this catalyst were found, including short reaction times, excellent yields, lower loading of the catalyst, easy workup, and recyclability. It was showed that the obtained catalyst exhibited the catalytic stability and the reusability for a minimum of five times without any noticeable decrease in its catalytic activity. All synthesized compounds were characterized by spectral methods such as ^{1}H & ^{13}C-NMR, FTIR, Mass spectral data. It is expected that the fundamental knowledge discussed in the work will serve as a powerful tool for carrying out Green Chemistry.

OIL-04 : Synthetic Approach of Different Heterocycles Fused Ring System : Their in Vitro Antimicrobial, Anti-Mycobacterium, Anti-Malerial, Anti-Oxidant and Anti-Protozoal Evaluations as well as and in Silico Molecular Modelling

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The lack of efficacy, development of resistance and tolerance, unexpected toxic side-effects and incompatibility with other drugshas been found in vast majority of drugs available in today's market. This provide an urgent need to synthesize the novel biologically active safe candidates which are expected to meet current medical need with improved potency, less toxicity and fast acting. The synthesis ofheterocyclic hybrids has been recognized in the field of medicinal chemistry because of their wideapplicability. This provides a great opportunity to synthetic chemists for the synthesis of new moieties possessing lower cytotoxicity and with better antimicrobial potency.The ability of various heterocyclic compounds to undergo different chemical reactions has made them important for molecule planning, such as, 1,2,4-triazole, 1,3,4-oxadiazole, chalcone, pyrimidine, Manich base, Schiff base, etc., using various amino benzimidazoles, qunaxolines, benzothiazoles etc. with enormous biological potential. All the newly synthesized scaffolds were subjected to in vitro anti-bacterial (S. aureus, S. pyogenes, E. coli, and P. aeruginosa), anti-fungal (C. albicans, A. niger, and A. Clavatus), anti-mycobacterial (M. tuberculosis H_{37}Rv), anti-malerial(P. falciparum) anti-tryponosomal (T. cruzi) and anti-leishmanial (L. Mexicana) activity.Moreover, short-term in vivo model on Trypanosoma cruzihas also been studied with one of the derivative containing 1,3,4-oxadiazole. We have also carried out in silico molecular docking study of our targeted compounds with different PDBs as

biological target to understand binding interaction of targeted compounds. The molecular dynamics (MD) simulations are performed for up to 20 ns simulation time investigating the stability of a ligand–protein complex.

OIL-05 : Syntheses of Biologically Potent Scaffolds Employing Triarylphosphine Based Reagents

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Triarylphosphine based reagents plays important role organic and inorganic synthesis and specifically in synthesis of biologically potent scaffolds, synthesis of organometallic complexes&in the generation of potential agrochemicals. Extensive synthetic explorations of these reagents have already been made by various researchers around the globe, through the involvement of a number of reactions such as Mitsunobu's reaction, Wittig reaction, Appel reaction, Deoxygenation, Sulphonation etc. & formation of complexes with transition metal complexes etc.

In search for potential scaffolds, our group have been synthesized various kinds of structurally diverse biologically potent scaffolds starting from various kinds of starting materials employing Triarylphosphine based reagents. In the present talk, I will be discussing some of our efficient and novel synthetic strategies for the syntheses of biologically potent scaffolds such as carbamates, dithiocarbamates, xanthates, S,S-dialkyl carbonates, trithiocarbonates, carbazates, dithiocarbazates, substituted ureas & α-amino nitriles employing triarylphosphine based reagents.

OIL-06 : Green Synthesis of Diverse Macrocyclic and Heterocyclic Library as Potential Biological Agents

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Macrocyclic and heterocyclic compounds are the most often encountered scaffolds in chemical biology and are essential for the human well-being. The remarkable ability of nuclei of these compounds to serve as effective pharmacophores has largely contributed to their unique value as traditional key elements of many drugs. Certain possible modifications on the macrocyclic and heterocyclic moieties may lead to new compounds with better biological profiles. Heterocyclic and macrocyclic rings are commonly found structural units within the frame work of a variety of natural products, which is the main reason for the growing importance of such types of compounds. Among the top prescription drugs there are many macrocyclic and heterocyclic compounds. Therefore, methods for the synthesis of such systems are of significant interest. The environmental protection has become a global concern and the synthetic organic chemists are searching the ways of developing and applying more efficiently and environmentally benign strategies for future sustainable growth. One of the thrust areas for achieving this target is use of green synthesis. The salient features of green synthesis are enhanced reaction rates, easy workup, high yields, operational simplicity, greater selectivity and experimental ease of manipulation, low cost and economy. In view of these advantages of the above environmental benign approach and as a part of our ongoing research program towards the non-traditional methods, the concept of green synthesis has been adapted for the rapid and efficient synthesis of diverse macrocyclic and heterocyclic library.

OIL-07 : Current Integrated Approach for the Search of New Bioactive Leads from Medicinal Plants

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Recently, new drug discovery program is facing serious challenges due to decreasing in number of new drug approvals coupled with exorbitant rising cost. Search of the new chemical entities by use of combinatorial chemistry has provided new hope, but even this scientific approach has failed to improve the success rate in new drug discovery. In the last few years, there has been an exponential growth in the field of discovery of new drug from plants and gaining popularity both in developing and developed countries because of their biocompatibility and less side effects. Some of these plants derived substances that can either be directly used as drugs for therapeutic purposes or may be precursors/ lead molecules for the synthesis of semisynthetic drugs. Medicinal plants continue to be an important source of new therapeutic aid for alleviating ailments of humankind. Keeping in view the importance of medicinal plants in the discovery new therapeutic agents and our continuous work to search the new leads in parasitic area, recently, in our laboratory we have isolated and identified the many

bioactive lead molecules viz. anthraquinones, spirostan saponins and triterpenoids from medicinal plants by using various separations and spectral techniques. Current integrated approach toward the discovery of new bioactive leads from medicinal plants will be discussed in detail during the presentation.

OIL-08 : Nucleophilic Sulphur Enabled Assembling of S, N, C in A Row and Umpolung C-N Bond Formation in Water Medium

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Assembling S and N in a row with 'C' bonds in water can access diverse structural designs. Accordingly, the presented reaction protocols pave the way for assembling distinct bond structures with hetero atoms in a novel product using no catalysts and additives. The nucleophilic activation of sulfur is manipulated to insert elemental sulfur in the organic framework, followed by distinct S-N bond formation. The post-modification of the nitromethyl group to an electrophilic carbon center paved the way for 'umpolung' C-N bond formation. The concomitant further reaction induces the framework's distinct bond, enabling the desired product in a single step. The method presents direct access to the unusual assembling of different heteroatoms initiated by nucleophilic sulfur activated by dissolved amine in water.

OO-CYSA-01 : A Sustainable Approach to Green Synthesis of Substituted-3-Acetylcoumarin using DABCO Catalyst : A Physical and Spectral Evidence

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Derivatives of 3-acetylcoumarins have intriguing many useful applications such as fluorescence brightener, anti-breast cancer, antimycobacterial, anti-inflammatory and analgesis, etc. According to previous studies, 3-acetylcoumarins have been synthesised using various catalysts having advantage and disadvantage. Herein, we have come up with more efficient, green and user-friendly approach in synthesis of library of 3-acetylcoumarins from easily available ethylacetoacetate (EAA) and o-hydroxyaldehydes in water at room temperature has been achieved in excellent yield by modifying novel methods. Hence, the experimental method is very simple and more economic, no further purification required and the experimental conditions have been optimized in gram scale. Also, we have examined the reaction under physical and spectroscopic aspects showed good results too. The reusability of catalyst resulted quite excellent yield at shorter time, also the byproduct ethanol formed in the reaction was distilled out. All products were identified by comparison of their physical and spectroscopic data.

OO-CYSA-02 : Copper Catalyzed Intermolecular Heteroannulation Reaction between O-acyl Oximes and 4-thiazolidinones for the Synthesis of 2H-pyrrolo[2,3-d]thiazole

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An intermolecular copper catalyzed heteroannulation reaction using Csp^3-Csp^3 radical coupling approach has been accomplished to synthesize 2H-pyrrolo[2,3-d]thiazole. C-C coupling between 4-thiazolidinones and O-acyl oximes under Cu catalyst further cyclizes to the target molecule “Thiazolidine-Fused Nucleus.” This unified method offers access to novel fused heterocycles with pyrimidines bearing 4-thiazolidinone in moderate to higher yields. The optimization study includes various copper catalysts, oxidants, bases, and solvents at different temperatures.

OO-CYSA-03 : Ultrasonication-Assisted Synthesis of Benzo[d]imidazo[2,1-b]thiazole Scaffolds Catalyzed by Hydromagnesite sheets Crowned with Cobalt-Ferrite Magnetic Nanoparticles: A Green and Sustainable Approach with In silico and Quantum Computational Studies Insights

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The present work elicits an ultrasonication-assisted strategy utilizing pioneering hydromagnesite sheets embracing cobalt×ferrite magnetic nanoparticles ($CoFe_2O_4$×HMS) as an environmentally benign catalyst leading to the synthesis of pharmacologically significant benzo[d]imidazo[2,1-b]thiazole scaffolds. This catalytic approach for the synthesis of biologically active synthetic equivalents was achieved through an A^3-coupling strategy under aerobic conditions. The fascinating features of this protocol include higher product yield (up to 94%) with a miniature reaction time and modest catalyst loading

as demonstrated by higher ecological compatibility and sustainability factors. The synthesized nanocomposite was thoroughly characterized using various spectroanalytical techniques, including PXRD, FE-SEM, EDAX, HR-TEM, Raman, FT-IR, TGA-DTA-DTG, magnetic studies, and nitrogen porosimetry analyses. The structures of synthesized compounds were accomplished through FT-IR, ^{1}H NMR,^{13}C NMR, mass, and elemental analysis data. The scalability of the reaction protocol to a multi-gram scale enhances its potential industrial applications.

The virtual screening of synthetic moieties was performed to ascertain the in silico selectivity and binding affinities against biological targets. Furthermore, a quantum computational study was computed at the B3LYP/6-311G++(d,p) level of theory to investigate the density functional theory-based chemical reactivity parameters and HOMO–LUMO energy gap of the synthesized derivatives. These studies pave the way for in vitro and in vivo testing of the synthesized derivatives as potent inhibitors with an improved pharmacological profile against biological receptor agonists.

OO-CYSA-04 : Ionic Liquid an Exceptional Reaction Medium for the Room Temperature Synthesis of Substituted Pyrimidones via Biginelli Pyrimidone Synthesis

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We report the syntheses of derivatives of pyrimidones by Biginelli pyrimidone synthesis, uniquely made possible with Ionic Liquid. The protocol provides highly efficient and selective route for the synthesis of structurally diverse pyrimidones under milder reaction conditions. Our conditions tolerate differently substituted aldehydes and ketones offers products in synthetically useful yields. Furthermore, for the first time camphor, benzil, benzoin and ethylacetoacetate were utilized for the Biginelli reaction and to our delight the resulting pyrimidones were obtained in excellent yields.

OO-CYSA-05 : Arylsulfenylation of 4-thiazolidinone with Elemental Sulphur and Aryl Halide : C-S Coupling

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The generation of carbon–sulphur (C–S) bonds is a crucial step in the quest to create valuable organic entities due to their widespread applications in various biological systems. Alongside, 4-thiazolidinone is considered a highly proficient heterocyclic scaffold, constituting tremendous pharmacological properties which have driven us to develop a one-pot synthesis of thioarylated 4-thiazolidinones with elemental sulphur and aryl halides using copper(I) iodide as catalyst. The basic nucleus 4-thiazolidinone was generated through trivial synthesis. The method has a broad substrate scope with various substituted aryl halides. Optimisation has been carried out through varieties of catalyst loading, base, temperature and solvent. The reaction is highly efficient and affords thioarylated 4-thiazolidinones in good yields with broad functional group tolerance.

OO-CYSA-06 : Fluorine Effect on Conformation of α/β hybrid peptide

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Protein secondary structures are extensively stabilised by non-covalent interactions. Substitution of hydrogen atom with fluorine in drugs shows improved stability and cell permeability. This method is even used to the construction of peptides containing one or more fluorine atoms on the side chains of non-natural amino acids. Although fluorine and hydrogen atoms are about the same size, their electronegativity is quite different. These results modified peptide folding pattern and can have an effect on the peptide overall shape. The position of the fluorine substitution may affect the peptide overall structure and variations in dihedral angles.

In this work, we illustrate the fluorine effect on conformation of short hybrid peptide. NMR, SC-XRD, and CD studies are used for synthesis, characterization, and conformational analysis.

OO-CYSA-07 : Synthesis, Characterization in-Silico and in-Vitro Diabetic Screening with Various Biological Assays of Thieno(2,3-d) Pyrimidine based Isoxazole Derivatives

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The goal of our research was to create new thienopyrimidine based isoxazole derivatives (6a–j), analyze their pharmacokinetic studies, molecular docking studies and anti-diabetic screening by using various biological assays such as MTT assay, glucose utilization assay and lipid peroxidation assay. The thieno[2,3-d]pyrimidine based isoxazole derivatives have been synthesized by reacting chalcone derivatives with hydroxylamine hydrochloride and sodium acetate in methanol (6a–j). IR ^{1}H NMR, ^{13}C NMR, and Mass spectra were used to evaluate the newly synthesized compounds. In the present study, in-silico predictions of pharmacokinetic parameters such as Absorption, Distribution, Metabolism, Excretion and Toxicity have been performed. Docking studies of all the synthesized compounds were carried out against the insulin receptor tyrosine kinase 1ir3 protein with the help of Auto Dock 4.2 Suite software. The docking study showed that compound 6c has good binding affinities. Further in-vitro anti-diabetic activity was observed with various concentrations of synthesized compounds.

OO-CYSA-08 : Calorimetric, Spectroscopic Human Serum Albumin Binding Studies and In vitro Antiviral Studies of Synthesized Dipyridodiazepinone Derivatives

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Present study has been aimed to develop novel dipyridodiazepinone derivatives via amination, amidation and cyclocondensation. All the synthesized compounds were characterized using spectral techniques. Further, binding interaction of the synthesized derivatives with human serum albumin (HSA) was studied using isothermal titration calorimetry (ITC) in combination with fluorescence spectroscopy. Furthermore, drug-protein binding interaction was evaluated by ^{1}H-^{15}N HSQC NMR. Later, molecular docking and molecular dynamic simulation studies were also performed to validate their binding potential with HSA. Lastly, in vitro antiviral activity of compounds was examined against HIV-1 reverse transcriptase.

OO-01 : Microwave Mediated Organic Reaction : A Convenient Approach for Rapid and Efficient Synthesis of Biologically Active Betti Reaction

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Betti reaction is a typical Mannich reaction, is one of the most important fundamental carbon–carbon bond-forming reactions in organic chemistry. The optical Betti base isomers are valuable ligands in asymmetric synthesis. Recently, the importance of Betti bases was well established in pharmaceutical chemistry because of their bioactivities, including anti-bacterial, antipain, antihypertensive and bradycardiac activities. The new type of Betti bases were synthesized by green method in good yield from the three component reaction of 1H-indazol-6-amine, and substituted Aryl aldehyde. five new compounds have been synthesized by this method. Which take place under solvent free method five compounds were synthesized. Synthesized compounds characterized by FT-IR Spectra, ^{1}H NMR spectra, and Mass spectra.

OO-02 : Synthesized 1,3,4-Oxadiazole, 1,3,4-Thidiazole,1,2,4-Triazole & their Derivatives shows Potential Anti-Cancer Drug Activity Targeting EGFR Kinase Domain Drug Target

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In our research we synthesized about twenty-four compounds of 2-alkyl/aryl substituted & 5-amine substituted 1,3,4-Oxadiazole, 1,3,4-Thidiazole, 1,2,4-Triazole & their derivatives. In vitro & In Silico studies we find influential antimicrobial activity of these molecules. Literature survey shows diverse biological activity of these derivatives containing symmetrical hetero ring containing, O, S & N hetero atoms. To find out their anti-proliferative effects associated with mechanisms, such as inhibition of growth factors, enzymes, kinases and others, deserve attention virtual screening of these molecules has been done which is entitled as Molecular modeling and docking studies of novel 24 compounds targeting EGFR kinase domain drug target towards finding their potential to act as anti-cancer drug like small molecule based on SBDD. The activity of these compounds was tested on drug target (PDB ID: 1M17) Epidermal Growth Factor Receptor tyrosine kinase domain with 4-anilinoquinazoline inhibitor erlotinib.

Docking results of these compounds targeting EGFR kinase domain (PDB ID: 1M17) for anticancer activity was tabulated as their Binding Energy in Kcal/mol& Predicted IC50 value. ADME parameters & Toxicology profile of these synthesized compounds are also studied. All the docking studies are done using AUTODOCK 4.2 version and the images are rendered using

Accelry's Discovery studio visualizer v4.0 interface. Best molecules are TDA-A-2 & TDA-A-1, TDA-D-2 represents it's 2D,3D, surface interaction with EGFR. In our synthetic library we tried to synthesized small molecules which can acts as an API which promote, motivate us to synthesized these molecules containing 1,3,4-Oxadiazole & 1,3,4-Thidiazole ring. In future they can be used to cure various types of cancer cells. Day by day cancer patients number are increasing due to over use of agrochemicals in food products. In silico study of these molecules reveals that they showed potent anticancer activity.

OO-03 : Exploring Isocyanide Organic Chemistry Beyond Conventional Flasks : Our Recent Progress

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Isocyanides, known for their historical importance in the field of organic chemistry, have found applications in both academic research and industrial contexts. Among the various stable divalent carbon nucleophiles, isocyanides stand out due to their exceptional ability to form multiple bonds on the terminal carbon atom. However, the incorporation of isocyanides into diverse areas of organic chemistry offers an exciting opportunity to explore uncharted chemical territory and potentially discover novel lead compounds. Nevertheless, this pursuit remains a significant challenge. In this presentation, I will discuss our recent progress in merging isocyanide chemistry with organic electrosynthesis, resulting in the synthesis of a wide range of medically valuable molecular frameworks (see the schematic references.

OO-04 : Fluoro Capsulated Benzylidene Schiff Bases: Synthesis, Spectral Study (^{1}H NMR, ^{19}F NMR, IR, Mass) and Screening their Microbial Properties

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Fluorine moiety shows feasibility in various metabolic processes and thus can be employed as a building block for the synthesis of new motifs. Multifaceted biological activity of acyl hydrazone accompanied with eases synthetic reaction between carbonyl carbon and hydrazide. Acyl hydrazides on getting fused with heterocyclic nucleus forms another peculiar molecule of high biological importance. Number of therapeutics utility of such compounds unveils by chemical moiety containing hydrazides. Among it some of the critical application are analgesic, antioxidant, cancer and for medicament of infection, treatment of Schizophrenia, hypertension. The chemical structures of synthesized fluoro based acyl hydrazone schiff bases were ascertained by FTIR, ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, Mass spectra and Elemental composition. Thermal study concluded its stability in vast temperature range so a variety of physical properties can be assessed. The synthetic motif was also subjected to test for their antimicrobial activity against six strains. As per the result Schiff base comprising hetero-atom displayed strong potential against the tested microbes and other scaffolds display moderate activity.

OO-05 : Photochemistry of 2,4,5-Trisubstituted-1-Hydroxy Imidazole Derivatives

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Imidazole derivatives are known to be potentially biologically active molecules. Initially imidazole derivatives are employed in agriculture as potent herbicide. Later it has been reported to be having potential anti-fungal activity to be employed on the body and not to be consumed due to toxicity. Many anti-fungal agents based on imidazole nucleus are in the market. 1-hydroxy imidazole derivatives are not explored much. 2,4,5-Trisubstituted-1-hydroxy imidazole derivatives were synthesized from easily accessible starting materials. Some of them are quite photo-active. A detail study on their phot-activity in particularly exposure to sunlight has been studied. Thus, this paper deals with the photo-chemical aspect of the synthesized imidazole derivatives.

OO-06 : Optoelectronic and Charge Transport Properties of Benzotrifuran (BTF) based Organic Molecules

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The key motive of the present work is the detailed study of charge transport and optoelectronic properties of Benzotrifuran (BTF) based organic molecules for organic electronic devices. To predict the desired properties, Density Functional Theory (DFT) calculations were performed on BTF based organic molecules. Time Dependent-Density Functional Theory (TD-DFT) is used to determine the absorption properties and the results are compared with corresponding known experimental results. Frontier molecular orbitals (FMOs) i.e.; Highest occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO), Hole Extraction Potential (HEP), Electron Extraction Potential (EEP), Ionization potentials (IP), Electron affinities (EA) and Reorganization energies (λ) of all the isomers are investigated. All the studied organic molecules are having low electron (λe) and hole (λh) reorganization energies and hence they can be used in organic electronic devices.

OO-07 : Water Extract of Piper nigrum Seed Assisted Synthesis of Iron Nanoparticles and Reduction of Various Nitro Compounds by $NaBH_4$ in the Presence of FeNPs as a Catalyst

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An attempt has been made for eco-friendly synthesis of iron nanoparticles by water extract of Piper nigrum seed. Formation of FeNPs and their morphology was confirmed by using different advanced characterization techniques such as UV-Visible spectroscopy, XRD and FE-SEM images of FeNPs. Further we wish to report for the first time reduction of various nitro compounds to corresponding amines by $NaBH_4$ in the presence of FeNPs as a catalyst. After reaction course, FeNPs can be recycled and reused without any apparent loss of activity which makes this process cost effective and hence eco-friendly. The structures of all the corresponding reduced products were confirmed by comparing their IR, ^1H NMR, spectra with the authentic samples.

OP-CYSA-01 : In Silico Approach for Designing Thiazolidinone based Analogues for Anti Inflammatory Activity

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Present communication covers docking studies of some thiazolidinone based analogues and its biological activities in order to identify prominent binding pockets for inhibiting cyclooxygenase (COX), lipoxygenase (LOX), and tumor necrosis factor (TNF-á). Additionally for these enzyme binding pockets, prediction of binding affinity, fragments responsible for the interaction with enzyme binding sites, and their modes of interactions with the active site have been investigated. This study discloses some structural features for binding to LOX, COX, and TNF-α, thus providing the prominent way to design new anti-inflammatory agents based on thiazolidinone moieties with better inhibition potency.

OP-CYSA-02 : Synthesis, Characterization and Docking Studies of Phthalimide Base α-helix Mimetics

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Protein-preotein interactions (PPIs) play a significant and crucial role in many biological processes which includes cell growth, cell differentiation, signal transduction, cell apaptosis and many more. The p53 (also know as “guardian of the genome”) is the major tumor suppressor protein and plays a fundamental role in apoptotic signaling and cell-cycle arrest through the binding at the hDM2 cleft. Three key hydrophobic residues Phe19, Trp23 and Leu26 of p53 protein generally imply for the p53-hDM2 PPIs. Overexpressed of hDM2 or inactivation of p53 through the mutation leads to loss of its pro-apoptotic activity, which is responsible for various kinds of diseases. More than 50% of all human cancer cells contains mutant or deactivated p53.

In this work we demonstrate the solution phase synthesis of phthalimide base á-helix peptides and their characterisation through

various characterisation technics. Using single-crystal XRD structure it will be clear to demonstrate that phthalimide base peptides can be rationally mimic the p53 α-helix. Docking studies of these peptides with hDM2 shows these mimetic peptides can be a potential inhibitor of p53-hDM2 PPIs through the binding to the hydrophobic cleft of hDM2

OP-CYSA-03 : Facile Carboxylic Ester Synthesis from Thioamides by Cleavage of C-S and C-N Bonds

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Facile synthesis of esters from thioamide precursor is successfully demonstrated in one pot under mild reaction conditions. The domino reaction of of stable thioamides results in the cleavage of stable C-N and C-S bonds to C-O and C=O bond formation in valuable ester. Readily available starting material makes this method attractive with broad substrate scope and facile at room temperature. Besides esters are integral components of natural flowers and fruits due to their attractive aroma, and they are frequently used in the fragrance industry[1]. Esters find application as precursor in synthesis. Presented technique may be useful in fragrance industry for synthesis of these essential materials.

OP-CYSA-04 : Magnetite-Chitosan Schiff Base Cu(II) Complex as A Novel and Recyclable Catalyst for the Oxidation of Ethylbenzene

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A magnetite-chitosan schiff base Cu(II) complex was developed using magnetite-chitosan composite, ortho-hydroxyl acetophenone (HACP) and cupric chloride which is abbreviated as {[Mag-Cs]HACP-Cu(II)}. The newly prepared heterogeneous catalyst was characterized by scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) etc. Its catalytic activity was tested for the oxidation of ethylbenzene with 70% tert-butylhydroperoxide (TBHP) as an oxidant. The 40.21% conversion of Ethylbenzene was obtained with 83.94% selectivity for acetophenone, when the reaction conditions are; amount of catalyst (50mg), substrate to oxidant ratio (1:1) and reaction temperature (80°C) for 5h was considered The catalyst was easy to separate and recyclable for several cycles.

OP-CYSA-05 : Copper Catalyzed Green Synthetic Protocol for the Synthesis of Triazoles via Click Chemistry

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The current review article highlights some recent significant advances in heterogeneous catalysis employing the "click reaction" to produce 1, 2, 3-triazoles via Cu-catalyzed 1, 3-dipolar azide-alkyne cycloaddition (CuAAC). In this review paper, we have divided the "click reaction" into two groups: the first is the CuAAC reaction, and the second is the other metal-catalyzed azide-alkyne cycloaddition (MAAC). The CuAAC reactions are also sub categorized into two groups: Cu(I)-nanoparticle-catalyzed azide-alkyne cycloaddition (Cu-NPs-AAC) and simple Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reaction. The 1,2,3-triazole synthesized by the click reaction has been shown to have anti-cancer, anti-tubercular, anti-diabetic, anti-bacterial, anti-viral, anti-convulsant, and anti-inflammatory activities. Additionally, the structural characteristics of 1,2,3-triazole allow for the copying of various types of functional groups, which hold up its application as a bio-isostere in the synthesis of novel molecules with potential medicinal applications, which have been described precisely.

OP-CYSA-06 : Amphipathic Hybrid Foldamers as Antimicrobial Agents

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Bacterial infections that are resistant to antibiotics are beginning to threaten public health globally. This spotlight on application provides a brief summary of our research investigation, with a particular emphasis on the investigation of small compounds that imitate host-defense peptides (HDPs) and have membrane-active antibacterial activity. Recently, membrane-active foldamers have been identified as promising antimicrobial peptide (AMP) mimics. Small molecules are selected for development because of their potential for more beneficial applications and low production costs. Innate defense peptide development and use are hampered by issues with absorption, off-target toxicity, and pharmacokinetics. They have broad-spectrum

activity against both Gram-positive and Gram-negative bacteria, including two strains that were multidrug resistant, according to in vitro studies.

In this work, we illustrate the confirmation of short hybrid foldamers, synthesis, characterization, conformational analysis, and antibacterial studies are included.

OP-CYSA-07 : Formation of α-Ketoamides through Oxidative Amidation and Amides via Degradative Amidation by using Aerial Oxygen

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Ketoamides and amides moieties are widely found in many bioactive molecules and natural products and are precursors for various organic transformations. Easily accessible gem-dibromoalkenes with N,N-dialkyl formamides gives oxidative amidation product α-ketoamides and under similar conditions with N-alkyl formamides gives degradative amidation product Amide. Aerial oxygen has proven to be an efficient oxidant for the formation of α-ketoamides and N-alkylated amides without the involvement of any transition metal and other oxidants. The versatility of this protocol is highlighted by its broad substrate applicability and compatibility with various functional groups. The degradative amidation follows a distinct mechanism that involves the neighbouring group participation of amines for the formation of amides.

OP-CYSA-08 : Synthesis of 4-Phenylpiperazin-Tetrahydropyrimido[4,5-b]quinolin-6(7H)-one Derivatives and in Silico-in Vitro Evaluation of their Antimalarial Activity

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A series of (4-phenylpiperazin-1-yl)-5,8,9,10-tetrahydropyrimido[4,5-b]quinolin-6(7H)-one have been synthesized and investigated for their in vitro antimalarial activity toward P. falciparum. All molecules exhibited excellent inhibition with IC_{50} values ranging from 0.61 to 0.82 µg/ml. Structure-activity relationship analysis indicated that the para-substituted derivatives significantly influenced the maturation of ring stage parasites into trophozoites and schizonts while the ortho-substitution counterpart outperformed moderate potency. The most potent compound in this series was a 1g bearing para-substitution motif with IC_{50} of 0.61 ìg/ml. Molecular docking and ADME studies were also performed to verify the SAR.

OP-01 : Design, Synthesis and Characterization of [1,3,4] Thiadiazolo and [1,2,4] Oxadiazolo- substituted 2,4-dicyclopropylamino-6- phenoxy-s-triazines

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s-Triazine is an important heterocycle and has gained much synthetic popularity due to its broad spectrum of biological properties. Recent studies, based on the s-triazine scaffold showing major pharmacological activities as anti-microbial, anti-viral, anti-tumour and anti-HIV activity have led these to be considered as most promising molecule to be employed as lead structures in the discovery of newer medicinally potent chemotherapeutic agents. A convenient synthetic procedure has been designed for the formation of [1,3,4]thiadiazolo- and [1,2,4]oxadiazolo- substituted 2,4-dicyclopropylamino-6-phenoxy-s-triazines by utilizing the versatility of thiosemicarbazone and amidine intermediates respectively. This approach attributes a wide substrate scope, high chemo and stereoselectivity, with simple operation.

OP-02 : Synthesis, Charactrization and DFT Study of 1,4-Disubsitutes 1,2,3-triazole through Click Chemistry utilizing Barbiturate Linked Aryl Hydrazone Moiety as Terminal Alkyne and Substituted Azide Precursors

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A series of 1,4-disubsituted 1,2,3-triazole derivatives synthesized from barbiturate with excellent yield using a catalytic approach through click reaction. The hybrid compounds were synthesized from terminal alkynes and pertinent azide derivatives in the presence of a copper catalyst in an ethanolic medium. The structural characterization of these compounds was confirmed through various Spectroanalytical techniques, including FTIR, NMR, mass spectrometry, and elemental analysis. This new protocol has several advantages such as recyclability, of the catalyst, cost-effectiveness, short reaction times, milder reaction conditions and a straightforward workup procedure. The optimized structures were calculated and obtained using at the B3LYP/6-31G(d) level of Density Functional Theory (DFT). Furthermore, the HUMO-LUMO energy gap were also calculated to determine the stability of the synthesized compounds.

OP-03 : Bismuth Oxide Assisted Synthesis of Pyridopyrimido Annulated Azepinone Derivatives

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Pyridine and pyrimidine have demonstrated as an important nucleus in the development of futuristic medicinal agents. Azepinone derivatives are also recorded to exhibit broad range of biological activities and considered as pharmaceutically active moiety. In view of this, novel pyridopyrimido annulated analogues of azepinones have been synthesized on the premise that the presence of these moiety could engender an interesting sequence of compounds with upgraded biological activities. To achieve this, a convenient and efficient catalytic approach of annulation of pyridopyrimidine nucleus with azepinone skeleton using the 2,4,6-trichloro-1,3,5-triazine and dimethyl formamide reagent have been developed. This approach attributes a wide substrate scope, high chemo- and stereoselectivity, and simple operation.

OP-04 : Palladaelectro-Catalyzed C–H Activation/ Arylation of Arenes using Aryl Diazonium Salts

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The emergence of resource-economical, environmentally benign strategies is one of the primary objectives of synthetic organic chemists. This can be achieved by minimizing waste product, avoiding the use of harsh chemicals and minimizing the cost of a chemical transformation. Transition metal-electro catalyzed C–H functionalization is one of the best alternative to traditional methods. This strategy is used in late-stage and site-selective functionalization(5) for the assembly of complex molecules. Herein, we developed a method of palladaelectro catalyzed C–H activation/ arylation of arenes using diazonium compounds which avoids the use of stoichiometric amounts of chemical oxidants and pre-functionalized starting materials, and reduce undesired waste generation.

OP-05 : Design, Synthesis and Characterizations of Some Halogenated Poly-Functionalized Pyrimidines for their Antimicotic Potency

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Nitrogen containing heterocyclic such as pyrimidine ring is a promising structural moiety for the designing of many therapeutic agents and currently plays a significant role in pharmaceutical industries. Pyrimidine ring form a component in a number of useful drugs and is associated with many biological activities such as anti-microbial, analgesic, anti-viral, anti-inflammatory, anti-HIV, anti-tubercular, anti-tumour, anti-neoplastic, anti-malarial, diuretic and cardiovascular agents. Pyrimidine compounds are also used as hypnotic drugs for the nervous system. Keeping in view the importance of pyrimidine moiety in drug discovery research, recently, we have synthesized the some new series of π electron deficient polyfunctionalized halogenated pyrimidines and evaluated their antimycotic activity in vitro against some human pathogenic fungi. In this presentation, the detailed synthetic procedure, biological screening profiles and characterisations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

OP-06 : Synthesis of Oxepin-, Oxocin and Oxonin-Annulated Coumarins by Ring-Closing Metathesis

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Coumarins fused with other heterocycles are known to have interesting biological and photodynamic properties which, in turn, have encouraged research with regard to procedures for the preparation of families of these compounds. Thus a number of methodologies have been reported for the synthesis of various 3,4-, 6,7- and 7,8-fused furo- and pyranocoumarins. Some members belonging to these two families have shown useful levels of biological activities. On the other hand, very little information is known about medium ring oxacycle fused coumarins which may, in part, be due to lack of general methods for the synthesis of such ring systems. In recent years, ring-closing metathesis (RCM) has emerged as a valuable tool for the construction of various carbocyclic and heterocyclic ring systems especially for medium to large rings.

Olefin metathesis is a unique carbon skeleton redistribution in which unsaturated carbon- carbon bonds are rearranged in the presence of metal carbene complexes. With the advent of efficient catalysts, this reaction has emerged as a powerful tool for the formation of C-C bonds in synthetic organic chemistry. Although alkene metathesis constitutes, for example, the most widely utilized type of metathesis reaction, recent years have witnessed the discovery and development of a number of related processes employing a broader range of substrates. Prominent amongst these are the enyne metathesis, which involves the union of an alkyne with an alkene to form 1,3-diene system. Enyne metatheses are wholly atom economical and are, therefore, driven by enthalpic rather than entropic factors.

In present work, we have demonstrated that the combined Claisen rearrangement and ring-closing metathesis reactions is a viable strategy for the synthesis of some potentially bio-active oxepin, oxocin and oxonin -annulated coumarins and synthesized some new coumarin based macrocyclic compounds using Grubb's-II catalyst.

OP-07 : Organocatalyzed Synthesis of Quinolino Annulated Azepinones Derivatives

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The versatility of dimedone synthon is explored for the synthesis of quinolino annulated azepinones derivatives. Primarily dimedone was treated with i) anthranilic acid, ii) isatoic anhydride to achieve acridone intermediate followed by reaction with hydroxylamine hydrochloride in the presence of Hyamine catalyst. Secondarily, the formed oxime underwent Beckmann rearrangement when treated with organocatalyst derived from the reaction of TCT and DMF to obtain desired azepinone in high yield. The use of organocatalysts has significant impact in Beckmann rearrangement due to their efficiency, good catalytic activity and mild condition. The compounds were characterized by spectral analysis through IR, ^{1}HNMR, ^{13}CNMR, Mass spectrometry.

OP-08 : Nickel Catalysed Heck and Suzuki Reactions using Dissipated Marble Slurry as Solid Support

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Transition metal catalysed coupling reactions such as C–C bond forming Mizoroki-Heck and Suzuki-Miyaura reactions have been prevalent and extensively used methods in the synthesis of bioactive molecules, pharmaceuticals, agrochemicals, drugs and fine chemicals. In modern synthetic chemistry, nickel has sustained with massive recognition as catalyst in the field of transition metal-catalysed C–C cross coupling reaction. Easy access of multiple oxidation states of nickel and facile oxidative addition has facilitated its use as an effective catalyst for many valuable and difficult transformations. However, most of the methods are based on homogeneous catalysis in which the catalyst is not recyclable and reusable and requires costly ligands.

Heterogeneous solid-supported catalytic systems have prominent interest in coupling reactions because of their high efficiency and reusability. Herein, we report the efficiency of marble slurry-supported nickel catalyst for Mizoroki-Heck and Suzuki-Miyaura cross-coupling reactions under ligand-free and aerobic conditions. Marble slurry-supported nickel catalyst (Ni@MS) was prepared by the wet impregnation method and used for the catalyzing Mizoroki-Heck and Suzuki-Miyaura reactions. The developed method was recyclable upto three cycles with moderate stability of catalyst. Thus, this study paves a way to develop an environmentally friendly method that offers a waste-to-wealth concept.

OP-09 : Molecules to Masterpieces: The Science of Organic and Polymer Synthesis in Ink and Lamination Adhesive Production

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Within the intricate interplay of science and art, the ink and coatings industry stand out as a beacon of innovative fusion. Transitioning from fundamental molecular structures to refined masterpieces embodies a blend of creativity and complex science. This work seeks to provide a comprehensive review of the latest strides in polymer and organic synthesis, with an emphasis on their applications in printing inks and flexible packaging. As the landscape evolves in response to stringent regulatory benchmarks, polyurethanes and their derivatives, especially Polyurethane Dispersions (PUDs) for water-based inks, have become indispensable. Their unmatched adaptability, resilience, and compliance with regulatory standards highlight their significance. Additionally, polyurethanes' innate benefits in lamination adhesives, including superior bond strength and longevity, accentuate their growing prominence. By intertwining these advancements with the introduction of eco-centric, bio-based additives, the industry is affirming its commitment to a sustainable and regulatory-aligned future. This review endeavors to illuminate the journey of how molecules, through cutting-edge synthesis, are transformed into functional masterpieces.

OP-10 : Design, Synthesis and Evaluation of Coumarin–Chalcone Hybrids Derivatives as Biologically Active Pharmacophores

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Based on the realistic biological activities of coumarins and chalcones, we have synthesized coumarin–chalcone hybrids with the aim of evaluating their antimicrobial properties. By applying standard Vilsmeier-Haack reaction condition, reaction of 4-Hydroxy Coumarin (1) with Vilsmeier-Haack reagents gives 4-Chloro-2-oxo-2H-chromene-3-carbaldehyde (2) which on further react with morpholine (3) gives 4-Morpholino-2-oxo-2H-chromene-3-carbaldehyde (4) which on further react with 4-Aminoacetophenone(5) gives chalcones (6) The structural variations were selected by introducing various amine at chloro acetyl group as well as various isothiocyanate and isocyanate at amine group. The structures of all the newly synthesised compounds were confirmed by their FTIR, ^{1}H NMR, ^{13}C NMR, mass spectral as well as elemental analysis data. All the newly synthesized compounds were screened for non automated in vitro antimicrobial and antimycobacterial-activity against selected pathogens. Some of the newly synthesized compounds exhibited excellent antimicrobial activity and said to be the most proficient members of the series compared to standard drugs and for future scope.

OP-11 : Exploring the Synthetic Methodology and an Antimicrobial Activity of 2-Aminothiazole and 2-Aminooxazole Derivatives

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In the last two decades, among five-membered heterocycles, thiazole & oxazole have been emerged as promising scaffolds in medicinal chemistry and drug discovery research considering their broad pharmacological spectrum. Especially 2-aminothiazole and 2-aminooxazole have privileged positions in antimicrobial, anticancer etc. research and constitute many highly active compounds. Currently many drugs are there in the market containing these two moieties, e.g., alpelisib, aztreonam etc. There had been challenges in synthesizing 4-substituted-2- amino oxazole derivatives because of low yielding reactivity.

OP-12 : Quantum Chemical and Molecular Docking on Pyrimidine Derivatives

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2,4-Dioxo-1,2,3,4-tetrahydropyrimidine-5-carbaldehyde (DTHPC) ($C_5H_4N_2O_3$) was computed theoretically via the DFT approach. ^1H, ^{13}C NMR, FT-IR, and UV-Vis analysis experimentally characterized DTHPC. The molecular structure, vibrational spectra, MEP and FMO analysis of DTHPC ($C_5H_4N_2O_3$) in the ground state were estimated using DFT/B3LYP using the 6-311++G(d,p) basis set. Calculated NMR chemical shifts (^1H and ^{13}C) and discrete regions in IR active vibrations are in good concurrence with their experimental counterparts. FT-IR spectra of DTHPC were obtained in the 4000-500 cm^{-1} range. The compound's electronic properties were analysed in different solvents by the TD-DFT method. The estimated HOMO and LUMO energies revealed that charge transfer may take place within the molecule. 3-D and 2-D interactions in the crystal were studied by Hirshfeld surface analysis. Finally, molecular docking was conducted on the DTHPC molecule to find the ligand-protein interactions.

OP-13 : Synthesis and Biological Evaluation of Difluoromethoxybenzimidazole Derivatives

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The present study reports the synthesis of novel benzimidazole derivatives possessing substituted difluoromethoxy ($-OCHF_2$) functional group. Formation of the titled derivatives was confirmed using IR, ^1H NMR, ^{13}C NMR, mass spectra, and elemental analysis. These were screened for therapeutic potential against a broad spectrum of bacteria and fungi and their minimum inhibitory concentration (MIC) values were recorded. Molecular docking analysis against critical microbial target DNA gyrase was performed to aid in understanding the possible binding modes and interactions between the synthesized compounds and protein target. Structure-Activity Relationship (SAR) study could provide insights into the structural fragments (functional group of an atom) responsible for the in-vitro antimicrobial activity.

OP-14 : Synthesis and Characterization of Chemically Modified Polysaccharide-based Nano-bio Carrier in Drug Delivery System

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As a result of its two key features-controlled drug release and biocompatibility nanoparticles made of biodegradable polysaccharides, such as modified maize starch (Butylated or Acetylated maize starch), are being thoroughly researched as drug delivery methods. This study aims to create butylated maize starch nanoparticles loaded with an Antihypertensive drug by employing the emulsion solvent evaporation process. Polyvinyl alcohol, Tween-20, Tween-80 etc used as a stabilising agent. The anti-hypertensive medication propranolol-HCl and Atenolol is frequently used to treat anxiety disorders and cardiovascular disease. This study looks at how certain preparation factors affect the form of nanoparticles and size made using the emulsion solvent evaporation technique. FE-SEM was used to characterise these nanoparticles. A study on zeta potential was conducted in order to comprehend the surface charge of nanoparticles. The drug release from drug-loaded nanoparticles was investigated using the dialysis bag technique, and the in vitro drug release information was examined using several kinetic models.

OP-15 : Identification of Polyalcohols from Peltophorum Ferrugineum Benth. Seeds Periodate Oxidized Polyaccharide by Smith Degradation Technique

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Peltophorum ferrugineum Benth. plant belongs to family-Caesalpiniaceae and commonly called known as Gulmohar Ke Yellow Flower. Water soluble polysaccharide were extracted from seeds yielded sugars as D-galactose and D-mannose in 2:5 molar ratio. Acid hydrolysis of fully methylated polysaccharide by Srivastava, Hakomari and Purdie's method, produced methyl sugars as : 2,3,4,6-tetra-O-methyl-D-galactose; 2,3,6-tri-O-mthyl-D-galactose; 2,3,6-tri-O-methyl-D-mannose and 2,3-di-O-methyl-D-mannose in 1:1:4:1 molar ratio. Periodate oxidation studies of polysaccharide with sodium metaperiodate which liberated 0.23 moles of formic acid per equivalent of polysaccharide with the periodate consumption of 1.32 moles of periodate for each anhydrohexose sugars after 55hrs. The linkages between D-galactose and D-mannose sugars with (1→6)-α-type at nonreducing end while D-galactose and D-mannose sugars unit by unit by (1→4)-β-type at main polymer chain. On the basis of methylation results a proposed polysaccharide structure and linkages are also confirmed by the periodate oxidation results.

OP-16 : Site-Selective Post-Modification of Short α/γ hybrid foldamers: a powerful approach for molecular diversification towards biomedical applications

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The extensive research work in the exhilarating area of foldamers (artificial oligomers possessing well-defined conformation in solution) proved them as promising candidates in biomedical research and material science. Post-modification approach is successful in peptides, proteins, and polymers to modulate their functions. To the best of our knowledge, site-selective post-modification of a foldamer resulting in molecules having different pendant functional groups within a molecular scaffold is not yet reported. We demonstrate for the first time the late-stage site-selective functionalization of short hybrid oligomers as an efficient approach to afford molecules with diverse functional groups. In this article, we report the design, synthesis of hybrid peptides with repeating units of leucine (Leu) and 5-amino salicylic acid (ASA), regioselective post-modification, conformational analyses (based on solution-state NMR, circular dichroism, and computational studies) and morphological study of the peptide nanostructures. The novel feature of the current work is that we utilized the difference in reactivity of two phenolic OH groups in short peptides to attain site-selective post-modification. It is challenging to apply the same approach to short á-peptides as they are poorly folded, and their structural modification may considerably affect their conformation. As a proof-of-concept for the site-selective modification strategy and its usage, we demonstrated the applications of differently modified peptides as drug delivery agents, imaging probes, and anticancer agents.

OP-17 : Kinetic Study of Acid Hydrolysis of di-4-chloro, 3-methyl Phenyl Phosphate Esters Eatalysed by Hydrochloric Acid

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Phosphate ester are play an important role in the physiology of cells is the participation of phosphate esters as a structural and functional part of DNA, RNA and its monomeric building blocks. The occurrence as a post-translational signal in proteins and as a head group in phospholipids. Phosphate is an indispensable nutrient that is usually taken up by plant cells and stored interacellularly which helps in photosynthesis, energy transformation and activity of some hormone in both plant and animals. Kinetic study of acid catalyzed hydrolysis of di-4-chloro, 3-methyl phenyl phosphate was studied in the acid region from 0.1 to 6.0 mol.dm^{-3} hydrochloric acid at 97±0.5ºC in 20% dioxane- water mixture. The rate of reaction increase with increase in hydrochloric acid molarity upto 4.0 mol.dm^{-3} HCl which was largely contributed by the conjugate acid species. Rate data at constant ionic strength was used to identify the reactive species as to determine the theoretical rates. Hydrolysis of di-ester via conjugate acid species was assigned the biomolecular behavior of the reaction on the basis of Arrhenius parameters. Solvent effect on hydrolytic reaction was found to indicate the formation of a transition state in which charge dispersion occurs. The first order rate coefficient have been calculated by using integrated form of corresponding rate equation.

OP-18 : Smith Degradation Method used for the Identification of Polyalcohols from Periodate Oxidised Seeds Polysaccharide of Erythrina Indica Lam. Plant

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Erythrina indica Lam. plant belongs to Papilionaceae family and commonly called as Indian Coral tree or Pangra, is a medium to large size tree upto 30 feet in height. It occurs in Northern India, Malaysia and Peninsula. Plant is medically used in Indigenous system of medicine for the treatment of diarrhoea, asthma and other human diseases. Seeds yielded a water soluble polysaccharide as D-galactose and D-mannose in 2:3 molar ratio by TLC. Column and Paper chromatographic analysis. Present investigation mainly deals with the determination of polyalcohols from periodate oxidised seeds polysaccharide by Smith degradation method for the confirmation of seeds polysaccharide structure. Seeds polysaccharide was reduced after periodate oxidation with sodium borohydride and sulphuric acid and obtained hydrolysate produced polyalcohols as glycerol and erythritol in 1.98:3.86 molar ratio by chromotropic acid method on paper chromatogram. The derivative of polyalcohols were produced from seeds polysaccharide as glycerol-tri-O-p-nitrobenzoate and tetra-O-tosyl-erythritol. Colour intensity and absorbance were recorded in photoelectrocolourimeter at 540 mu for glycerol and erythritol.

OP-19 : Synthesis and Characterization of Polyurethane Acrylate Oligomers Derived from 2-Methyl 1,3 Propane Diol

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This research focused on the synthesis of polyurethane acrylates derived from 2-Methyl 1,3 propane diol (MP diol). The condensation polymerization of MP diol with Adipic acid was employed to produce the polyol intermediate. Hydroquinone bis(2-hydroxyethyl) ether (HQMME) served as an aerobic antioxidant throughout the process. The generated polyol was then utilized to synthesize polyurethane acrylate (PUA), which subsequently found applications in UV-curable inks and coatings. The structural attributes and molecular weight of the developed Polyester polyol were characterized using Fourier transform infrared spectroscopy, gel-permeation chromatography, and hydroxyl value determination via titration. The performance attributes of the UV-cured coating were evaluated through thermogravimetric analysis and scanning electron microscopy. Results showcased the coating's notable flexibility, hardness of 3H, and grade 1 adhesion. Further, the coatings exhibited excellent thermal stability and chemical resistance, affirming the efficacy of the synthesized Polyester polyol with a well-defined molecular weight distribution.

PHYSICAL CHEMISTRY SECTION

Acting Sectional President's Address

Pradeep K. Sharma
Former Head, Department of Chemistry, Director, UGC – HRDC and Registrar, J.N.V. University, Jodhpur (Rajasthan)
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Dear Colleagues, Scientists, Researchers, Scholars and Students…..

A very good morning & warm greetings of coming New Year 2024

It’s a matter of great pleasure & pride to be the part of this ICC-2023 Mega Scientific & Academic event of the year, organised by University of Kota. I have been associated with ICC since last more than thirty years and witnessing its growth & overall development in the scientific community to leave an impact on highly quality research and interface the central science, chemistry in all the leading research areas.

Friends, I would like to press upon the good quality of research which should be applicable to the society and community at large. You must have heard Vocal for Local, Think Global & Act Local, Global Science for Global Wellbeing. Excellence in research can be achieved only when you have Integrity & Ethics in thinking, action and applications.

Integrity, ethics and excellence in research is a set of values & practices that expect each and every researcher / scientist to act with honesty, trust, fairness, respect and responsibility. As an emerging scientist / researcher, the questions and their answers may lead you and your colleagues into uncharted waters of knowledge. In conducting the research and then disseminating the results having the accountability to the colleagues, community, country and the world. Academic integrity is about who you are as a person, and how you act when it matters.

Ethics in Research involves the application of fundamental ethical principles to research activities which include the design & implementation of research, respect towards society & others, the use of resources & research outputs, scientific misconduct & the regulation of research. There are many ethical considerations when undertaking research. Key amongst these is the protection of human participants, welfare of animal subjects, handling of personal data and respect for intellectual property. Ethics are a personal code of conduct based on respect for one's self, others and surroundings and is governed by the principles or assumptions underpinning the way individuals or organisations ought to conduct themselves. Intellectual property is the output of intellectual endeavour in literary, artistic, dramatic, industrial, scientific and engineering fields, which is generally capable of being identified and protected.

Excellence in research or impact measurement may be calculated using researcher specific metrics such as the h-index, or by quantitative methods such as citation counts or journal impact factors. This type of measurement is also referred to as bibliometrics. This is based on the best work published or appeared in the journals of repute, have indexed in Scopus, Web of Science and Google scholar. The idea here is that the evaluation of a development researcher should take into consideration three major aspects: Research output & publications. The researcher's profile, his / her personal characteristics & record, The environment, scientific as well as ecological. Measures of esteem are additional factors which may provide evidence of research quality, including awards & prizes, membership of professional or academic organisations, research fellowships, patents or other commercial output, international collaborations, and successfully completed research grants or projects.

PIL-01 : Ionic Liquids as Biocompatible Solvents for Enhanced Structural and Thermal Stability of Enzymes

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Ionic liquids (ILs) have evolved as novel solvent systems fulfilling the requirements of biotechnology and bioengineering. In recent years, large numbers of ILs have been synthesized and their effect on protein stability has been illustrated. However, harsh process conditions, such as temperature, pH, and presence of organic solvents, are the major barriers to the effective use of enzymes in biocatalysis. We demonstrate the suitability of ILs as potential media for enzymes, in which remarkable enhanced activity and improved stability of proteins against multiple stresses were obtained. The catalytic activity of the enzyme in presence of ILs was retained against several external stimulus, such as chemical denaturants (H_2O_2 and GuHCl), and temperatures up to 120 °C. The observed enzyme activity is in agreement with its structural stability, as confirmed by UV–Vis, circular dichroism (CD), and Fourier transform infrared (FT-IR) spectroscopies. Finally, it is demonstrated that protein can be successfully recovered from the aqueous solution of ILs and reused without compromising its yield, structural integrity and catalytic activity, thereby overcoming the major limitations in the use of IL-protein systems in biocatalysis.

PIL-02 : Effect of γ-Irradiated Surfactant on Drug and Drug-Protein Binding in Aqueous Solution

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In the present work, gamma irradiated surfactants in aqueous solution was examined for solubilizing hydrophobic drugs. Two pluronic surfactant solutions in aqueous medium were subjected to gamma-irradiation with two doses 75 kGy and 135 kGy. These irradiated amphiphilic solutions were tested for solubilizing five drugs. They were, ciprofloxacin, ornidazole, tinidazole, aceclofenac, and methyl parapen. Their solubilized capacity was compared with that of unirradiated surfactant solutions. The irradiated surfactants had better solubilizing power compared to the unirradiated ones. In another experiment, with low dose irradiation of 30 kGy was applied to four nonionic surfactants. The presence of the irradiated surfactant was examined in drug and Bovine serum albumin (BSA) interaction. There was enhanced binding of Drug-BSA in presence of irradiated surfactant compared to its unirradiated counter parts. Our observation was that the interaction was very much specific to the drug and the surfactant combinations.

PIL-03 : PIL-03 : Tuning the Optical Blue shift in Zinc Oxide Nanoparticles by Greener Methods

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Zinc Oxide Nanoparticles (ZONPs) are well known for their great potentials in the multifaceted applications in sun screens, cosmetics, paints, light emitting diodes, solar cells, biocatalysis, photocatalysis etc. The conventional synthesis of ZONPs require either harsh physical conditions or hazardous chemical treatments owing to various environmental disadvantages, there is a growing need for eco-friendly methods suitable for low-cost production of ZONPs. This study deals with reviewing and comparing the methods of metal ion doping with greener cost-effective and eco-friendly methods used for tuning the optical properties of ZONPs. The UV-visible spectra were used to evaluate the optical band gap (standard value 3.37eV) values of the ZONPs nanoparticles in literature reviewed and found to be in the range of 3.43-3.64 eV which indicated the presence of blue-shift with enhanced absorption of sunlight irradiation by ZONPs. The present study reveals that eco-friendly methods for ZOPN synthesis are relatively inexpensive and eco-friendly methods over the conventional metal doping which may be used preferentially for various applications.

PIL-04 : Enhancement and Evaluation of Chiral Selectivity of Modified Chitin and Chitosan

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Resolution of optically active components of a racemic bio-active organic compound has drawn substantial attention of the researchers. Chromatographic enantio-separation is one of the most versatile approaches for such resolution. Numerous synthetic and natural materials have been employed as chiral stationary phase for enantio-separation studies. Carbohydrates of almost all kinds too have been studied. This study report about immobilization of quinine on chitin and chitosan. Quinine is a well-known chiral reagent that has been used for enantio-separation by conventional methods. However, polysaccharides show only limited ability for real application. Quinine immobilized cellulose and starch have been reported for improved enantio-selectivity. Guaran, a seed polysaccharide with abundance of cis-1, 2-hydroxyl groups when anchored with quinine significantly improved chiral selectivity. Racemic borate complexed mandelic acid and bio-active oflaxacin are efficiently resolved by chromatography using Quinine modified chitin and chitosan. All the materials used for the current study are natural, non-toxic, readily available and inexpensive. Methods employed are simple and results clearly establish a correlation between structural component and enantio-separation.

PIL-05 : Oxidation Kinetics of DL-Methionine, a Sulfur Containing Amino Acid by Tripropylammonium Chlorochromate : A Mechanistic Approach

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Oxidation of methionine (Met), a sulphur containing amino acid, by tripropylammonium chlorochromate (TPACC), a mild and selective Cr(VI) oxidizing reagent in dimethylsulphoxide (DMSO) as a non-aqueous solvent, is leading to the formation of its corresponding sulphoxide. The reaction is found to be of first order with respect to TPACC. Michaelis-Menten type kinetics is observed with respect to methionine. The reaction is catalysed by hydrogen ions. The hydrogen-ion dependence has the form: $k_{obs} = a + b [H^+]$. The oxidation of methionine is studied in nineteen different organic solvents. The solvent effect is analyzed by employing linear salvation energy relationship (LSER) of Kamlet's and cation- and anion-solvating power of solvents of Swain's multi-parametric equations respectively. Solvent effect indicated the importance of the cation-solvating power of the solvent. A suitable mechanism has also been proposed.

PIL-06 : Functionalized Polymer Nanocomposites as a Promising Materials for Industrial Applications

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Functionalization of polymers has recently become better understandable as a good tool to prepare composite materials possessing excellent thermal, mechanical, and other specific required properties. Polymers are promising candidates to solve existing

engineering problems, due to its low density and excellent mechanical performance. Large number of functional groups was successfully introduced in the past decades and there is still work is going on in this domain. Functional groups as like hydroxyl, epoxy, carboxylic or amino groups introduced into polymer backbone to achieve specific required properties in that polymer. In the present research work discussion were made on different properties of functionalized polymer nanocomposites materials by using different functional groups of poly(methyl methacrylate) (PMMA). Synthesis of amino functionalized PMMA using post polymer functionalization method by treating with four different amino compounds to obtain functionalized PMMA. Bonding behaviour of functionalized PMMA was characterized with Fourier transform infrared (FTIR) spectroscopy. Studies were highlighted on functionalized PMMA to prepare functionalized polymer nanocomposites by the addition of nanoclay and Ag nanoparticles into the polymer matrix. Behaviour of these nanocomposites were studied against thermal and antibacterial properties. Sophisticated analytical techniques i.e., thermal gravimetric analysis (TGA), differential thermal analysis (DTA) and derivative thermogravimetric curve (DTG) were reported to characterize the thermal properties of nanocomposites.

PIL-07 : Kinetic and Biochemical Study on 2-Iodoxybenzoic Acid : A Greener Oxidant

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The development of greener protocol for transformation of organic compounds has emerged as a need in current time. Hypervalent iodine compounds have emerged as potential oxidants with mild nature, high selectivity and ecofriendly approach.2-IODOXYBENZOIC ACID (IBX) belong to λ^5 iodanes class of hypervalent iodine compounds. It has emerged as green oxidant in comparison to conventional chemical oxidants. The study on amino acid oxidation has found the significance in various fields of sustainable approach towards environmental protection. The kinetics of amino acid oxidation in acetic acid-water solvent system was investigated during present study. Dynamics measurements study showed Lineweaver-Burk relationship suggesting towards Michaelis-Menten type of kinetics with respect to amino acids's concentration wheras first order dependence with respect to oxidant. The mechanistic determination involved detection of free radical, validation of isokinetic and Arrhenius relationships. Thermodynamic and activation parameters point towards formation of ordered complex in the mechanistic pathway. Based upon structure activity correlation analysis suitable mechanism has been proposed. Growth supporting potential of IBX was investigated on selected stage of plant system. Defined IBX concentration was found to be non-necrotic and growth stimulatory. IBX treatment favoured seed germination under controlled conditions. The positive effect of IBX on growth was correlated with the protein content in cotyledon stage. Total protein concentration was altered after IBX treatment. The increased accumulation of protein in cotyledon with the non-necrotic effect highlighted the greener character of IBX towards its possible application as an eco-friendly oxidant to be used in the field of organic synthesis and pollutant remediation.

PIL-08 : Decipherment of Alteration in Suspected Documents using Spectral Comparision Technique & its Implimentation in Forensic Document Cases

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Ink analysis may be an important part of the investigation of suspected documents, including forged checks, wills, or altered records. Although all blue or black inks may look the same, there can be some important differences in their chemical composition. These can be revealed by laboratory analysis and the results can help assess whether there have been any additions or alterations to a document.

Analysis of documents under a microscope can be informative as a first step. The investigator may be able to see slight changes in ink color, not visible to the naked eye, that could be indicative of alterations, or there may be suggestions of obliteration and overwriting. The ink itself may be analyzed by non-destructive or destructive testing, depending on whether a sample needs to be taken from the document, a process that would alter it. It is preferable to try the non-destructive approach first, so that the document is left intact.

The characterization of ink on paper is of importance for dating and comparing questioned ink entries in forensic document examination. Inks are commonly characterized by their colorant profile that is identified by well-established analytical methods.

The document examiner often encounters cases regarding alteration in documents if any and has to decipher the original contents of writing to establish the forgery. In this paper examination of Forensic document cases using IR luminescence and IR reflectance technique, regarding differentiation in ink has been discussed in relation to cases involving decipherment of addition or alteration in original documents pertaining to detection of forgery.

PIL-09 : Oxidation Kinetics of some Lower Oxyacids of Phosphorus by Picolinium Chlorochromate: Determination of Reactive Reducing Species

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Picolinium chlorochromate (PICC) in dimethylsuloxide (DMSO) oxidizes lower oxyacids of phosphorus, forming matching oxyacids with phosphorus in a higher oxidation state. The reaction shows stoichiometry of 1:1. In relation to PICC, the response is first order. Regarding the reductants, a kinetic behaviour of the Michaelis-Menten type was noticed. Acrylonitrile does not undergo polymerization as a result of the reaction. Hydrogen ions function as catalysts for reactions. The form of the hydrogen-ion dependency is: $k_{obs} = a + b[H+]$. Deuterated phosphinic and phenylphosphinic acids showed a significant primary kinetic isotope impact during oxidation. Nineteen different organic solvents were used to study the oxidation. The multiparametric equations of Taft and Swain were used to analyze the solvent effects. The influence of the solvent shows that the polarity of the solvent is crucial to the process followed. The penta-coordinated tautomer of the phosphorus oxyacid has been shown to be the reactive reductant, and it has been determined that the tri-coordinated forms of phosphorus oxyacids do not take part in the oxidation process. It has been hypothesized that the rate-determining phase involves the transfer of a hydride ion.

PIL-10 : Potentiality of Raman Spectroscopy in Ascertaining the Chronological Sequence of Intersecting Ink Strokes in Forensic Examination of Questioned Documents

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The determination of the sequence of line crossings is still a current problem in the field of forensic documents examination. Optical examination, lifting technique, ESDA technique, and electron microscopy are the most widely used methods for the determination of the writing order of crossing texts. However, at present many examinations of intersecting lines result in an inconclusive opinion, particularly if the same type and colour of ink is involved. This paper presents the potentiality of the Raman Spectroscopy in determination of sequence of homogenous and heterogeneous strokes. Raman Spectroscopy is a relatively new technique that is being increasingly applied in forensic science. This is a non-destructive method that determines the composition of a given sample accurately. Scientists have recently begun to use it in investigations to differentiate inks.

In this work, attempt has been made to assess how useful it is in ascertaining the order in which intersecting lines have been drawn. Both homogenous (i.e. drawn by the same type of instrument) and heterogeneous ones (i.e. drawn by different types of instrument). The samples studied were intersecting graphic lines made by popular writing instruments (e.g. ball point pens, fiber tip pens, gel pens) in different combinations, and intersections in which one line was made by an ink jet printer and the other by various writing materials (ballpoint inks and fluid inks). Raman spectra were obtained using RL-633 Raman Spectroscope by RENISHAW,UK. The examination was carried out on samples prepared on the same type of paper. Five readings were taken for each sample, and the spectra obtained were averaged and compared with spectra of pure inks.

PIL-11 : Chitosan Functionalised Iron Oxide-Incorporated Peanut Shell Biomass : A Novel Green Adsorbent for Chromium (VI) Removal from Aqueous Media

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In the realm of environmental remediation, biomass adsorbents stand as secret weapons, championing sustainable adsorption of toxicants to ensure safe water resources. This study focuses on the development and application of green sorbents derived from peanut shell biomass, functionalized with chitosan and incorporated with iron oxide, for the efficient removal of chromium (VI) from aqueous media. The innovative material was thoroughly characterized using modern spectroscopic methods to confirm successful embedding. Batch adsorption experiments were conducted, revealing robust chromium removal. The kinetic and equilibrium studies supported the efficacy of the developed adsorbent. The sorption data demonstrated an excellent fit with the pseudo-second-order kinetics model, reinforcing the conformity with the Langmuir isotherm model. The adsorption studies explored the effects of pH and time, reusability, ionic strength, and the presence of coexisting ions.

At pH 4 and an optimal contact time of 40 minutes, the maximum sorption capacity reached an impressive 14.28 mg/gm. Remarkably, the green adsorbent exhibited resilience over multiple cycles, with efficient chromium removal for up to four cycles. The impact of background electrolytes on uptake efficiency was minimal, showcasing the versatility of this novel adsorbent.

In conclusion, the chitosan functionalized Iron Oxide-Biochar Composites emerged as unbeatable, recyclable, and highly efficient adsorption tools for chromium desalinization. The utilization of peanut shell biomass not only enhances the sustainability of the adsorption process but also contributes to waste management by unlocking the latent power of agricultural by-products. The successful incorporation of chitosan and iron oxide further enhances the adsorption capabilities, providing a green and cost-effective solution for chromium removal from aqueous media.

PO-CYSA-01 : Physicochemical Profile of BSA, Hb, and dsDNA with aq-NaCMC at 298.15-310.15 K Interfaced via UV-Vis Fluorescence Circular Dichroism Spectroscopy and *in-silico*

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The 0.2-0.8 mg% @ 0.2 mg% bovine serum albumin (BSA 66), hemoglobin (Hb 64.5), and double stranded deoxyribonucleic acid (dsDNA 130 kDa) with water and 0.25, 0.50, and 1.00 g% aqueous carboxymethyl cellulose sodium salt (NaCMC) thermodynamically stable homogeneous solutions via resonating energy transfer were designed. Density (ρ,10^3kgm^{-3}), viscosity (η,10^{-3}kgm^{-1}s^{-1}), surface tension (γ,mNm^{-1}), friccohesity (σ,sm^{-1}), apparent molar volume (V_2,10^{-6}m^{3}mol^{-1}), and isentropic compressibility ($\kappa_{s\phi}$,10^{-3}m^{4}kg^{-1}s^{-1}) at 298.15, 304.15, and 310.15K were studied. UV-Vis spectrophotometry, fluorescence spectroscopy, circular dichroism (CD), and *in-silico* study via reorientational activities have elucidated structural recognition. The ρ, η, γ, σ, V_2, and $\kappa_{s\phi}$ physicochemical properties (PCPs) have studied the interacting activities of salt bridges (peptide bonds) of proteins and base pairs (adenine, thymine, cytosine, guanine) of dsDNA on developing nanohydration sphere (NHS) with water and 0.25-1.00 g%

aq-NaCMC. Regression constants of PCPs have elaborated the interacting mechanism of internal linkages of BSA, Hb, and dsDNA for solubilizing them without unfolding assisted by glycosidic bonds of glucopyranose units of NaCMC.

PO-CYSA-02 : Cadmium Sulfide (CdS) Quantum Dots/ Polymer Nanocomposite for Electrical Ammonia Sensing

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Quantum dots are zero-dimensional semiconducting nanomaterial of size ranging from 1 to 10 nm. They exhibit properties like high photostability, high quantum yield, excellent photoluminescence properties and tunable size confinement effect. In this report Fluorescent CdS quantum dots have been synthesized using hydrothermal method with citric acid as capping agent. Polythiophene was prepared by oxidative polymerization process by using thiophene monomer. Nanocomposites of CdS quantum dots and polythiophene were obtained by ex- situ method by loading different volume percentage of CdS QDs over PTh. These synthesized polymer nanocomposites have been characterized by different characterization techniques like UV- Visible, Photoluminescence, FTIR analysis and XRD. These characterization techniques confirm the successful formation and interaction between CdS quantum dots and polythiophene nanocomposites. These nanocomposites were tested for electrical gas sensing. Maximum sensitivity was obtained for ammonia. The sensor shows linear response which is useful for device fabrication. For optimized nanocomposite, the sensitivity was found to be maximum with response and recovery time in few seconds.

PO-CYSA-03 : Expanding the Potential Role of Cholinium Citrate based Deep Eutectic Solvents toward Facilitating the Structural and Thermal Stability of α-Chymotrypsin

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In view of the global environmental and economic challenges of conventional organic solvents, most of the Deep Eutectic solvents

(DESs) have proved themselves as a "greener" group of cosolvents, especially for enzymes. However, there is a lack of fundamental knowledge on the greener aspects of various multicationic DES systems on biomolecules. In this regard, we have synthesized the monocholinium citrate-ethylene Gycol ([Chn][Cit] -EG), dicholinium citrate-ethylene Gycol ([Chn]2[Cit]-EG) and tricholinium citrate-ethylene Gycol ([Chn]3[Cit]-EG) DESs and employed them to explore their suitability for α-chymotrypsin (α-CT). This study specifically addresses the effect of increased cationic ratio of of hydrogen bond donor(HBD) on stability and activity of α-CT with the help of various spectroscopic techniques. Various spectroscopic analysis showed that there is improved structural stability and activity of α-CT as the cationic ratio of DES increase. We found better structural stability of α-CT in ([Chn]3[Cit]-EG) and ([Chn]2[Cit]-EG) as compared to that in ([Chn]3[Cit]-EG) Interestingly, temperature-dependent fluorescence spectroscopy results explicitly elucidate that transition temperature (Tm) of α-CT enhancement in the presence of ([Chn]2[Cit]-EG) when compared to Tm of α-CT in buffer solution. Ultimately, these results establish that through an increase in the molar ratio of aqueous cholinium cation in [Chn][Cit] intensifies the capability of DESs to stabilize the α-CT structure. Our results suggested that multicationic HBD system sensitivity to cosolvent exposure may be utlized in the future as a new approach to explore new biocompatibility toward proven stability studies.

PO-CYSA-04 : Impact of Acylthiourea Based Rhodium Complexes on Proteolytic Activity and Conformational Stability of α-Chymotripsin

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In this research study, a series of four acylthiourea ligands and their corresponding rhodium(III) pentamethylcyclopentadienyl complexes, designated as Rh1, Rh2, Rh3 and Rh4 were successfully prepared. Through meticulous analysis of the spectroscopic data, it was convincingly established that the acylthiourea ligands served as neutral and monodentate ligands in their interaction with the Rh(III) ions. Specifically, the spectroscopic evidence confirmed that the sulfur (S) atoms within the acylthiourea ligands formed coordinated bonds with the Rh(III) ions. This crucial finding elucidates the specific coordination mode and binding interactions between the ligands and the central Rh(III) metal ion, which has been seldom investigated.The biomolecular interactions of the all the Rh complexes with áchymotripsin have also been studied in detail using various spectroscopic and microscopic methods, such as UV-Visible spectroscopy, Fluorescence spectroscopy, FTIR spectroscopy, Raman spectroscopy, Dynamic light scattering (DLS). Thermal denaturation study was also performed using Fluorescence spectroscopy. Further, our results deliver that all the Rh complexes are able to interact with α-chymotripsin with maintenance of structural stability as well as enzymatic activity of enzyme. Further, the proteolytic activity of α-chymotripsin in presence of all Rh complexes increases to higher extent.

PO-CYSA-05 : Degradation of p-Nitrophenol by H_2O_2/ Nanoparticles in Micellar Media

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Removal of recalcitrant PNP pollutant from water bodies is a critical challenge while dealing with water pollution and its treatment. A novel approach to enhance the H_2O_2 production along with Fe-Co nanoparticle to increase efficiency of PNP degradation by various methods is studied. Fe-Co NPs was synthesized using the hydrothermal method and characterized by SEM, EDS, TEM, XRD, FTIR, TGA, VSM. Kinetics and efficiency of oxidation are studied under various condition like temperature, pH, CPC, DOSS, CPB, CTAB, SDS, Triton X-100, H_2O_2 conc, PNP conc. Findings highlight the fundamental mechanism of H_2O_2 production along with its enhanced production and determination of degradation rate constant of PNP under various conditions.

PO-CYSA-06 : The State of Understanding Electrochemical Behaviours of A Valve-regulated Lead-Acid Battery Comprising Manganese Dioxide-impregnated Gel Polymer Electrolyte

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Gel electrolyte plays a vital role in the valve-regulated lead acid battery. To address this, we formulate a gel polymer electrolyte containing poly(vinyl alcohol) as the base matrix and manganese dioxide as an additive. The addition of manganese dioxide into poly(vinyl alcohol) increases the ionic conductivity of the gel. Chemical interaction

between poly(vinyl alcohol) and manganese dioxide is confirmed by Fourier transform infrared spectroscopy. Electrochemical characterizations such as cyclic voltammetry, electrochemical impedance spectroscopy and potentiodynamic polarisation suggest that 3 wt% manganese dioxide at poly(vinyl alcohol) gel system displays better electrochemical performance. The galvanostatic charge-discharge technique reveals that the battery device with an optimized gel system showed the highest discharge capacity of 9.080 µAh at a current density of 87.5 μAcm^{-2} and 81 % discharge capacity after 500 steady cycles.

PO-01 : Cosmic Chemistry: Contribution of Few Elements: C,H,N,P,S,O For Molecular Rearrangement for the Life Living and Non Living Materials on the Basis of Law of Conservation of Mass and Energy

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The present paper is based on the correlation of molecular energy with life molecule after degradation, decomposition or after decay. This study will be a key guide for upcoming research in the field of physical chemistry and biologist to unhide the mystery of energy of life molecule.

PO-02 : A Mechanistic Investigation of Ruthenium (III) Catalyzed Oxidation of D-Mannitol by Diperiodatocuprate (III) in an Aqueous Alkaline Medium

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The study investigates the kinetics associated with the oxidation of D-Mannitol (D-Mann) by diperiodatocuprate(III) (DPC) in an aqueous alkaline medium using spectrophotometric methodin presence of catalyst Ru(III). Reaction medium's ionic strength was maintained constant at 0.60 mol dm^{-3}. First-order kinetics was seen in [DPC] and it exhibitedless than unit order for [D-Mann] and [alkali]in the reaction. It was of the negative fractional order in [periodate]. Current study revealed that order of the reaction concerning [Ru (III)] was determined to be unity. Moreover, no influence was observed on the reaction rate

due to variations in ionic strength and dielectric constant.It was determined that Ru(III) catalyzed reaction of substrate D-Mann with DPC in an alkaline medium shows 1(D-Mann):4(DPC) stoichiometry. The products of reaction were identified by FTIR and confirmed by LC-ESI-MS spectral data. The catalytic constant (Kc) was calculated at distinct temperatures. The reaction constants for each step of the mechanism were determined. For the rate determining step of reaction mechanism, activation parameters were calculatedand discussed. Further, thermodynamic quantities for the reactions were also estimated. The studies indicated that active species of DPC is $[Cu(H_3IO_6)_2(OH)_2]^{3-}$and that of Ru (III) is $[Ru(H_2O)_5OH]^{2+}$.

PO-03 : Spectral Investigations and Thermal Analysis of Chromium Soaps

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The spectral investigations of Chromium soaps (Palmitate, Laurate and Caprate) were investigated in solid state. The infrared results revealed that the fatty acids exist with dimeric structure through hydrogen bonding between two molecules of fatty acids whereas the metal –to-oxygen bonds in chromium soaps are not purely ionic but possess considerable covalent character. The X-Ray diffraction results showed that these soaps possess double layer structure with molecular axes slightly inclined to the basal plane. The results of thermogravimetric analysis have been explained by using Freeman-Carroll's and Coats-Redfern's equations. The decomposition reaction for metal soaps is found kinetically of zero order and the values of the energy of activation for the decomposition process are in the range to 2 to 16.6 kcal mol^{-1}.

PO-04 : Ru (III) and Os (VIII) Catalayzed Oxidation of Sulfanilic Acid with Alkaline Hexacyanoferrate (III)- A Kinetic and Mechanistic Aspect

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The kinetics and mechanism of oxidation of sulfanilic acid by hexacyanoferrate (III) have been studied in presence of osmium (VIII) and Ruthenium (III) as catalyst. The reaction simultaneously occurs without these catalysts which have been suspected due to the trace metal ion catalysis present as an impurity either in reagents or water.

The rate of reaction is retarded by hexacyanoferrate (II) which has also been accounted for in the reaction mechanism and the rate law.

The energy and entropy of activation are evaluated in all such reactions. A plausible reaction mechanism has been suggested.

PO-05 : Nanohybrid Comprising Electropolymerized Glycine and MWCNT for Electrochemical Analysis of Diclofenac in Diverse Matrices

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The Carbon Paste Electrode (CPE) blended with Multi-Walled Carbon Nanotubes (MWCNTs) and electropolymerized with Glycine (Gly) was used to study the electrochemical behaviour of Diclofenac (DCF). The electrochemical performance and analytical applications were investigated by employing voltammetric techniques like cyclic voltammetry and differential pulse voltammetry. To determine the surface morphology, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) were utilised. The modified sensor showed high electrocatalytic properties displaying an enhanced peak current at the developed electrode compared with bare Carbon Paste Electrode (CPE). The modified electrode displayed faster electron transfer, excellent reproducibility and repeatability features. The parameters affecting the DCF peak current like immersion time, pH variation, scan rate, and concentration were examined. The limit of detection was calculated to be 7.96×10^{-8} M. The fabricated electrode was used to determine DCF in biological and pharmaceutical test samples also.

PO-06 : Fabrication of Terpolymer Magnetite Nanocomposite of Chitosan for Efficient Removal of Nitrate

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The removal of nitrate ions from waterbodies is essential to reduce eutrophication and nitrate-induced health hazard like blue baby syndrome. In the present study, a hybrid polymer nanocomposite has been developed for adsorptive removal of nitrate from wastewater. The preparation of the nanocomposite has been achieved by microwave irradiation of the aqueous mixture of chitosan (CS), poly(diallyldimethylammonium chloride) (PDADMAC) and N-(2-

hydroxyethyl)acrylamide (HEAAm), N,N'-methylenebis(acrylamide) (MBA) in the presence of a radical initiator followed by incorporation of magnetite nanoparticles. A semi interpenetrating network appears to be formed by entanglement of PDADMAC chains with the MBA crosslinked network of chitosan-graft-poly(N-(2-hydroxyethyl) acrylamide) within which Fe_3O_4 nanoparticles are held. The material (CS-g-PHEAAm)-PDADMAC and (CS-g-PHEAAm)-PDADMAC/Fe_3O_4 was characterized for the physicochemical structure using FTIR, XRD, SEM, EDS, and TGA techniques. Its utility for nitrate removal was evaluated through adsorption studies. The nitrate adsorption process was optimized for contact time, solution pH, adsorbent dosage, temperature, and initial adsorbate concentration. The adsorption data showed a close fit with Freundlich adsorption isotherm model and pseudo-second-order kinetic model. The presence of Fe_3O_4 nanoparticles is observed to enhance the adsorption capacity of the gel significantly from a value of 45.87 mg/g to 53.76 mg/g. The thermodynamic studies indicated the adsorption to be a spontaneous and endothermic process. The results indicated the possibility of using the developed nanocomposite as an adsorbent for effective removal of nitrate ions from water.

PO-07 : Role of Sugarcane Bagasse Biochar Supported Titanium Dioxide Composite in Waste Water Treatment

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The sugarcane bagasse is a natural, biodegradable, free of cost and easily available material. Their chemical compositions have drawn interest as a highly promising and adaptable component in composite materials. This green material with low pollutant indices,eco-friendliness and affordability are being sought after by material science researchers.Sugarcane bagasse wastes are chosen as an ideal raw material manufacturing new products because of its low fabricating cost and high quality green end material. In the present research article, titanium dioxide nanoparticles were loaded on sugarcane bagasse biochar to enhance its adsorption capacity of methylene blue dye. The sugarcane bagasse biochar was synthesized through microwave- assisted pyrolysis method. The ultrasonication method employ for impregnation of nanoparticles of titanium dioxide on biochar. The newly synthesized sugarcane bagasse biochar composite were characterized through various techniques like XRD, FTIR, XPS, etc.

which elucidate the size, morphology, and surface area of composite. The porous titanium dioxide modified biochar shows excellent adsorption potential against methylene blue dye and helpful in waste water treatment.

PO-08 : Removal of Some Agrochemicals by Activated Carbon and it's Evaluation by Thermodynamic Parameters

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Adsorption of some agrochemicals activated carbon from it's dil.aqueous solution has been studied under laboratory conditions with the help of thermostat. For this work four granular activated carbons were used.GAC383 (native form), experiments have been conducted with the help of 'Thermostat' constructed with a tub, two motors, electronic relay, Teflon stirrer, simple glass stirrer etc. Experiments are carried with concentration, temperature, time and equilibrium conditions. Extent of adsorption is studied using Langmuir adsorption isotherm and Freundlich adsorption isotherm.

PO-09 : Rapid Charge Transport of Carbon Quantum Dots and Reinforced Polypyrrole Network as A High Performance Symmetric Supercapacitor

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In this work, we report PPy, PPy-CQD1, PPy-CQD2, PPy-CQD3, and PPy-CQD4 composites synthesized by the in-situ polymerization method as electrode materials for supercapacitors. The as-synthesized composites are characterized and investigated by Ultra violet visible spectroscopy (UV), Fourier infrared spectroscopy (FTIR), X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The performance of the PPy-CQD3 supercapacitor device shows outstanding supercapacitive properties compared to other fabricated devices. It was found that PPy-CQD3 demonstrated the highest specific capacitance of 1093 Fg^{-1}at 10 mV/s as well as high energy density (66 $Whkg^{-1}$), power density (1090 Wkg^{-1}) and capacitance retention of 95% of its initial specific capacitance after 10,000 cycles at current density. The outstanding electrochemical performance of the PPy-CQD3 device is maybe due to the synergistic effect of CQDs on the PPy matrix, where rich pores and network structures made the electrolyte ions more easily accessible for faradaic reactions.

PO-10 : Adsorption of Some Organic Dyes from their Dilute Aqueous Solution on Graphin and it's Evaluation by Thermodynamic Parameters

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Adsorption of some organic dyes on activated carbon from it's dil.aqueous solution has been studied under laboratory conditions with the help of thermostat. For this work four granular activated carbon used, coconut shell based activated carbon. (native form), experiments have been conducted with the help of 'Thermostat' constructed with a tub, two motors, electronic relay, Teflon stirrer, simple glass stirrer etc. Experiments are carried with varied concentration, temperature, time and equilibrium conditions. Extent of adsorption is studied using Langmuir adsorption isotherm and Freundlich adsorption isotherm.

PO-11 : Comparative Study of Adsorption of Phenol and Cresols on Granular Activated Carbon and It's Evaluation

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Adsorption of phenol, ortho, para and metacresols from their dilute aqueous solution on Granular Activated carbon was studied under the laboratory conditions using batch reactor/thermostat. This comparison was studied at three different temperatures. In order to conduct the research smoothly, experiments were carried out using a thermostat. It is a simple water bath (tub) of 30 litres capacity, two separate stirrers, heater, electronic relay, motors etc. Granular activated carbon was used for this investigation. Adsorption of all the phenols is separately studied at 25°C temperature conditions and their adsorption data is comparatively studied. This evaluation is studied using Langmuir and Freundlich Adsorption Isotherms. It is observed that Langmuir adsorption data is best fitted for this evaluation. Other

thermodynamic parameters like free energy change, entropy change and enthalpy change shown that reactions are spontaneous and irreversible. This data highlighted that extent of adsorption of phenol is less than the substituted cresols.

PO-12 : Ab-Initio Investigation of Dielectric Properties of α-CdP_2

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An ab-initio investigation of the dielectric properties of the alpha phase of CdP_2 is carried out with the help of the CRYSTAL Program under the coupled perturbed Hartree-Fock (CPHF) method. In this study, GGA-functional PWGGA is utilized. The computations for dielectric, polarizability and first-order electric susceptibility tensors for á-CdP_2 are performed at ~ 0 eV. The analysis of optical anisotropy is carried out through optical indicatrix. The computed principal refractive indices of α-CdP_2 crystal system are 6.23, 6.64 and 7.22. The first-order principal electric susceptibility components of the alpha phase of CdP_2 are 5.23, 5.64 and 6.22. The calculated value of mean polarizability is nearly 906 $Bohr^3$.

PO-13 : Kinetic and Biochemical Study on 2-Iodoxybenzoic Acid : A Greener Oxidant

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The development of greener protocol for transformation of organic compounds has emerged as a need in current time. Hypervalent iodine compounds have emerged as potential oxidants with mild nature, high selectivity and ecofriendly approach.2-IODOXYBENZOIC ACID (IBX) belong to ë^5 iodanes class of hypervalent iodine compounds. It has emerged as green oxidant in comparison to conventional chemical oxidants. The study on amino acid oxidation has found the significance in various fields of sustainable approach towards environmental protection. The kinetics of amino acid oxidation in acetic acid-water solvent system was investigated during present study. Dynamics measurements study showed Lineweaver-Burk relationship suggesting towards Michaelis-Menten type of kinetics with respect to amino acids's concentration wheras first order dependence with respect to oxidant. The mechanistic determination involved detection of free radical, validation of isokinetic and Arrhenius relationships. Thermodynamic and activation parameters point towards formation of ordered complex in the mechanistic pathway. Based upon structure activity correlation analysis suitable mechanism has been proposed. Growth supporting potential of IBX was investigated on selected stage of plant system. Defined IBX concentration was found to be non-necrotic and growth stimulatory. IBX treatment favoured seed germination under controlled conditions. The positive effect of IBX on growth was correlated with the protein content in cotyledon stage. Total protein concentration was altered after IBX treatment. The increased accumulation of protein in cotyledon with the non-necrotic effect highlighted the greener character of IBX towards its possible application as an eco-friendly oxidant to be used in the field of organic synthesis and pollutant remediation.

PP-CYSA-01 : Influence of Urea and TMAO Osmolytes on Conformational Transition of Poly (N-isopropylacrylamide)-b-poly(acryloylmorpholine) block Copolymer

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Studies have provided evidence for the disruption of the hydrogen bonds of poly(N-isopropylacrylmide)-b-poly(acryloylmorpholine) PNIPAM-b-PACMO block copolymers in the presence of osmolytes such as trimethylamine N-oxide (TMAO) and urea. Herein, we synthesized poly(N-isopropylacrylamide)-b-poly(acryloylmorpholine) (PNIPAM-b-PACMO) by reversible addition”fragmentation chain-transfer (RAFT) polymerization and explore the effect of a mixed osmolytes environment on the aggregation behavior of copolymer. The investigation of the globular or collapsed state of aqueous PNIPAM-b-PACMO solution in the presence of co-solvents is exploited using various biophysical techniques like UV-visible spectroscopy, fluorescence spectroscopy, dynamic light scattering studies (DLS) and Fourier transform infrared spectroscopy (FTIR). The decrease in the lower critical solution temperature (LCST) with the addition of osmolytes and their mixed environment may be due to the different types of interactions (direct or indirect) with the hydrated, extended, coiled and globular states of PNIPAM-b-PACMO. TMAO is a better inducer for the collapsed state of PNIPAM than urea, and their mixture shows a drastic decrease in the LCST of block copolymer, because of the LCST decrease in both osmolytes individually, but the limited number of binding sites of PNIPAM is the main reason the mixture of urea and TMAO is not able to show an additive effect on PNIPAM agglomeration. Varying ratios of TMAO and urea are compared for a clear understanding of their behavior toward PNIPAM. Their mixed environment is a very good inducer of the globular form, compared to individual urea at higher concentration. The collapsed state of the polymer may provide sites or domains for drug encapsulation and release at the target by changing its conformation.

PP-CYSA-02 : Impact of Imidazolium type Zwitter Ion Ionic Liquids on Peroxidase Activity and Conformational Stability of Cytochrome C.

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There is considerable interest in the use of structurally stable and catalytically active enzymes, such as cytochrome c (Cyt c), in the pharmaceutical and fine chemicals industries. However, harsh process conditions, such as temperature, pH, and the presence of organic solvents, are the major barrier to the effective use of enzymes in biocatalysis. Functional Zwitter Ions (ZIs) developed from Ionic Liquids (ILs) are anticipated to exhibit IL-like characteristics because the word "zwitterion" itself indicates an ion pair where the cation and anion are covalently linked. There are some particular characteristics that ZIILs alone can display like cytochrome c gets renatured dissolved in polar phosphonate type ionic liquids by using highly polar ZIs, Phosphonate type zwitter ion used as an additive to improve the saturated water content of phase separated ionic liquid from aqueous phase towards reversible extraction of proteins. We demonstrate the suitability of imidazolium-based ZIILs as potential media for enzymes, in which remarkable enhanced activity and improved stability of Cyt c against multiple stresses were obtained. Among the several ZIILs studied, we observed the increase conformational stability and activity of Cyt c in the aqueous solutions of 4-(3-methyl-1H-imidazol-3-ium-1-yl)butane-1-sulfonate, 4-(3-ethyl-1H-imidazol-3-ium-1-yl)butane-1-sulfonate and 4-(3-butyl-1H-imidazol-3-ium-1-yl)butane-1-sulfonate compared to the commonly used phosphate buffer solutions (pH 7.2). The observed enzyme activity is in agreement with its structural stability, as confirmed by UV–vis, circular dichroism (CD). Moreover, it was found that the imidazolium-based ILs studied herein protect the enzyme against protease digestion and allow long-term storage at room temperature monitored by UV-vis spectroscopy and activity.

PP-01 : Synthesis of Carbon Quantum Dots as Rapid Charge Transport and Reinforced Polypyrrole Network as A High Performance Symmetric Supercapacitor

Gyan Singh*, Shumaila[1], Sushma Kumari* and Samina Husain*

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In this work, we report PPy, PPy-CQD1, PPy-CQD2, PPy-CQD3, and PPy-CQD4 composites synthesized by the in-situ polymerization method as electrode materials for supercapacitors. The as-synthesized composites are characterized and investigated by Ultra violet visible spectroscopy (UV), Fourier infrared spectroscopy (FTIR), X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The performance of the PPy-CQD3 supercapacitor device shows outstanding supercapacitive properties compared to other fabricated devices. It was found that PPy-CQD3 demonstrated the highest specific capacitance of 1093 Fg^{-1}at 10 mV/s as well as high energy density (66 $Whkg^{-1}$), power density (1090 Wkg^{-1}) and capacitance retention of 95% of its initial specific capacitance after 10,000 cycles at current density. The outstanding electrochemical performance of the PPy-CQD3 device is maybe due to the synergistic effect of CQDs on the PPy matrix, where rich pores and network structures made the electrolyte ions more easily accessible for faradaic reactions.

PP-02 : Microwave Assisted Synthesis, Characterization and Anti Corrosion Study of Imidazolium based Ionic Liquid.

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Nowadays, Ionic Liquids are widely synthesised by microwave irradiation due to their eco-friendly, less time consuming and easy to handling nature compare to the conventional methods. In this paper, we report the microwave synthesis and characterization of imidazolium based ionic liquids namely 1-ethyl-3-Benzylimidazolium Chloride [EBzImCl]. Microwave irradiation is a non-conventional heating source which is fast, efficient and solventless method for green synthesis. The above Ionic Liquid was prepared by microwave irradiation of equimolar mixture of Ethyl Imidazole and appropriate Alkyl halide. Prepared ILs was washed by Ethyl Acetate and dried by the help of Vacuum Oven. Further the structural conformations of the IL were carried out by IR, ^{1}H-NMR, ^{13}C-NMR spectroscopy and Mass-Spectrometry. The anti-corrosion properties of synthesized IL at different temperature on mild steel in 0.5M H_2SO_4 medium was calculated by various techniques such that weight-loss method (WL), potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS) and scanning electron microscopy (SEM). The WL results indicated that the maximum inhibition efficiency was obtained 91.75% at 1000 ppm concentration and 303K temperature. PDP and EIS results revealed the mixed type of behaviour and enhancement in the inhibition efficiency with the increasing concentration of IL. Thermodynamic data favour the physisorption behaviour. It is best fit with the Freundlich modal of adsorption isotherms. SEM confirmed the protective layer formation of IL on mild steel surface. ILs are good replacement of classic and toxic organic corrosion inhibitor and have a big impact on industrial fields and environment revolutions.

PP-03 : Photocatalytic Degradation of Ibuprofen Drug in Visible Irradiation using Nanosized $NiTiO_3$ Perovskite

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Nickel titanium oxide ($NiTiO_3$) nanoparticles were synthesized at low temperature in non aqueous medium by modified pechini method. The structural and morphological characteristics of the products were studied by powder X-ray diffraction, fourier transform infrared spectroscopy (FT-IR), UV-Visible Diffuse Reflectance Spectroscopy (UV-DRS), scanning electron microscope (SEM) and energy dispersive X-ray spectroscopy (EDAX). XRD patterns of powder revealed crystalline rhombohedral $NiTiO_3$ obtained at 700 ° C and this crystalinity increased with temperature. The DRS spectra reveal two peaks, one at around 440-450 nm and another one at around 740-750 nm. The band gap energy was calculated using Tauc plot and it was found to be 1.67 eV. Photocatalytic properties of $NiTiO_3$ on ibuprofen drug degradation is being investigated in the present study which has not been reported elsewhere and results shows that it is a prominent material for photodegradation of drug in the range of visible light.

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NOTE

NOTE

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(i) To advance and promote the cause of chemical research & education in the country.

(ii) To strive for strengthening co-operation on the national level and promoting contacts amongst scientist of the country.

(iii) To publish such proceedings, journals, transactions and other material as may be considered desirable.

(iv) To organize symposium, discussions, special lectures, exhibitions and other related activities for a better understanding of chemical research and its applications for the economic, social and industrial progress of the country.

(v) To under take any or all other acts, matters and things as are conducive to, or incidental to, or necessary for, the above objectives.

(vi) To work in association with International Societies of Chemistry and to co-operate with other organizations having similar objectives

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