XXXX1
ANNUAL CONFERENCE
INDIAN
COUNCIL OF CHEMISTS

27th - 29th DECEMBER, 2022

DEPARTMENT OF CHEMISTRY
INSTITUTE OF BASIC SCIENCES, KHANDARI
DR. BHIMRAO AMBEDKAR UNIVERSITY, AGRA

ABSTRACTS BOOK - 2022

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ABSTRACTS BOOK

Department of Chemistry
Institute of Basic Sciences, Khandari
Dr. Bhimrao Ambedkar University, Agra

27th - 29th DECEMBER, 2022

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 XXXXI Annual Conference of ICC from 27th - 29th December, 2022 at School of Chemistry, IBS Khandari, Agra-282002.

The leading researchers and key opinion leaders in Chemistry have been invited to facilitate sessions and deliver lectures at XXXXI 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 Agra the City of Taj. You can enjoy there too.

Thank you for your participation.

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

PROVISIONAL PROGRAMME

Tuesday, 27th December, 2022

04.00 to 05.30 pm	Registration at **Department of Chemistry, IBS**
05.30 to 08:00 pm	Inauguration, Award Ceremony and Keynote address at **Hotel Clarks Shiraz, Agra**
08:00 pm onwards	Dinner

Wednesday, December 28th, 2022

All Events at Department of Chemistry, IBS

08:00 to 09:00 am	Breakfast
09:00 to 11:00 am	Symposium on "Materials, Health & Environmental Sciences"(MHE) (common to all delegates)
11:00 to 01:00 pm	Sectional Presidents address in respective sections Invited lectures and paper presentations
01.00 to 02.00 pm	Lunch
02:00 to 06:00 pm	Invited lectures and paper presentations
06:00 to 07:30 pm	Poster presentations
07:30 to 08:30 pm	Cultural Programme (J.P. Sabhagar, Khandari)
08:45 pm onwards	Dinner

Thursday, December 29th, 2022

All Events at Department of Chemistry, IBS

08:00 to 09:00 am	Breakfast
09:00 to 12:00 noon	Invited lectures and paper presentations
12:00 to 01:00 pm	International online presentations
12:00 to 01:00 pm	Poster presentations
01:00 to 02:00 pm	Valedictory Function
02:00 to 03:00 pm	Lunch

The detailed programme of each day and each section shall be circulated in the Conference.

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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 XXXXI Annual Conference at Agra on 27th - 29th December, 2022 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 41 years of its existence.

The Council is grateful to Prof. Ajay Taneja, Prof. Devendra Kumar, Prof. Gautam Jaiswar, Staff Members and Students of School of Chemistry, IBS Khandari, Agra for their utmost cooperation in organizing this 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
MHE-SP	-	Symposium

Life Time Achievement Awardee Lecture to be given as Key Note Address

Chemistry is all that "Clicks" : Case of Versatility of Thermal Analysis

Ranjit K. Verma

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The phenomenon of "snapping together of the molecular building blocks" has taken "click chemistry" to new heights and this year's Nobel Laureate, Carolyn Bertozzi has shown how this concept can be utilized in living organisms. This has further proved the 'versatility' of chemical sciences. As an example, the versatility of Thermal Analysis shall be discussed. Being a group of techniques monitoring temperature dependent properties has some application in almost all branches of science involving synthesis, characterisation or suitability of substances. Differential Scanning Calorimetry, Dynamic Mechanical Analysis Nanocalorimetry/ultra-chip calorimetry and some coupled techniques shall briefly be overviewed. Properties of nano materials and their applications are dependent upon the synthetic technique and the sintering temperature that can be optimised using DSC etc. Ferrites, chromites and aluminate spinels have been synthesised using optimisation technique, and studied.

In a similar way, the thermooxidative decomposition in edible oils is of great concern. Thermal stability and shelf life of mustard oil was studied using oxidation induction period method. It has been found that stability of the oil increases with decreasing partial pressure of oxygen in the reaction atmosphere at lower temperatures. In air atmosphere, the stability is approximately 3 times higher than in O_2. Stability of the curcumin-doped samples was found to be independent of partial pressure of O_2, at higher temperature. This may be because of reactions involving curcumin and different fatty acids.

To be presented in Inauguration Session

Prof. W. U. Malik Memorial Awardee Lecture

Metal-based Potent Anticancer Therapeutic Drug Candidates : Structure Elucidation, Validation of Cytotoxic Response Against Chemo Resistant Cancers

Sartaj Tabassum

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Metal-based chemotherapeutics gained prominence as a potent class of anticancer drugs owing to their distinct physico-chemical properties, geometrical preferences in biological spaces and multimodal mechanism of cell death via myriad pathways, apoptosis, ROS-mediated cell death , anti - angiogenesis and proteasome inhibition etc and reduced toxicity profile. In lieu of above, we undertook to design a series of tailored potent metallic-based drug formulations, that were isolated and fully characterized by various spectroscopic methods and single X-ray crystal diffraction studies. *In vitro* binding studies of the promising candidates were carried out with therapeutic target biomolecule, ct-DNA by using various complementary biophysical techniques and molecular docking studies. To predict the mechanistic pathway of these newly designed metal-based drug candidates, gel electrophoretic assay was performed with plasmid pBR322 DNA ascertaining the cleavage efficiency of the compounds via hydrolytic/oxidative discernible pathway. To understand the drug-bio-macromolecules interactions and the affinity of compounds towards proteins was also investigated. The cytotoxicity activity of potent metal-based drug candidates showed high inhibitory activity against a panel of chemosensitive cancer cell lines validating that these metallic drug candidates could kill cancer cells effectively at a low intracellular concentration.. The mode of cell death induced by complexes was apoptosis, as revealed by AO/EB staining and Hoechst 33258 staining. The selected compounds were evaluated *in vivo* and found highly effective at lower doses as compared to the existing drugs.

To be presented in
Inorganic Section

Prof. S.P. Hiremath Awardee Lecture

Enhanced Sensing Performance of Morphology and Size Dependent Novel Nanomaterials

Navinchandra Gopal Shimpi

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Spherical shape copper (Cu) doped ZnO nanostructures of various amount (3, 6, 9 and 12%) were synthesized. The XRD, FTIR, UV-Visible, HR-TEM, FESEM, EDS, SAED and XPS were done to understand the structural, optical, morphology and shape of Cu doped ZnO nanostructures. To achieve the best gas reaction, doping concentration was optimized. ZnO and Cu doped ZnO nanostructures were exposed to various oxygenated volatile organic compounds (OVOCs) and found to be more selective towards acetaldehyde sensing. For 50 ppm acetaldehyde gas, temperature study was done at various temperatures (RT, 50, 100, 150, 200°C) which showed optimal at 100! for maximal gas response. The response and recovery time was 16.53 and 18.36 seconds for 50 ppm of acetaldehyde gas. The gas sensing study was carried out at different humidity rates (11, 32, 51, 63 and 84%) using different saturated solutions. 9 % Cu doped ZnO shows maximum response (61.53%) as compared to pure ZnO and 3, 6 and 12% Cu doped ZnO. The spherical shape Cu doped ZnO sensing response was increases with increase in concentration of gas from 10 to 300 ppm. Acetaldehyde gas shows enhanced selectivity towards spherical shape Cu doped ZnO sensors as compared to the other OVOCs like acetone, ethyl methyl ketone, methanol, ethanol, n-propanol, n-butanol, formaldehyde, acetaldehyde, propionaldehyde and acrolein. The reproducibility of Cu doped ZnO was studied for 50 days. Also, after acetaldehyde gas sensing change in morphology study of sensor was done. Moreover, Spherical ZnO nanostructures doped with Sn nanoparticles (2%, 5%, 7%, and 10%) were created using the hydrothermal technique. Characterizations included XRD,

FTIR, XPS, HR-TEM, FESEM, SAED, EDS, BET and UV-Visible. Maximum gas response was achieved by optimising doping concentration. When ZnO and Sn doped ZnO nanostructures were examined at various temperatures (room temperature, 100, 150, 200, and 250 °C), it was discovered that 150 °C provided the best gas response. Using several saturated solutions, the gas sensing study was conducted at various humidity rates (11, 32, 51, 63, and 84%). In comparison to the undoped and doped sensors (2, 7 and 10%), the 5% Sn doped ZnO sensor has the highest response (75%). Compared to other gases, acetone gas exhibits improved selectivity towards Sn doped ZnO sensors. Response and recovery times for 5% Sn doped ZnO are 30.19 and 63.54 seconds, respectively, and repeatability was examined for roughly 60 days.

To be presented in
Inorganic Section

Prof. Kaza Somashekhar Rao Awardee Lecture
Women Scientist Award

Next Generation Electrochemical Sensors and Biosensors

Nimisha Jadon

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Disposable electrodes gained attention in recent years due to its electrochemical and economical characteristics, in the analysis of various types of inorganic and organic compounds in different matrices. Disposable sensors based on screen printed electrodes (SPEs), carbon paste electrodes (CPEs), pencil graphite electrodes (PGEs) including microelectrodes and modified electrodes have led to new possibilities in the detection and quantitation of many target analytes such as biomolecules, pesticides, antigens, DNA, microorganisms and enzymes. Disposable sensors are in tune with the growing need for performing rapid and accurate in-situ analyses and for the development of portable devices. Application of disposable electrodes modified by different modifiers has also proved to be powerful tools for analysis of a vast array of compounds. Miniaturization of modified disposable sensors via microchip format may decrease the analysis time, sample volumes, reagent consumption and improve portability for in situ determinations. Microfluidic devices have attracted considerable attention during last few years for detection of compounds but more work is needed to integrate the different functionalities and overcome the challenges related to miniaturization of disposable analytical devices. Much has been done in the field of fabrication of disposable sensors; yet many new avenues remain to be opened and followed.

To be presented in
Environmental & Analytical
Chemistry Section

Dr. Arvind Kumar Memorial Awardee Lecture

Nanostructured-based Electrochemical Sensors for Toxic Molecules

Nagaraj P. Shetti

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In the present scenario, environmental pollution is the biggest problem that has become difficult to tackle, as many emerging pollutants are continuously introduced into the environment. This substance poses a significant threat to the environment and humans due to its difficult decomposition and high toxicity. Therefore, developing a safe and simple method for detecting toxic pollutants is essential. Among many detection methods, the electrochemical method shows many advantages, including high sensitivity, low limit of detection (LOD) and low cost. One such technique is voltammetry, which can quantify a trace amount of the toxic substances; out of all voltammetric techniques, cyclic voltammetry (CV) and square wave voltammetry (SWV) find extensive applications. Furthermore, carbon-based and metal-based nanomaterials are excellent electrode modifiers due to their large specific surface area and strong electron transmission performance. Therefore, the selectivity and sensitivity of the electrochemical system toward toxic pollutants could be enhanced by modifying the electrode. Further, using the SWV technique, trace-level toxic substances such as pesticides can be detected. The agricultural and environmental relevance of the developed method was successfully used for monitoring toxic substances in ecological samples, viz., water, soil, vegetable and fruit samples. In addition, advanced state-of-the-art nanostructured materials have the potential for application in electrochemical sensing platforms as they demonstrate high-performance electrochemical sensitivity, selectivity and long-term stability.

To be presented in
Physical Chemistry Section

Prof. S. T. Nandibewoor Awardee Lecture

Development of Advanced Super-Capacitive Charge Storage Materials

Raj Kishore Sharma

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Unveiling the role of active sites is of great significance for the design and development of high performance energy storage materials. Defects in the form of vacancies and edges act as charge storage active sites and are not considered as imperfections. These defects have the ability to modulate electronic, surface and electrochemical properties. The active research on the supercapacitor these days involves the exploration of the fact that defects not always act as imperfections to the material but can be treated as energy storage sites. A number of questions that needs to be answered for the proper understanding of the field includes, which kind of lattice defects enhanced the performance of electrode material? How these defects can be generated in controlled, low-cost, scalable, and reproducible manner? How they can be identified and estimated in an appropriate way? How do they improve the activity of the material and what is the exact relation between structure and activity of the material? In recent years, oxygen vacancies rich perovskite oxide based supercapacitor has seen an unprecedented popularity due to their structure/composition flexibility and anion intercalation charge storage mechanistic path. Still, a number of questions are left unanswered for the proper understanding of this field. Such as, what kind of structure modulation enhanced the stability of perovskite electrode? How the leaching of metal cations during electrochemical process can be prevented? What kind of doping positively influences the charge storage? How do oxygen vacancies contribute in the entire charge storage process? In this regard, we have tried to answer the above questions on the basis of experimental and theoretical investigations. Thus, we have made an attempt to comprehensively and critically review the factors favorable for design of high rate perovskite oxide based supercapacitor electrode.

To be presented in
Physical Chemistry Section

Prof. S.M.L. Gupta Memorial Award

Application of Doped Nanomaterials and Nanocomposites for the Advanced Oxidation Processes to Remove Organic Water Contaminants from the Aqueous Medium

Vinod S. Shrivastava

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Advanced oxidation processes (AOPs), such as photolysis, photocatalysis, ozonation, Fenton, and wet air oxidation, have been investigated extensively for the removal of a wide range of trace organic contaminants (TrOCs) from the water. Doping to minimize band gap energy and improve morphology is the established process however, recently doped semiconducting materials are extensively coupled with carbonaceous materials like carbon fibers (CF), graphene oxide (GO), graphitic carbon nitride (g-C_3N_4) and carbon nanotubes (CNT). The discussion in this section is based on the development of the metal-doped, metal non-metal doped multi-doped semiconducting materials and, nanocomposites of MWCNT decorated by doped semiconducting materials of ZnO, ZrO_2, and Bi_2O_3. The materials were characterized by advanced characterization techniques like TEM, SEM, XRD, EDAX, FT-IR, UV-RDS, etc. Variable organic contaminants like organic dyes and pesticides were tested for degradation. The catalysts synthesized were tested for degradation in different conditions by altering the pH, organic contaminant concentration, concentration of dopants, etc. The effectiveness of the degradation was tested by techniques like TOC and LC-MS. The reusability of the material is a critical factor for the effectiveness and it was tested for all the materials. Overall, the metal-doped, metal-nonmetal multi-doped, and, carbonaceous nanocomposites prepared can be some potential candidates for advanced oxidation processes for water purification.

To be presented in
Inorganic Chemistry Section

SYMPOSIUM ON "MATERIALS, HEALTH & ENVIRONMENTAL SCIENCES"

Chairman Remark

Prof. Ajay Taneja

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Materials, Health and Environment represent three aspect of human life. With materials providing the stem of human growth, every discovery in material science adds a small step for development of human kind. Benefits such as identification of biomarker and early detection of various diseases has been proved beneficial for complete treatment. The field of materials have not just held the advancement in various fields in science and innovation but also additionally contributed towards the change of nature of human life all things considered.

Environmental issues such as non-biodegradable plastics, pollution, global warming have been becoming increasingly challenging. Scientists from different fields have been trying to solve these challenges. Many studies have been undertaken in the last decade to provide scientific evidence for policies to reduce the threats to health posed by the many environmental hazards to which people are exposed in their daily lives.

The Symposium's specific objectives are:

• to highlight issues in environment and health research so that it can be solved by cost effective interventions.

• to explore viewpoints covering areas with metals ceramics glasses polymers, electrical material, composite materials, Nano structured materials, biological and biomedical materials and their application to various fields of environment and health.

Present symposium on "Materials, Health and Environmental Science" will try to bring expertise in from different aspects to interact which each other in the historical city of Agra. It is believed that this symposium will provide best forum to the best talents in academia and research institute to collaborate and address the current challenges, to seek new windows for discovery and exploration and to promote the new horizon of science and technology for sustainable future. Outcome of this symposium will improve our understanding the way we should face these challenges.

MHE-IL-01 : Starbon Mediated porous Metal Oxide Nanocomposites as Efficacious Catalytic Materials

Surinder Kumar Mehta

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Starbons™ are a family of mesoporous carbonaceous materials derived from polysaccharides.Starbons™ possess high surface area, large accessible space, electrical conductivity, thermal stability, scalability, low density and interconnected hierarchical porosity at different length scales, which are very favorable for adsorption, photocatalysis, separation, energy storage and conversion.

One recent development in this field is directed towards the incorporation of foreign metal oxide nanoparticles into the matrix of porous material. A novel MoO_3 nanoparticle-Starbon composite is fabricated using microwave technology. Due to the inherent properties of Starbon (mesoporous, high surface area) and MoO_3nanoparticles, this composite serves as a proficient catalyst for the abatement of common water pollutant i.e., 4-nitrophenol which is a known carcinogen, teratogenic and mutagen. Further, CeO_2 decorated Starbon matrix is also explored as an efficient catalyst for the dephosphorylation of 4-nitrophenyl phosphate disodium salt hexahydrate. Therefore, these studies present an endeavor to contribute to burgeoning research in the fields of scalable synthesis and catalysis by manufacturing green metal oxide-based nanostructures.

MHE-IL-02 : Miraculous Chemistry of sp^2hybrid Carbons

C. P. Bhasin

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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 upto a few micro-meters and even the larger but the thickness is only single or a few-atoms thick (typically less than 5 nano-meter). Although their exploration dates back a few decades, 2004 year marked the ultrathin 2D nanomaterials resurgencewhen Gem & Novoselovsuccessfully exfoliated graphene from graphite using Scotch tape. 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 materialswith special reference to their application for fluoride removal in the drinking water will be highlighted.

MHE-IL-03 : Green 2D Nanostructured Materials for Environmental Remediation

Rengaraj Selvaraj

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Renewable and green energy research has been attracted much attention worldwide because renewable resources are a promising approach to address the global environmental pollution and energy production complications. Recently a substantial progress has been made in the development of highly active photocatalytic 2D nanomaterials for environmental applications. Especially metal free photocatalysts such as modified and unmodified graphitic like carbon nitride (g-C_3N_4) materials. Metal free semiconductor has attracted a lot of attention due to its exceptional electron mobility properties. The presence of pharmaceuticals in the aquatic environment has received increasing attention as environmental issue. This is due to improper discharge of industrial, hospital and wastewater or household

activities. These contaminants can cause severe adverse effects in human and wildlife. Therefore, removal and degradation of pharmaceuticals is of a great concern in environmental and health risk management. So far, many pharmaceuticals compounds has been detected in the wastewater and ground water. Recently, our research group have developed modified and unmodified photocatalytic 2D nanostructure materials for environmental applications. We demonstrate that several process parameters strongly influence the morphology and the efficiency of the final product. The synthesized products have been characterized by different advanced analytical methods, which includes XRD, FE-SEM, EDX, XPS, UV-DRS. Furthermore, the photocatalytic activity studies revealed that the synthesized 2D nanostructured materials exhibited an excellent photocatalytic performance in rapidly degrading various pharmaceuticals, where more than 95% efficiency achieved within short period under solar or visible-light irradiation. Also we have applied this materials for the effective removal of oil from oil contaminated wastewater.

MHE-IL-04 : Clean Energy Initiative through Solar-Hydrogen Generation : Opportunities and Material Challenges in Photoelectrrochemical Water Splitting

Rohit Shrivastav

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Production of renewable and non-polluting fuels by the direct utilization of solar energy is a fascinating challenge for the scientific community in the 21st century and one of the pre-requisites to improve the living standard of the world's population and support economic growth. Sunlight that represents clean, renewable and abundant energy-source on earthcan be converted to hydrogen by photo-splitting of water. The processoffers long-sustainable and environmentally-benign alternative to the fast-depleting global-stock of fossil fuels, and respite from burgeoning concerns on adverse climatic changes and other environmental problems associated with large-scale burning of fossil fuels.Of the many approaches to produce renewable-hydrogen, solar-light-induced direct electrolysis of water in photoelectrochemical (PEC) cell is distinctly the most promising method.PEC water splitting is a process thatinvolves illuminating the semiconductor electrode by light/solar light, with the absorbed photo energy used to split water into hydrogen and oxygen. This one step process eliminates the need to generate electricity from solar energy and subsequently feeding it

into an electrolyser, as in the case of photovoltaic-electrolysis system. However, the key challenge to be taken in the field of PEC cell is to develop efficient, corrosion resistant photoelectrode material. To date no ideal water splitting photoelectrode material being available, research is being pursued on the design of novel materials with desired properties. The greatest requirement for fundamental research concerns doping for bandgap shifting and surface chemistry modification. Corrosion and photocorrosionare other major concerns that need to be addressed most, particularly usingthe best available material options. Computational approach may be a tool in this screening to yield necessary insight into different materials and identify the most suitable one for PEC system.This talk deals with an overview of the basic principle, recent advancements, challenges and opportunities on solar-hydrogen generation by photoelectrochemical water splitting.

MHE-IL-05 : Design and Optimization of a Bioprocess for Bioremediation of Malathion by Micrococcus Aloeverae

Mohd. Ashraf Dar **and Garima Kaushik**

Department of Environmental Science, School of Earth Sciences, Central University of Rajasthan, Bandarsindri, Ajmer, 305817, Rajasthan
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Malathion is widely used as an agricultural insecticide, but its toxic nature makes it a serious environmental contaminant. To screen indigenous bacteria for malathion degradation, a strain MAGK3 capable of utilizing malathion as its sole carbon and energy source was isolated from agricultural soil. Based on morphological and biochemical characteristics and 16S rDNA sequence analysis, strain MAGK3 was identified as Micrococcus aloeverae. The strain was cultured in the presence of malathion under aerobic and energy-restricting conditions, and reverse-phase UHPLC–DAD analysis indicated that a considerable degradation (66.79%) was attained with malathion (0.03%) being the sole carbon source after 240 h of incubation. To enhance malathion biodegradation, effects of co-substrates, pH, temperature, initial malathion concentration, agitation (rpm), and inoculum size were evaluated using Taguchi methodology. Experiments with various combinations of factors were conducted, and results in respect of malathion biodegradation were evaluated in the Qualitek-4 software to determine the key effect of individual factors, their interaction effects, and optimal levels of process factors. All parameters contributed to malathion biodegradation, and Taguchi DOE's ability to predict optimum response, was established by experimentation via optimized

levels of factors. Results confirmed that pesticide concentration caused the maximum impact on malathion degradation. Before optimization, Micrococcus sp. MAGK3 had an average degradation of 57.94% within 168 h, but after optimization, the rate of biodegradation improved to 87% within 38 h. Confirmation of malathion degradation to malathion mono, diacids, and phosphorus moiety was performed by Q-TOF–MS analysis, and a pathway of biodegradation was proposed.

MHE-IL-06 : Alleviation of Bioaerosol by Chitosan Basednanofabric Material : A Promising Approach towards Antibacterial Applications

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Exposure of airborne pathogenic microorganisms to human being can aggravatea numerous adverse health effects viz. infections, allergic reactions and majority of respiratory diseases. The associated risk of infections caused by the exposure of these airborne pathogens has led to the interest in development of antimicrobial materials for emerging sustainable environment in terms of better air quality. Keeping these views in mind, present study screened the airborne pathogenic bioaerosol mitigation potential of biopolymer based nanofibers (Chitosan/PVA) loaded with silver nanoparticles as a biocide by an environmental friendly approach. Successive formation of AgNPs by using Aloe-vera plant extract has been confirmed by characterizing these particles and average size was found to be approximately 50nm. In order to enhance the biological reactivity, AgNPs have been assimilated into the biopolymers and fabricated through the electrospinning method resulting in the formation of uniform bead free nanofibers of smaller diameter ranging from 30-80 nm Specific ratio of CS/PVA (30:70) fibers with different concentration of AgNPsnano-filler exhibited an adequate surface area (39.6-83.1 m^2g^{-1}) for releasing the essential functional groups in order to prevent the microbial growth. No evidence of cytotoxicity of these scaffolds was observed in cell-viability test, suggested their biocompatible nature. The pore diameter of these fibers was found to be in between 115-130 nm with % porosity concentrated in 45 %, favorable for air-filtration applications. Results of antibacterial efficiency of these fibers demonstrated their promising antibacterial action against airborne pathogens, and fibers embedded with maximum content of AgNPs showed maximum inhibition on microbial growthwhich has been further confirmed by flow- cytometric analysis. Results derived from the

current study showed the reliability of these scaffolds in terms of their efficacy, cost effectiveness and biocompatibilityfor developing different products such as individual protection (masks), air filters and can also be feasible for incorporating them as window screening in reducing the exposure to environmental bio-contaminants of emerging concern.

MHE-IL-07 : Industrial Waste Management: Challenges and R&D Perspectives in India

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India is rapidly moving from an agricultural-based economy to one that is industrial and services-oriented. The management of industrial waste disposal has become more challenging as a result of the current economy's rapid growth. Every year, there are enormous amounts of industrial trash produced and most of them are dumped or burned, which eventually create environmental problems like ecological degradation and health risks to living beings. In contrast, numerous sustainable approaches to integrated solid waste management have emerged as a result of recent advancements in environmental policies. Reuse, remanufacturing, and recycling techniques for handling industrial waste have drawn a lot of attention as a result of their ability to reduce costs over time and support profitable recovery firms. A weak institutional structure, a dearth of sufficient environmental laws, and low enforcement of laws governing industrial waste management all serve to exacerbate these effects. The primary industrial waste management challenges, R&D perspectives, and accessible treatment methods are highlighted in this article.

MHE-SO-01 : A Study on Indoor Radon, Thoron and their Progeny Level by Nuclear Track Detectors : A Brief Report from the State of Nagaland

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There has been an increasing concern regarding exposure to radon (^{222}Rn), thoron (^{220}Rn) and their progeny due to their detrimental effects on human health. In fact, radon, thoron and their progeny contribute a major fraction of total dose to human beings from all possible sources of natural radioactivity. Epidemiological studies have discovered

significant evidence of a relationship between indoor radon and lung cancer, even at relatively low radon levels. There have been several studies on radon and thoron measurements by several authors using passive methods. It had been the usual practice to calculate both the radon and thoron progeny concentration from the measured gas concentration using an assumed equilibrium factor. However, this process of progeny concentration estimation involves a lot of uncertainty especially in the case of thoron progeny Thus in order to provide a realistic assessment of these species in the indoor environment, it is necessary to conduct direct measurements of radon and thoron and its progeny, since inhalation doses are predominantly due to decay products of radon and thoron, and not due to the gases themselves. With the development of pinhole twin cup dosimeters, Direct Thoron Progeny Sensor (DTPS) and Direct Radon Progeny Sensor (DRPS), one can measure the radon, thoron and its progeny concentration directly with these detectors. Although radon problem is so far not seen as a major concern in India, there is still a need to delineate the variability of radon levels in Indian dwellings. This requires systematic studies for collecting, centralizing and interpreting the data obtained through different groups with reliable techniques. Thus it was felt that a detail study on the presence of radon and thoron would be very useful for data base creation for the state of Nagaland. Present paper present results of this study

MHE-SP-01 : Analysis of Fluoride Ground Water of Bareilly District (U.P) India

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The Physico-Chemical condition of ground water of Bareilly district (U.P) has been studies and four water samples 2 from hand pumps and 2 from tube well were collected from two different villages near by Bareilly City. The duration of study was from Jan 2022 to March 2022. The Physico-Chemical parameters analysed were pH, temperature, turbidity, DO, BOD, COD, Chloride, fluoride, sulphates, nitrates and total hardness. It was observed that all other parameters were within range when compared with WHO standards, only fluorides and chlorides were present in excess amount in tube well water of Faridpur and Bhojipura two villages. It has also been observed fluoride ions Concentration as compared to hand pump water samples.

MHE-SP-02 : Photosensitized Degradation of 4-Methylaniline using TiO_2 as Photocatalyst

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The photocatalytic action of the TiO_2 has been studied on4-methylaniline. Photocatalyticdegradation of 4-methylaniline solution in a suspension of titanium dioxide was carried with the use of artificial light sources (UVA). The effects of various process variables on degradation performance such as concentration of substrate, catalyst concentration, pH and intensity of light have been investigated. Photoproduct was characterized by physical, chemical and spectral methods. A tentative mechanism has been proposed with overall reaction.The results show that the degradation of the substrate can be carried out conveniently and efficiently using TiO_2 semiconductor as photocatalyst.

MHE-SP-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.

MHE-SP-04 : Development and Validation of RP-HPLC Method for the Estimation of Clonazepam in Tablet Dosage Form

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Validation is an important feature in any method of quantitative drug analysis because it is closely related to the quality of the results. So, there is always a need to develop validated analytical method. Only such methods are used for routine analysis and for study of stability of the drug products. The aim of the present investigation is to develop a validated analytical method using RP- HPLC for clonazepam in tablet dosage form. The Chromatographic separation was done using a mobile phase of anhydrous dibasic ammonium phosphate, methanol and tetrahydrofuran in the ratio60: 52:13 respectively, using C8 5µcolumn (4.6 × 150mm), UV detector maintained at 254nm. The method was validated in terms of system suitability, specificity, linearity, accuracy, precision, robustness and stability studiesaccording to the ICH guidelines. The retention time of clonazepam was 8.92 min.The calibration curve waslinear in the range of 80 to 140mcg/ml with correlation coefficient of 0.999; theaverage recovery was found to be 100.52%, 99.87% and 100.13% at various concentration.The percentage relative standard deviation for precision was 0.38%.Stability studies at different time intervals starting from one hour to 22hours by keeping at room temperature was done.This demonstrates that the proposed method was simple, sensitive, precise, accurate, linear, robust and stable for the estimation of clonazepam in tablet dosage form.

MHE-SP-05 : Copper Oxide Encapsulated Zeolite Catalyst from Coal Fly Ash for the Degradation of Crystal Violet Dye by Wet Catalytic Method

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Water contamination caused by colours/dyes from many industries, including textile, paper and pulp, tannery, dye and dye intermediary, and Kraft bleaching, is a severe issue for wealthy nations. Wet catalysis involving environmentally benign oxidants like H_2O_2, peroxo mono and disulphates, etc., is a green method and an efficient advanced

oxidation process (AOP) for the degradation of organic contaminants. In this work, a new active zeolite supported copper catalyst was developed from coal fly ash by immobilization of copper nanoparticles. Zeolite (Zeo) was synthesized from FA by acid and hydrothermal treatment. Copper nanoparticles are synthesized from Catharanthus roseus leaf extract. The formed copper nanoparticle was encapsulated into the zeolite framework by mechanical stirring followed by calcination at 550ºC. The prepared CuO-Zeo catalyst was characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Scanning electron microscope (SEM) and Energy dispersive X-ray (EDX) techniques. Catalytic activity of the synthesized CuO-Zeo material was investigated by crystal violet dye degradation by wet catalytic method in the presence of H_2O_2. The effect of catalyst dosage, catalyst variation, dye concentration, volume of H_2O_2 and pH were studied. It was observed that the catalytic activity of base Zeo is negligible and is enhanced by copper encapsulation and also the efficiency of the catalyst is tested and .95% is maintained.

MHE-SP-06 : Metamaterials : The Future Material

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Metamaterials are the artificial materials designed to obtain the exotic physical properties that do not exist in natural materials. The Physical properties of metamaterials are not primarily dependent on the intrinsic properties of the chemical constituents, but rather on the artificial internal structures. These artificial structures function as the atom and molecules in traditional materials while through regulated interaction with the electromagnetic light waves they can generate novel properties that are difficult or even impossible to obtain with natural materials. Metamaterials offered the capability of researchers in the limit of their facilities to design material properties at will. This paper focuses on the fundamentals, recent developments and forthcoming directions in the research of metamaterials. This paper starts with an overview of metamaterials and then goes into great depth about how to create metamaterials with previously unheard-of electromagnetic properties. A number of intriguing phenomena and applications associated with metamaterials are discussed, including negative refraction. Finally, we conclude offer an outlook on future directions of metamaterials.

MHE-SP-07 : Electroless Plating Loaded Cr-P 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 herein used the 3% CrP-cocatalyst modified graphene oxide(GO) by usingtwo step electroless plating method. As-synthesised materials shows 10.8foldsincrement inphotocatalytic H_2 production rate ofGO/Cr-P (491.078 ìmol$g^{-1}h^{-1}$) in comparison to the pristine GO (45.470 ìmol$g^{-1}h^{-1}$) in 20% CH_3OH under 300W Xenon light source.The apparent quantum efficiency of the system was calculatedi.e. 1.49%.Based on advance analyses techniques photocatalytic electron transfer mechanism is proposed Cr-P accelerated the separation of photo e^-- h^+ pair to relay the photoe- via Cr-P particles to H_2O that improves the photocatalytic water splitting of pristine GO.

MHE-SP-08 : Preparation & Characterization of Ag/AgBr@MoS2 NCs using bio-based Surfactant Choline Deoxycholate and their Application in Degradation of Rhodamine B

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We exfoliated bulk MoS_2 into few-layer 2D nanosheets by ultrasonication[1,2] method using choline deoxycholate as a surfactant and stabilizer.Techniques such as AFM analysis, Raman spectroscopy, XRD, and UV-Vis-NIR spectroscopy were used to characterize exfoliated 2D MoS_2 nanosheets.After separation using centrifugation, the exfoliated 2D MoS_2 nanosheets were used as a substrate for in-situ preparation of the Ag/AgBr[3] NPs on the surface of the 2D MoS_2 nanosheets to form Ag/AgBr@MoS_2 nanocomposites(NCs) in the presence of sunlight.Ag/AgBr NPs were also prepared using the same method in the absence of nanosheets. The prepared Ag/AgBrNPs and Ag/AgBr@MoS_2[4] NCs were characterized employing UV-Vis-NIR spectroscopy, XRD , XPS, TEM, and HRTEM analytical techniques,

and were further utilized for the degradation of the Rhodamine B dye under sunlight. The Ag/AgBr@MoS_2 NCs showed enhanced catalytic activity as compared to the Ag/AgBr NPs because the 2D MoS_2 nanosheets provide greater surface area for the adsorption of the reacting molecules and prevent charge recombination by delocalizing electrons and holes throughout thesurface. In this way, a new sustainable method for the preparation of photo-catalytically active nanocomposites is reported.

MHE-SP-09 : Potentiality of Low-Cost Adsorbent for the Sequestering of Synthetic Dye from Aqueous Solution

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Dyeing is a key process in textile industries. In which the decolorization of dyeing bath has to be done for providing higher efficiency of dyeing of apparels. A substantial part of this process deals with pigments, which are released to the environment after decolorization due to incomplete dye fixing. Most of the dyes having synthetic origin and usually denoted to be highly toxic substances. Wastewater from these industries poses serious environmental problems.One of the widely used water treatment technologies is biosorption, biosorbents are recognized as a green, cost-effective and efficient alternative. Therefore, the search for locally or regionally available biomass for dye removal has gained rapid attention. In this context, a comprehensive understanding of the biosorption capacity of different biosorbents is necessary.

In this study, the adsorption potential of an adsorbent prepared from Araucaria plant leaves was evaluated for the removal of Methyl Orange (MO) dye from aqueous solution. Batch adsorption experiments were performed with different operational parameters such as adsorbent dosage, initial dye concentration and contact time. The adsorption capacity of experimental leaf powder for the removal of MO dye was correlated by both Freundlich and Langmuir isotherms. The kinetic study revealed that the second-order kinetics were in better agreement with both first- and second-order kinetics. The thermodynamic adsorption parameters showed that the adsorption process is exothermic. Experimental data show that Araucaria plant leaf powder was effective in removing MO from aqueous solutions.

MHE-SP-10 : Optimization and Batch Studies of Cationic Dye Removal using Plant Leaf Powder

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Pollution emanating from effluents containing residual dyes which are not biodegradable has become a serious environmental problem in the last decade due to the increasing and fast-growing usage of dyes in different applications. Even small amount of dye in water effects the aesthetic value and water transparency in water bodiestherefore the contaminated dye in waste water needs to be removed before released to natural stream. The dye removal process which is the low cost of operation and occurred through the green reaction under the usage of the natural waste is the interested method.Biosorption is leaded to the decolorizing the waste water by using the agricultural waste through the adsorption technique.

In this study the Malachite Green (MG) adsorption onto Plumeria alba leaf powder was investigated in terms of both adsorption efficiency and kinetic study. The effect of various parameters i.e. initial dye concentration, contact time, adsorbent dosage, pH and temperature were investigated. The adsorption data fitted the isotherm model such as Langmuir, Freundlich. Thermodynamic parameters (Such as ΔG^0, ΔH^0, ΔS^0) were also determined to find out the spontaneity of the adsorption process. The experimental results showed that the adsorbent has heterogeneous surface activity and the adsorption of dye on it follows pseudo-second order kinetics and the adsorption is spontaneous and exothermic.

MHE-SP-11 : Bio-Inspired Synthesis of Catalytically and Biologically Active Silver Nanoparticles using Camelusbactrianus Urine

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Silver nanoparticles are synthesized by reducing Ag ions using the liquid metabolic waste of Camelusbactrianus urine. Various bio-molecules present in camel urine are effectively used to reduce silver ions to silver nanoparticles in a single step. The synthesized nanomaterials were characterized using advanced characterizations which ensures the formation of silver in nano form. The synthesized bio-inspired AgNPs show potential antimicrobial and antioxidant

activities. Both of the antimicrobial and antioxidant activity helps in study application of nanoparticles in medical and veterinary sciences.

MHE-SP-12 : Water Extract of Piper nigrum Seed Assisted Synthesis of Palladium Nanoparticles and Reduction of Various Nitro Compounds by $NaBH_4$ in the Presence of PdNPs as a Catalyst

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An attempt has been made for eco-friendly synthesis of palladium nanoparticles by water extract of Piper nigrum seed. The formation of PdNPs and their morphology is assured using different advanced characterization techniques such as UV-Visible spectroscopy, XRD, and FE-SEM images of PdNPs. Further, we wish to report for the first time reduction of various nitro compounds to corresponding amines by NaBH4 in the presence of PdNPs as a catalyst. After the reaction course, PdNPs 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.

MHE-SP-13 : Preparation of Ag/AgBr@MoS_2 NCs using Bio-based Surfactant Choline Deoxycholate and their Application in Degradation of Rhodamine B

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In this study, we exfoliated bulk MoS_2into few-layer 2D nanosheets by ultrasonication[1,2] method using choline deoxycholate as a surfactant. The exfoliated 2D MoS_2 nanosheets were characterized by AFM analysis, Raman, XRD, and UV-Vis-NIR spectroscopy.Exfoliated 2D MoS_2sheets were separated from the unexfoliated part by centrifugation method. After centrifugation, the exfoliated 2D MoS_2 nanosheets were used as a substrate for in-situ preparation of the silver nanoparticles (AgNPs) on the surface of the 2D MoS_2 nanosheets to form Ag@MoS_2 nanocomposites[3] in the presence of sunlight.Ag NPs were also prepared using a similar protocol in the absence of nanosheets. The prepared AgNPs and Ag@MoS_2 NCs were characterized by using UV-Vis-NIR

spectroscopy, XRD analysis, XPS, TEM, and HRTEM analysis. The prepared AgNPs and Ag@MoS_2NCs were used for the degradation of the Rhodamine B dye[3] under sunlight. The Ag@MoS_2NCs showed greater catalytic activity as compared to the AgNPs because the 2D MoS_2 nanosheets provide greater surface area for the adsorption of the reacting molecules. The 2D MoS_2nanosheets also carry the electron generated by the localized surface plasmon resonance of the AgNPs.In this way, a new sustainable method for the preparation of photo-catalytically active nanocomposites is reported.

MHE-SP-14 : Studies of Chemical Parameters in Ground Water of Kaman Tehsil of Bharatpur District (Rajasthan)

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The ground water is the major source for drinking water. The ground water resources include hand Pumps, tube wells, and open wells. The availability of fresh, safe ground water is very scarce and restricted due to peculiar hydrological, geological, geomorphic and demographic features. A variety of chemical substances like fluoride chloride, nitrate, calcium carbonates & Bicarbonates and other dissolved solids are dominant in the ground water Contamination. A study has been carried out for the determination of chemical parameters such as Fluorides, Chlorides, Nitrates, Hardness, Alkalinity and Total dissolved solids in the ground water resources in Kaman Tehsil of Bharatpur district, Rajasthan.

This study shows a huge variation in these chemical parameters such as fluoride ranges from 0.5 ppm to 8.36 ppm, chlorides ranges form 40 ppm to 2700 ppm, Total Hardness ranges from 70 ppm to 4500 ppm, Total dissolved solids ranges from 228 ppm to 10450 ppm and Alkalinity ranges from 30 ppm to 2400 ppm.

MHE-SP-15 : Fatty Acids Composition and Elements Analysis of Cassia Siamea Lam Seed Oil

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Cassia siamea Lam is well known Ayurvedic medicinal tree. Cassia siamea Lam is a genus of family Fabaceae and sub-family Caesalpinioideae which is selected for investigation. In this study, we determined the fatty acid composition and elements analysis of Cassia siamea Lam seed oil. The oil was extracted from Cassia siamea Lam

seed using a Soxhlet extractor with n-hexane as solvent. The fatty acid composition was analyzed by using the GC-FID technique and elements were analyzed by the ICP-MS instrument. Unsaturated fatty acids and saturated fatty acids are very important for pharmacological investigation. Linoleic and gamma linoleic acids are important unsaturated fatty acids that can be used in the synthesis of tissue hormones. Elements Pb, Cu, As, and Sn levels in this oil were measured. Although this oil contains lead and copper, it does not contain As or Sn. Cu is required in the body to prevent anemia, heart diseases and nervous disorders is found in this oil. A very small amount of Pb is present in this oil, which is not harmful to our bodies. Fatty acids and Elements of Cassia siamea Lam seed oil suggest that it may find application in both cosmetic and pharmaceutical natural product formulations.

MHE-SP-16 : A Facile Green Synthesis, Morphological and Antibacterial Studies of Mn and Cu Codoped ZnO Nanoparticles

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In the present study, a green, sustainable, simple and cost-effectivemethod was adopted for the synthesis of Mn and Cu codopedZnO NPs. The FTIR spectra of all samples showed bands in the lower region may be attributed due to stretching vibrations of M–O bond indicating the formation of nanoparticles.The size and morphology of the nanoparticles were determined by P-XRD and FE-SEM studies respectively. Energy-dispersive X-ray diffraction was used to determine the elemental composition of the synthesized nanoparticles.P-XRDresults revealed that the particle size of synthesized nanoparticles exist in the nanometer range.The morphology of the pure ZnO has been changedafter codoping with Mn and Cuas indicated by FE-SEM.The synthesizednanoparticles were screened for antibacterial activity in vitro against gram-positive bacteria Staphylococcus aureus and gram negative bacteria Escherichia coli by adopting disk diffusion method.The results of antibacterial studies exhibited potential antimicrobial activity.These investigations could be used in antibiotic development which further gives a direction for biomedical applications.

MHE-SP-17 : Morphological and Antibacterial Activity of ZnO Nanoparticles Synthesized by Plant Leaves Extract of Psidium Guajava

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Green synthesis is an emerging area in which nontoxic chemicals are generated using environmentally friendly and bio-safe reagents and also be considered as a convenient alternative to the physical and chemical methods. This research work involves the development of better and reliable method for the formation of zinc oxide nanoparticles through eco-friendly plant mediated Microwave Assisted synthesis. The formation of nanoparticles was confirmed by UV-Visible spectral studies and FTIR analysis. The size of the nanoparticles was determined by P-XRD studies that revealed the average particle size of synthesized nanoparticles exist in the nanometer range. The FE-SEM, EDAX images indicated rod shaped nanoparticles. The synthesized nanoparticles were screened for antibacterial activity in vitro against gram gram negative bacteria Escherichia coli and Klebsiella Pneumoniae by adopting disk diffusion method. The results of antibacterial studies exhibited that ZnO nanoparticle were potential antibacterial agent.

MHE-SP-18 : Optical, Structural and Morphological Studies of Plasmonic Ag-TiO_2 and Au-TiO_2 Nanocomposites and investigation of their Solar-mediated Photocatalytic activity by Degradation of Methyl Orange and Rhodamine-B Dyes

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Environment pollution have become major challenge in 21 century because of increase inworld population,rapid development of industrialization, shortage of clean water and water contamination has become a global issue. Therefore, research for producing materials is very urgent to solve these problems. In the present study, Ag-TiO_2 and Au-TiO_2 were synthesized by using sol-gel method. The synthesized nanocomposites were characterized by XRD, UV absorption studies and FESEM/EDX. The bandgap of nanocomposites was calculated by using Tauc-Plot which was found to be around 3.02eV (Ag-TiO_2) and

2.99eV (Au-TiO_2) lower the (3.29eV) TiO_2. The photocatalytic efficiency of synthesized nanocomposites was analysed by photocatalytic degradation of Rhodamine-B and Methyl Orange under solar and UV irradiation. The results of photocatalytic activity concluded that Ag-TiO_2 shows 83% degradation of MO after 35 minutes of solar irradiation and Au-TiO_2 shows 85% of degradation of Rh-B after 4 hours of solar irradiation.

MHE-SP-19 : Formulation of Anti-tuberculosis Drug Loaded Starch Propionate Microparticles for Controllable Drug Delivery

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The goal of this study was to use an emulsification solvent evaporation approach to formulate anti-tuberculosis drug (isoniazid, rifampicin, and pyrazinamide) loaded starch propionate microparticles (ATD-SPMPs). Fourier transform infrared spectrometry revealed that starch propionate (SP) exhibited new bands at 1749cm^{-1} and 1236cm^{-1}, whereas SPMPs had identical peaks. The A-type pattern of native starch was entirely changed into the V-type pattern of SP by X-ray diffraction, while SPMPs showed a similar type pattern with SP having reduced crystallinity. Propionylation improved the thermal stability of native starch by reducing the number of hydroxyl groups in the modified starch molecule. SPMPs have superior thermal stability than SPMPs due to their semi-crystalline structure. In the optimized formulation, the highest percentage encapsulation efficiency of isoniazid, rifampicin, and pyrazinamide was determined to be 37.6%, 45.2%, and 43.1%, respectively. Scanning electron microscopy revealed that propionylation partially disturbed the granule morphology of native starches, and the imperfections and porosity structures of SP granules were completely changed into the uniform-sized spherical shape of SPMPs. The geometric particle sizes of the blank SPMPs, isoniazid, rifampicin, and pyrazinamide loaded SPMPs were 1.243 ± 0.3 µm, 1.65 ± 0.2 µm, 2.73 ± 0.7 µm, and 2.69 ± 0.5 ìm, respectively. The dialysis bag method was used to study drug release from ATD-SPMPs and in-vitro drug release data was also analyzed using several kinetic models. The in-vitro drug release investigation revealed that drug release from SPMPs was controlled in comparison to pure ATD using the Korsmeyer-Peppas model, indicating drug release by anomalous diffusion, i.e., non-Fickian diffusion. Overall, the formulated ATD-SPMPs may be regarded as a potential anti-tuberculosis micro-drug, offers a path forward for tuberculosis clinics.

MHE-SP-20 : Nanotechnology in Food Packaging Applications

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Nanotechnology is a rapidly developing field and nanomaterials are of significant technological and economic interest and have a huge impact on many industries especially in the food packaging industry.Nanomaterials are often used to improve the properties of food packaging due to their antimicrobial, UV protection activity and possibility of oxidation prevention.The usage of nanotechnology in the food sector is focused on improving food quality and safety in form of the incorporation of nanoparticles in food or packaging materials. To create new food packaging functions, the use of nanotechnology enables possible improving the properties of food, such as healthier, tastier as well as improved nutritious food, when it is packaged. In the present presentation we will focus on the different materials or composites that will be used for making materials in the applications of food packaging.

MHE-SP-21 : Incorporation of Carbon Nanotubes as Transparent Conductive Electrode in ITIC-OE Accepter Organic Solar Cell

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The most common transparent conducting electrode, ITO, is delicate and prone to shattering under mechanical stress, which lowers the device's performance on flexible plastic substrates. Because of their exceptional optical transparency, low sheet resistance, and great mobility, carbon nanotubes have garnered a lot of interest as a Transparent Conductive electrode in organic solar cells. Molybdenum Trioxide (MoO_3) doping of carbon nanotube Transparent Conductive electrodes makes p-doping, good energy-level alignment, and improved hole transport possible.In the present study, the performance of Non-Fullerene ITIC-OE Acceptor Organic Solar Cells with a transparent electrode fabricated from Carbon Nanotubes doped with Molybdenum trioxide (MoO_3) is simulated using SCAPS 1-D.The optimized PCE of 24.94 %, Fill Factor (FF) of 74.02 %, J_{sc} of 35.32 mA/cm^2 and V_{oc} of 0.9539 V are shown in the current work by varying the band gap of MoO_3 doped CNTs. Also, upgrading the simulated cell's Electron transport Layer (ETL) with SnO_2, TiO_2, and ZnO yields an

optimized result with TiO_2 ETL, having PCE of 25.71%, FF of 76.30%, J_{sc} of 35.32 mA/cm^2, and V_{oc} of 0.9539 V.These results demonstrated the possibilities for ITIC-OE acceptor Organic Solar Cells with Transparent Conductive Electrodes made of carbon nanotubes to advance device performance in the near future.

MHE-SP-22 : Synthesis of Highly Reactive Supported Platinum Catalyst and its Characterization

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Being a precious metal catalyst, it is necessary that platinum must be highly dispersed on support material that results in a large specific surface area and consequently higher specific activity of catalyst. In order to obtain these objectives, we prepared nanostructured alumina supported platinum catalysts using wet impregnation technique. This catalyst has active metal component on the surface of a nano-structured support, a highly porous, thermo stable material (with a high surface area and suitable mechanical strength) and hence the catalyst life. Using different synthesis techniques, nanostructured alumina supported platinum catalysts were prepared in the laboratory by maintaining 0.1-0.2 wt% of platinum concentration and low heating rate (0.2!/min) during calcination. The percent of platinum exposed on surface and dispersion on alumina were characterized by using H_2-chemisorption technique. One of our synthesis method has given around 59 percent platinum exposed onto the support surface and most of the platinum particles within size range of 60 to 150 nm. Our best catalyst sample could only be determined by integrating the outcomes of hydrogen chemisorption, TEM and XPS results. It is also found when a volatile component was present in the impregnating solution it gave higher values of percent platinum exposed, better dispersion and preferential distribution of nano sized platinum near the surface of catalysts.

MHE-SP-23 : An Indigenous Tool for the Adsorption of Rare Earth Metal Ions from the Spent Magnet E-Waste : An Ecofriendly Bio-Polymer Nanocomposite Hydrogel

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Polymer bionanocomposite hydrogel (PNC-hydrogel) have attracted the focus and attention of young and dynamic researchers in water

remediation and its purification as well. The acrylic acid and acryl amide functionalized chitosan effectively enhances the usability capacity thousand times in comparison to the virgin biopolymer. The functionalization of the biopolymer is proficient enough for binding the rare earth ions from the waste water solution and it is done by grafting of biopolymer with variety of co-polymers. Herein, SiO_2 nanopowder embedded bionanocomposite hydrogel (SCB-hydrogel) has been prepared. The impact of various parameters such as pH, adsorbate doses, time of contact, concentration of metallic ions, kinetic parameters with proper isotherms, desorptivity, and reusability of the PNC was studied in batch adsorption mode. The adsorption efficiency by the PNC-hydrogel with increasing concentration of lanthanide ions was observed to be 99% from the waste diluted water followed by Langmuir model along with Pseudo second-order kinetics. The adsorption efficiency of these PNCs didn't alter much as with the original in reusability of maximum three times. So the PNCs can be effectively used as the novel bio-adsorbent for treatment of waste water containing pollutants along with transition rare earths (Nd^{+3}, Pr^{+3}).

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

Sectional President's Address

$MgFe_2O_4@SiO_2–SO_3H$: Environmentally Benign Catalyst for Green Synthesis of Benzoxazinone and Benzthioxazinone via Multicomponent Reactions under Solvent Free Condition

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Catalysis is a very rewarding field and magnetic recovery of catalyst added a greener approach to it. In the context of Green Chemistry catalysis has received a remarkable interest, both from a scientific and an industrial perspective. It deals with the reduction of the hazardous impact of chemicals and chemical process on the environment. Catalysis has been a central them in green chemistry since it inherently embraces waste minimization of materials as well as energy. During the recent year's silica-coated magnetic nanoparticles have been found very useful and interesting applications due to its unique characteristics which make it suitable for different applications. The surface functionalization of silica-coated magnetic nanoparticles using reactive organic and inorganic group allows synthesis of multifunctional of silica-coated magnetic nanoparticles. Moreover, structural, magnetic and optical environments in spinel ferrites can be quite different, due to the distribution of iron and the divalent metal ions among the tetrahedral and octahedral sites of the spinel lattice. Recently, we have developed a number heterogeneous supported catalysts which showed improved efficiency for several important reactions. In the present work we have described a sulfuric acid-functionalized silica-coated magnetic nanoparticles ($MgFe_2O_4@SiO_2–SO_3H$) and its characterization by XRD, FT-IR, TGA, SEM-EDS, TEM

and surface area measurements. The performance catalyst towards different multicomponent reactions such as benzoxazinones, benzthioxazinones, imidazole, pyranopyrazoles etc. have been explored under solvent free conditions. The product distribution pattern with the variation of different reaction conditions such as reaction temperature, solvent, molar ratio, effect of non-conventional energy source, concentration of catalyst and reaction time. The attractive features of this protocol are its greenness with respect to mild reaction conditions, high activity, and easy work-up, excellent yield and reusability of a catalyst. All synthesized compounds were characterized by various physiochemical techniques such as ^{1}H & ^{13}C-NMR, FTIR, Mass spectral data, melting points and compared with reported values. It is expected that the fundamental knowledge discussed in the work will serve as a powerful tool for carrying out Green Chemistry.

AIL-01 : Biodiversity of Medicinal Plants of Nepal-A Health Care Overview

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Medicinal plants are used as a source of drugs for the treatment of various human and livestock health. According to WHO, "A medicinal plant is any plant which in one or more of its organs, contains substances that can be used for therapeutic purpose, or which are precursors for chemo pharmaceutical semi-synthesis" Nepal is a country full of medicinal herbs and shrubs. Because of the diverse climatic conditions of Nepal, many types of medical herbs are available. Nepal has significant variation in altitude ranging from 67 meters in southeastern Terai to the tallest mountain on earth, Mt Everest, measuring 8,848 meters. This gives Nepal a remarkable variety of its flora and fauna resources. Nepal has 35 different types of forests and 118 different ecosystems. Most of the high-value medicinal herbs are available in northern Nepal. In Nepal, we use these herbs in Ayurveda medicine and also as home remedies. Nepal is one of the popular countries with medicinal herbs, shrubs, or trees. Our medicinal plants are useful for the treatment of various medical conditions. Moreover, medicinal herbs and plants come under one of the top export products of Nepal. These days too, we first try home remedies instead of going to the doctor for a checkup, if we have any of the medical conditions. If medicinal herbs in our home don't heal us, only after we choose hospitals and doctors for option. Thus, today in this lecture we will learn about top 20 best medicinal plants of Nepal and also some herbal products manufactured in Nepal with its composition and uses.

AIL-02 : Why Indoor Chemistry Matters

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Chemicals found indoors are a significant risk factor that can modify or degrade the indoor environment. Direct emission of chemicals into the indoor environment can occur from various sources, including building materials, paints, stoves, cleaning products, furnishings, and personal care products. Biological sources including microorganisms, plants, pets, other animals can also contribute to indoor chemistry. Why does indoor chemistry matter? It matters because people spend most of their time at home or in other indoor locations. Complex mixtures of chemicals in indoor environments may adversely impact

indoor air quality and human health. People are often in close proximity to sources and processes that, respectively, emit and transform chemicals. Whether exposures to indoor chemicals result in an adverse effect is dependent on exposure duration and additional factors, including the inherent toxicity of the chemical mixture, chemical concentrations in the environment, the route of exposure, and the susceptibility of the person. This study explores indoor chemistry from different perspectives including sources and reservoirs of indoor chemicals and the ability of these chemicals to undergo transformations and partitioning in the indoor environment. In some cases, indoor chemistry can result in the creation of potentially more or less toxic products, reactive intermediates, or products with different physiochemical properties. Understanding large differences in indoor exposures requires deeper insight on the societal and systemic context in which exposures occur in residential and nonresidential environments. This study provides a status report for indoor chemistry research. The goal is to improve our understanding of how indoor chemistry is linked with chemical exposure, air quality, and human health.

The presentation will also identify future research needs

AIL-03 : Water Recycle Treatment Plan of West Water -case study- Surat City

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In recent years lot of awareness and concern has developed over the environment issue of the chemical industries. The pollution control board is also becoming stricter in the implementation of the pollution control act. This has brought a lot of environmental pressure on the chemical industries. Environmental pollution affects our health. We expect Urbanization & Industrialization to bring in prosperity. But they lead to many environmental problems, related to polluted air, water& soil resulting in increase in various diseases Ensuring development of sustainable, green solutions in the fields of water treatment. We have to adopt and respond to new challenges more rapidly than ever before. We are learning that we need to innovate solutions and systems that are both locally appropriate and globally relevant. Surat is largest textile center in the world for production of synthetic fiber fabrics like Nylon& polyester. There are more than 400 textile processing units – water based industries situated in and around Surat city in various industrial clusters. Here I want to discuss the case study of Surat city west water treatment Plane & earning

Money. One process Mill for dying & Printing process per day require -100000 liter river water.

-Per day required 400 X 100000 = 400000000 liters water and all this water are wasted as effluent. One of my PhD student Dr. Nemish Vashi & SMC negotiated with Industries Association to make use of 40 MLD tertiary treated sewage water of Industrial grade to promote reuse and recycle of west water.

This would enable SMC to reduce pressure on ground water resources in the city and earn money.

AIL-04 : Design and Development of Nanoparticles-based Colorimetric Sensors

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Recently, the nanoparticles (NPs) based sensors have received significant attention for the detection of various types of analyte molecules possibly due to simplicity, rapidity and high sensitivity. The method is based on the color changes of NPs that is induced by aggregation of NPs after the addition of analytes. In addition, the attention has been drawn in the direction of preparation of flexible paper based chemical sensors using metal nanoparticles (NPs). Paper based devices have been emerging trend in developing a new analytical device for wide range of applications in the field such as clinical, food and environmental monitoring. The use of NPs based chemical sensor is found simple, rapid and can be used for multiple analyses with reproducible results and cost effective compared to spectroscopic and chromatographic methods.

AIL-05 : Eu-doped ZnO@graphene Oxide : A Winning Horse for Effective Photocatalytic Water Splitting

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In this study, the feather-like Eu-doped ZnO (particle size ~34.87mm and Eg ~3.13eV) nano-assembly was synthesized by using the capping agent CTAB (cetyltrimethylammonium bromide)-supported hydrothermal method. The Eu-doped ZnO was loaded onto the graphene oxide surface and as-synthesized Eu-doped ZnO@GO (particle size~23.07 mm and Eg~0.79eV) applied to measure the photocatalytic water splitting activity in 20% CH_3OH under 300W Xe light source. Eu-doped ZnO@GO exhibited the higher hydrogen generation activity of

255.8 $mmolh^{-1}g^{-1}$ that is 159 and 1.5 times more than the pristine GO and Eu-doped ZnO systems, respectively. The composite shows the 6.47% apparent quantum efficiency for the system at 420nm. Eu-doped ZnO enhances the photocatalytic activity of GO because the p-n junction formed between GO and Eu-doped ZnO might support the charge-transfer and suppression the charge recombination enhanced the light harvesting power of GO and ZnO makes the charge transfer smooth through GO network. Surface photovoltage and electrochemical impedance study of the Eu-doped ZnO@GO composite, GO acts as the p-type semiconductor and Eu-doped ZnO worked as an n-type semiconductor and their interface facilitates the p-n junction to ease charge separation that enhance the water-splitting efficiency.

AIL-06 : Developing Effective Remediation Technologies for Water Treatment : Challenges & Opportunities

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Contamination of aquatic system/water resources by heavy metals, radioactive waste, and microbes has become significant health concern globally. Extensive industrialization, exponential rise in population, anthropogenic and geogenic activities have been recorded as principle causes of water contamination. Investigators are making consistent efforts in developing smart functional materials viz. Carbon nano tubes (CNT), metal organic framework (MoF), and biogenic nanomaterials have evolved as reliable and efficacious materials for water remediation.

AIL-07 : Calix and Calix functionalized Metal Nanoparticles : Opportunities and Challenges

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Within the macrocyclic family, calixarenes are undoubtedly amongst the most popular members, due to their interesting chemical and physical properties. Indeed, since its renewal in the late 70's, calixarene has emerged as versatile macromolecules and found its way in most fields of molecular chemistry and materials. As a result, calixarenes are now very popular in diverse areas such as supramolecular systems, inclusion complexes, solid state architectures, ionic recognition, synthesis of nanoparticles-based architectures, catalysis, biological applications and so on. The basic calixarene

framework exists as a bowl shape macromolecular architecture. Its unique shape, tunable cavity, ease of preparation and potential applications makes it very attractive area of research. Our research interest are mainly focused on the design and synthesis of supramolecular architectures and investigating their photo physical properties toward their broader use of chemical sensors, catalytic activity and biomedical applications. Employing suitable functionalization, we have designed chromophores, that exhibits strong colorimetric and fluorescence signals. This photophysical properties are utilized to determine the binding behaviour of targeted guests including nitroaromatic compounds (NACs), organophosphorous compounds (OPs), cations, anions, chemical warfare agents (CWAs) etc.

AIL-08 : Interfacial Electrocatalysis for Green Energy and Clean Environment

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Today, energy crisis due to depleting fossil fuel supply and their negative impact on environment like global warming is probably the world's biggest problem. Efforts have been made to develop abundant, inexpensive and environment friendly renewable resources of energy among which water splitting using solar light is considered as one of the most potential approaches. Moreover, the exponentially increasing global CO_2 concentration in the atmosphere has stimulated an intense research activity towards the development of economically viable technologies for environmental remediation and search for carbon-neutral energy sources. In this regard, addressing CO_2 problem on the lines of the natural photosynthetic process continues to be a major challenge for the researchers. The use of electrochemistry and nanomaterials are considered as promising avenues to address this dual challenges. In this lecture, I shall discuss few recent examples of research that have been conducted by us at IIT Delhi, India to throw the lights on the numerous applications of electrochemistry in the field of materials science and technology for the green energy and clean environmental related applications. I shall focus on the photo-electrochemical water splitting process using semiconductor materials to convert solar energy directly into chemical energy in the form of H_2 and O_2 as well as the electrochemical conversion of CO_2 and N_2 using nanostructured materials.

AIL-09 : The Privileged Structures "Naphthoquinones", their Reactions with Primary Amines and Aminophenols, X-ray Structures and Biological Activity

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Naphthoquinones are privileged structures in pharmacology and medicines. The wide range of biological functions of quinones are because of their intrinsic redox nature. The clinically active anticancer drugs, doxorubicin, daunorubicin, mitomycin C, bleomycin, chlorambucil, etc., possess quinone chromophore in their framework. Aminonaphthoquinone moiety is found in a core structures of the antibiotics rifabutin, rifamycin(s), hygrosin A, Geldanamycin, Naphtomycin A, etc they exhibits anticancer, antibiotic properties. Plethora of synthetic naphthoquinones are known those possess several pharmacological activity such as anti-tuberculosis, anticancer, antibacterial, antifungal, and antimalarial activity. The unique biological properties of naphthoquinones are attributed to their ability to interact with biomolecules via $\pi\cdots\pi$ stacking, hydrogen bonding, van der Waals interactions, electrostatic along with hydrophobic and charge transfer (CT) interactions. Some of the recent applications of naphthoquinones includes photosensitizers in Dye Sensitized Solar Cells (DSSC) and chemosensors.

The present endeavour includes some of recent results obtained in our laboratory on naphthoquinone chemistry. The reactions of naphthoquinones with primary amines, amino phenols, pyridylamines, and oximes are discussed with respect to their single crystal X-ray structures, chemosensor and biological activity. Hydroxy naphthoquinones are also versatile ligands in coordination chemistry. First row transition metal complexes their X-ray structures, anticancer activity will be discussed.

AIL-10 : Spectrophotometric Determination of Validamycin Pesticide in Environmental Samples by Mixed Micellar Cloud Point Extraction

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Validamycin is a fungicide most widely used to treat the sheath blight disease of crops like rice, wheat, vegetables etc. which is harmful

for human organisms. The extraction and determination of this pesticide in vegetables and water surrounding paddy fields is therefore important. Cloud Point Extraction approach is a Green Separation method for the extraction and pre concentration of Validamycin fungicide residues in different water samples. The present work describes the results of a new mixed micellar surfactant Could Point Extraction (CPE) method developed using Sodium Dodecyl Sulphate (SDS) and TritionX-114 (TX-114) for preconcentration and UV-Visible Spectrophotometry for determination. To get the greatest extraction efficiency, parameters like pH of solution, surfactant concentration (SDS and TX-114), concentration of salting out agent (NaCl), equilibrium time and temperature were optimized. The experimental results show that the most effective conditions for the extraction of Validamycin are: pH-4.0, surfactant concentration SDS - 0.14 W/V%, TX-114 – 2.0 W/V%, concentration of NaCl-2.4 W/V%. The equilibrium temperature was found to be 50! & equilibrium time was found to be 15 min. Under these optimum conditions, calibration curves were found to be linear in the range of 0.153 – 3.074 mg/ml. The method was then successfully applied to the determination of Validamycin in vegetables and water samples of paddy fields.

AIL-11 : Assessment of Carbonaceous Aerosols Over India, Mass Level & its Impact on Regional Climate

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Carbonaceous aerosols (organic carbon: OC and black carbon/ elemental carbon: BC/EC) constitute a significant fraction (~10–70%) of the fine aerosol mass ($PM_{2.5}$) and have gain significant importance in aerosol research due to adverse effects on human health, environmental issues as visibility impairment, regional air pollution, climate change etc. The effects of these aerosols depend on particle size and chemical composition. In order to reduce the adverse impacts and to develop the mitigation strategies for air quality control, the knowledge of atmospheric aerosols and its chemical composition is very essential, especially over the developing countries in South Asia with the highest emissions. In view of the above importance, monitoring of mass PM, carbonaceous aerosols as well as it impact on climate were studied over India. The long term highest mass level of $PM_{2.5}$ were recorded (~120 μgm^{-3}) (annual mean) over Delhi which is around 10 times higher than the US-EPA standard (12 μgm^{-3}), however, the BC mass concentrations were around 7 μgm^{-3} (annual mean) with the highest (>20 μgm^{-3}) in the winter and lowest in the monsoon

(~ 4 μgm^{-3}). During the winter period, the contribution of OC was 7 times higher than the EC indicating significant influence of biomass and biofuel burning (burning of wood and agricultural waste). Radiative forcing due to aerosols and BC were studied and higher atmospheric heating rates up to 1.9-2.0 K day^{-1} was observed over Delhi. The BC DRF was found to be larger for air masses traversing North Western India, Indus Basin and Punjab, which were identified via the concentrated weighted trajectory analysis as the carbonaceous aerosol hot-spot areas over the Indian subcontinent. Our study indicates that the policy level changes is required to mitigate the excess carbonaceous aerosol over this region which ranks among the highest in India and elsewhere especially during the post-monsoon and winter seasons.

AIL-12 : Application of Kinetics in Environmental Analysis

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After the study of the rate of inversion of sucrose (hydrolysis into glucose and fructose in the presence of an acid in 1850 by Wilhelmy (Germany), the two great chemists Peter Waage and Cato Guldberg in 1864 pioneered the development of chemical kinetics by formulating a simple law called as 'the law of mass action', which states that the speed of a chemical reaction is proportional to the quantity of the reacting substances. This olden day development of the chemical kinetics has now opened door for its application in various fields in modern age. The thoughtful study of the kinetics and reaction mechanisms of transition metal complexes (redox or ligand substitution) began some around six decades ago and many of which opened the door for their direct applications. My laboratory at the University of the South Pacific (USP) has been involved in studying the kinetics and mechanisms of the redox as well as ligand substitution or redox reactions followed by their applications as analytical and environmental analysis tool. Therefore, several reactions such as redox reactions, ligand substitution reactions and metalloporphyrin formation have been utilised as indicator reactions for the development of catalytic kinetic methods for trace analysis.

In this presentation on 'Kinetics in Analytical and Environmental Applications', an attempt will be made to highlight brief principles and procedures along with the most recent research carried out in our laboratory for the trace determination of inorganic as well as

organic chemical species based on their catalytic/inhibitory effects on selected indicator reactions.

AIL-13 : Simultaneous Detection of Hazardous Skin Whitening Agents in Indian Cosmetic Products using a Novel Green Chromatographic Technique

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The present work mainly highlights the simultaneous detection of four skin whitening agents i.e. hydroquinone (HQ), resorcinol (RS), catechol (CC) and 3,3'-dichlorobenzidine (DCB) in facial creams and body lotion, which could initiate adverse effects on the human body. Among these, the first three are positional isomers of dihydroxybenzene so simultaneous separation is difficult with the conventional reverse-phase high-performance liquid chromatographic technique (RP-HPLC). The selected skin whitening agents were detected in facial cream and body lotion using micellar liquid chromatography coupled to a photodiode array detector (MLC-PDA). Optimization of the method was accomplished using response surface methodology (RSM) with central composite design (CCD). The optimized mobile phase was 0.15 M SDS-0.01 M NaH_2PO_4-7% (v/v) 1-butanol, pH 7 that provided a chromatographic run time of 7.5 min. for the simultaneous determination of selected analytes. The correlation coefficient (r^2) values were satisfactory between 0.998-0.999 over the linear concentration range of 0.125-10 ìg/mL. Limits of detection (LODs) and the limits of quantification (LOQs) for the four skin whitening agents were 0.01-0.02 ìg/mg and 0.04-0.09 ìg/mg, respectively. The developed method is fast, cost-effective, and green which could operate for complex matrix (facial creams, body lotion) without any pretreatment other than filtration. The results indicated that the MLC-PDA method proved to be more suitable for the simultaneous separation of selected positional isomers.

AO-CYSA-01 : Characterization and Microbial Nature of Aerosol in Ambient Air of Agra During Pre-winter Season

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Aerosol plays a very important role in climate change and public health. It affects cloud condensation nuclei and causes a number of epidemic diseases. The correlations of aerosol with epidemic diseases are due to the biotic components of aerosol. In the present investigation, the microbial activities, metal concentration, and particulate matter ($PM_{2.5}$ and PM_{10}) in the ambient environment of the city of Taj, i.e., Agra (India) were assessed. The composition of bacteria and fungi using a culture technique was also examined, which indicates that bacterial concentration was higher as compared to fungi. The levels of $PM_{2.5}$ and PM_{10} are much higher than the recommended value set by NAAQS in India. Bacterial and fungi count numbers and nomenclature were also reported in the study. Instead of the traditional culture method, BOD incubation techniques had been adopted in this study. Culture techniques had been used for microbial growth and biological characterization using different media, pH, temperature, and incubation periods. This study may help in developing a standard method for bacterial and fungal characterization.

AO-CYSA-02 : Particle Induced Toxicity in Association to Transition Metals and Polyaromatic Hydrocarbon Contents

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Air Pollution is regarded as one of the great existential challenges of the anthropogenic 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. Airborne particulate matter (PM) is a heterogeneous mixture of metals, inorganic ions, organic matter, PAHs originated from both natural and anthropogenic sources. Several epidemiological studies have clearly demonstrated strong linkage of PM and adverse health effects, such as cardiovascular and respiratory diseases, premature deaths, impaired pulmonary function, and other neurodegenerative disorders. Toxicological studies have provided an important clue in this direction by suggesting oxidative stress as the most important mechanism for PM-driven health effects. It has been demonstrated that ambient PM is capable of redox cycling the electrons from biological reductants to oxygen and generate reactive oxygen species (ROS) that oxidizing important biomolecules such as DNA and proteins.

In this work, a selection of datasets of studies done on PM characterization and toxicological assessment at Pune, India is presented. Sampling was undergone at university campus of SPPU, Pune to monitor PM_{10} and $PM_{2.5}$ concentration and assessment of toxicological profile of associated metals and polycyclic aromatic hydrocarbons (PAHs) was undertaken. The average concentration of both PM_{10} and $PM_{2.5}$ exceeded the Indian National Ambient Air Quality Standards and WHO guidelines. The ratios $PM_{2.5}/PM_{10}$ calculated in present study was found in the range between 0.48 and 0.80 with an average of 0.70 i.e. PM_{10} is composed of 70% of $PM_{2.5}$, indicating quite high proportion of fine particles in the city of Pune. The contribution of redox active metals (Fe, Cu, Cr, Ni and Mn) in PM was more as compared to non-redox metals (Pb, Cd and Co) indicating significant risk to the exposed population. The cytotoxicity induced by PM_{10} and $PM_{2.5}$ in A549 and PBMC cells varied from absolutely nontoxic blank to highly toxic one. A significant decrease in cell viability in a dose dependent manner was found in the cells treated with varying concentrations of PM. Regarding PAHs, the relative % distribution of Low molecular weight (LMW) three ring PAHs were found to be predominant for both PM_{10} and $PM_{2.5}$. The cytotoxic profile of PAHs determined by MTT assay demonstrated significant decrease in cell viability and PAHs associated with PM_{10} samples exhibited higher cytotoxic response. The redox activity measured by DTT assay exhibited the oxidative nature of PAHs associated with both sized PM. Source apportionment identified vehicular activity, industrial emissions, coal combustion, construction activities and soil and road dust were found to be the main source contributors to the PM bound metals at the sampling site. Results obtained in present study provides a basis for identifying the characteristics of PM sources and its related toxicity in Pune city that would aid in formulating effective strategies for source control and to address better community concerns.

AO-CYSA-03 : Carbon-based Material Obtained from Wheat Straw for the Adsorption and Photocatalytic Degradation of Organic Waste from Water

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Rhodamine B and Cr (VI) are the high-priority industrial pollutants and are known to cause serious effects to living beings, especially via accumulation in waste water. Their toxicity effects the organs of humans as well as aquatic ecosystem. Considering this, detoxification

of contaminated water is highly required. Photocatalytic degradation is one of the popular methods for degradation of organic waste in water. Many a times, the use of expensive reagents which are even not environmentally viable renders the process to be sustainable. Therefore, a sustainable, cost-effective and an eco-friendly method is essential for the degradation of water contaminants. Herein, carbonaceous material obtained from wheat straw after dissolution in Deep Eutectic solvent (DES) at optimum conditions is used as a photocatalyst for photo-degradation of Rhodamine B under sunlight along with the adsorption of Cr (VI) from waste water. The dissolved wheat straw in DES is regenerated using anti-solvent. The regenerated material is characterized using various spectroscopic techniques such as XPS (X-ray photoelectron spectroscopy), ^{13}C NMR, FT-IR (Fourier transform infrared), TGA (Thermogravimetric analysis), X-ray diffraction, UV-vis and Fluorescence spectroscopy. Further this carbonaceous material is employed for the adsorption of Cr (VI); adsorption and degradation of Rhodamine B in water under sunlight. The influence of concentration of Rhodamine B as well as regenerated material upon efficacy of photocatalytic degradation has been studied. Therefore, the results of present studies substantiate that material obtained from bio-mass is promising adsorbent for the removal and photocatalytic degradation for organic waste from water.

AO-CYSA-04 : Multivariable Regression Analysis Of Air Pollutant with Mobility Data in Agra City Uttar Pradesh

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Deterioration of air quality is a growing concern in the world. Air pollution causes serious health problems and also leading rise in death. The aim of this study is to quantify the magnitude and spatial variability of air quality parameters in the Agra region in the year 2021 and establish the relationship with the activity parameters. The actual data related to air quality in Agra (Sanjay Place) is obtained from Central Pollution Control Board (CPCB) website for four factors such as $PM_{2.5,}$ NO, NO_2, and OZONE. The mobility reports showing movement trends over time, geography across different categories of places such as retail and recreation, groceries and pharmacies, parks, transit stations, workplaces, and residential. The MINITAB software was used to analyze in depth. Minitab acts as a tool for applying Six Sigma principles (take air quality parameters as the dependent variable

and the other mobility factors as the independent variable to carry out multivariable regression analysis). The Multiple Regression Model demonstrated a positive relationship of mobility with $PM_{2.5}$ and No_2 concentrations, and NO concentration. $PM_{2.5}$ levels significant during the study period, and it was also related to the mobility data show a upward trend. In this study we see the $PM_{2.5}$ is the main air pollutant which effect on the human mobility. From the present study, it is evident that the air pollution scenario pertaining to the SPM concentration in the city is reached alarming stage at couple of sites.The findings are important for framing state and regional level policies for addressing air pollution problems in cities, and achieve the sustainable development goals (SDGs) linked to public health, reduction in the adverse environmental impact of cities, and adaptation to climate change, as indicated by SDGs.

AO-CYSA-05 : Core-Shell Chitosan Coated Lanthanum Iron Oxide for Electrochemical Determination of Food Freshness Level by Detecting Tyramine Contents

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Herein, the designing of chitosan (CS) loaded Lanthanum iron oxide (LFO) nanoparticles (CS/LFO) has been carried. The prepared x CS/LFO (x = 100, 200, 300, 400 and 500) were well analysed with several characterisation technique. The x CS/LFO modified glassy carbon electrode (GCE) was then utilized for electrochemical tyramine detection. Tyramine is a biogenic amine, the presence of which can be precisely related with the quality of the food products. The obtained electrochemical detection response was also compared with the pure constituents. The 400 CS/LFO modified GCE provided excellent electrochemical response for tyramine determination. The designed electrochemical sensor exhibited linear co-relation between anodic peak current and concentration of tyramine in the range of 0.02-100 µM with the detection limit of 0.6158 µM or 615.8 nM (by LSV method) and 0.5814 µM or 581.4 nM (by DPV method). Additionally, the designed 400 CS/LFO was also applied on the screen-printed electrode and further its stability was determined for a period of 30 days, in order to introduce a portable electrochemical sensor for tyramine detection. The real-time analysis proposed sensing platform was investigated via real sample analysis on various food products such as milk, beer, fish, meat and yoghurt.

AO-CYSA-06 : Exposure Assessment of $PM_{2.5}$-Bound Heavy Metals and their Association with Lung Cancer

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To better understand the toxicity associated with ambient $PM_{2.5}$-bound heavy metals, PM samples were collected using an SKC cascade impactor in November 2021, and blood samples of cancer patients were subsequently collected in Agra region from hospitals. The inductively coupled plasma mass spectrometry method was used for determining heavy metals in $PM_{2.5}$ and blood samples. The $PM_{2.5}$-bound average concentrations of Al, Cr, Cu, Fe, Mn, Ni, Pb, and Zn were 0.446, 0.036, 0.044, 0.392, 0.025, 0.006, 0.043, and 0.141 μg/m^3, respectively. The distribution of these metals followed the order: Al (39.39%) >Fe (34.62%) >Zn (12.46%) >Cu (3.91%) >Pb (3.76%) >Cr (3.13%) >Mn (2.18%) >Ni (0.56%). In blood levels of heavy metals (Al, Cr, Cu, Fe, Mn, Ni, Pb, and Zn) were 0.446, 0.087, 0.108, 16.723, 0.011, 0.025, 0.181, and 0.078 μg/L, respectively. The distribution of heavy metals in blood samples differed from that in $PM_{2.5}$, indicating the various bioavailability of these heavy metals. In addition, our results suggested that blood heavy metals levels are a good indicator for inhalable $PM_{2.5}$-bound heavy metals intake. Moreover, personal exposure to ambient $PM_{2.5}$-bound heavy metals and its relation with different health alteration in humans will be discussed in the presentation.

AO-CYSA-07 : Ag Modified TiO_2 Sensitized with CdS Quantum Dots for Photocatalytic Hydrogen Production

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Various concentration of Ag modified TiO_2 (Ag=1%, 2%, 3% and 5%) nanoparticles were synthesized by using the hydrothermal method. The synthesized material is characterized using XRD patterns which indicated only anatase phase. Further the binary hierarchical photocatalyst Ag-TiO_2/CdS was fabricated via a successive ionic layer adsorption and reaction (SILAR) technique. These Ag-TiO_2/CdS Composite materials were characterized using powder XRD, FE-SEM, EDX, UV–DRS and Photoluminescence (PL) spectra. UV–DRS spectra

propose the decrease in optical band gap of Ag-TiO_2/CdS with the increase of Ag content up to 5 mol%. The PL spectra suggest that, with the increase of Ag ion concentration into TiO_2/CdS, intensity of green emission band increases, which reflects the low recombination rate of photogenerated charge carriers which is responsible for higher photocatalytic H_2 production. The visible light photocatalytic performance of these materials was investigated for H_2 evolution with the solution of 0.35M Na_2SO_3 and 0.25M Na_2S under natural sunlight conditions. Extent of hydrogen production is affected by content of Ag in TiO_2/CdS.

AO-CYSA-08 : Hydrothermal Synthesis of Ni Doped Vanadium Pentoxide (Ni@V_2O_5) as An Efficient Electrode Material for Non-Enzymatic Urea Sensing

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We demonstrate a simple, inexpensive, enzyme-free electrochemical sensor for Urea detection in alkaline medium, based on the enhanced catalytic activity of Vanadium pentoxide with different levels of nickel doping (2.5 % - 10 % by weight) are prepared through facile hydrothermal method. Urea [$(NH_2)_2CO$], is extensively used as a nitrogen-release fertilizer in agriculture, animal feed additive and in consumer products such as detergents and cleaning products. It has been one of the major adulterant and pollutants, which has conflicting effect on human health and environment. Vanadium oxide(V_2O_5) nanoparticle is an attractive material due to its good catalytic, electrical and optical properties. Herein, Ni doped V_2O_5 has been synthesized using Ammonium metavanadate (NH_4VO_3), Nickel Nitrate ($Ni(NO_3)_2$ 6 H_2O and Hydrogen peroxide (H_2O_2) in the presence of capping agent. Doping with nickel in percentage has a great impact on the electrochemical properties, detection limit, and morphology. Thus, it is applied as an electrode modifier to develop an electrochemical sensor. The physiochemical properties of the as-synthesized material were probed by SEM, XRD, TGA, UV-DRS, XPS and BET. The working surface area of nickel foam was fabricated with the synthesized material using the screen painting method and electrode was employed to determine urea using cyclic voltammetry (CV). The electrode exhibited a good detection limit of 10ìM and was linear in the range of 50-500ìM with an R^2 value of 0.990. Real-world sample analysis to examine its practicability was conducted using a milk sample and tap water in an alkaline medium. The urea sensor showed good repeatability, stability and selectivity with an excellent anti interference ability against electroactive species.

AO-CYSA-09 : Quantification of Size Segregated Particulate Matter Deposition in Human Respiratory Tract and their Health Risk on Glass City Residents

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The present study aims to investigate the regional and lobar deposition of size-segregated PM in the respiratory tract and their toxic effect on human health by the MPPD version 3.04 and USEPA model. Size-segregated PM is collected using the Grimm portable environmental dust monitor during winter season in Firozabad; a Glass city of India. In MPPD, airway structures of infants, children and adults are considered for the study. From the results it was found that PM10 and PM2.5 was highest deposited in head region (0.3477-0.5622& 0.366-0.4704) followed by pulmonary region. The variation in deposition percentage in our study is mainly due to the airway geometry, PM size, and its deposition mechanisms. The coarse fraction due to its large size cannot follow the airway path and mostly gets deposited by inertial impaction in the head region and its bifurcations. The present study results inferred that fine PM deposition was highly visualized in 9 year and 3 month age category. For the chronic exposure scenario for normal and worst-case exposures, HQ>1.0 (Child, and Adults) & ELCR>10^{-6} for children and adults inferred that sensitive exposed population may be at risk of developing health-related problems and can cause carcinogenic and Non-carcinogenic diseases.

AO-CYSA-10 : La-doped Bi_2O_3 Nanoflowers : An Efficient Photocatalyst for the Degradation of Carbolfuchsin and Chlorpyrifos

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Photocatalytic degradation of organic dye by AOP's is an effective method to minimize water pollution. The semiconducting materials have a larger bandgap and difficult to fabricate in the form of 2 D-films. Here we report a simple method for the effective fabrication of undoped and La-doped Bi_2O_3 thin films by a chemical solution deposition method. The incorporation of lanthanum dopant was successfully done and confirmed with the help of SEM, EDAX, XRD, and other advanced characterization techniques. A brilliant flower-like morphology and incorporation of La ions in Bi_2O_3 lattice helped the fabricated doped

thin film for efficient degradation of carbolfuchsin (CF) organic dye, and Chlorpyrifos (CPS) organic pesticide under 120 min of stimulating light source irradiation. Detailed deposition effect on morphology is discussed. The narrowing of bandgap (2.85 eV) in the doped thin film as compared to undoped Bi_2O_3 film (3.01 eV) resulted in efficient degradation of CF up to 89% with rate constant 0.520 min^{-1} and CPS to 67% with 0.366 min^{-1}. The scavenger addition confirmed Ï%OH as the major ROS and, metabolites formed during the degradation are identified by LC-MC analysis of degraded samples of both CF and CPS. The reusability study confirmed the efficiency of films up to multiple catalytic cycles. The work confirmed La-Bi_2O_3 film was effective for the degradation of moieties from a separate class of organic framework.

AO-CYSA-11 : Title: Synthesis, Characterization and Application of Graphene/Zr Composite Supported on Activated Carbon for Efficient Removal of Fluoride from Drinking Water

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Fluoride is a serious public health issue in many regions of the world because of its elevated concentration in water resources. Defluoridation of drinking water requires cost-effective adsorbents. Graphene/zirconium/activated carbon (G/Zr/AC) nanocomposite has been synthesised and characterised via field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectrometry (EDX analysis), N_2 physisorption (BET analysis), Fourier transform-infrared spectroscopy (FTIR), and X-ray diffraction (XRD). In addition, the point of zero charge (pHpzc) was determined. The result showed that graphene/Zr nanoparticles have been successfully anchored onto the activated carbon, which plays a significant role in the defluoridation of water. The G/Zr/AC adsorbent study for the removal of fluoride from water was investigated in a batch system under various conditions. The adsorption studies were carried out by optimizing various parameters such as initial pH, adsorbent dose, adsorption time, agitation, and initial fluoride concentration. The results showed that at low pH values, the G/Zr/AC composite was more effective at adsorbing fluoride, with a maximum adsorption of 74.6%. Among the conditions of temperature and agitation evaluated, the best results were achieved at 30°C and 200 rpm. The system proved equilibrium after 4 h of operation. While the Langmuir isotherm (linear/non-

linear) best represented the equilibrium data, with a maximal adsorption capacity of 81.47 mg/g, the pseudo second order kinetic model best described the kinetic data. In other words, the findings we got prove that the material produced is effective adsorbent and can be used in the removal of fluoride from drinking water.

AO-CYSA-12 : Au / $BaTiO_3$ Nanocomposite based Humidity Sensor Applicable for Breathe Analysis

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Herein, we report, Au/$BaTiO_3$ based humidity sensor. The $BaTiO_3$ nanopowder has been synthesized using $Ba(OH)_2$ and TiO_2 via solid-state synthesis method. The obtained $BaTiO_3$ was further modified with Au with different Au % loadings (0.01, 0.1 and 0.6 wt%) . The as-prepared Au/$BaTiO_3$ nanocomposites have been characterized using XRD, particle size analysis, UV-Visible spectroscopy, FESEM, FETEM and FTIR analysis. The XRD analysis of the $BaTiO_3$ revealed the tetragonal crystal structure. The FESEM and FETEM analysis shows the irregular square disc shaped structure of the $BaTiO_3$ nanoparticles. The size of the particles ranges from 10 to 30 nm. All the synthesized nanocomposites as well as pristine $BaTiO_3$ were tested for humidity sensing in the relative humidity range of 11% to 92% RH. The Au/ $BaTiO_3$ nanocomposite with 0.1% Au has shown superior humidity sensing performance over 11% to 92% RH range than the remaining samples. The response of 0.1% Au/ $BaTiO_3$ nanocomposite was 3.3 M Ù / %RH. The humidity response obtained for this nanocomposite was linear and useful for device fabrication. Further using these nanocomposites, we have performed the breath sensing tests. The breath sensing results has generated the regular breathing pattern with response and recovery time of few microseconds.

AO-CYSA-13 : The Effect of Cholinium-based Ionic Liquids as A Major Formulation Component on the Stability of Immunoglobulin G Antibodies

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Access to protein-based vaccines is a big challenge in developing countries. Majority of the cost of production is due to cold-chain storage. Cold chain exists to preserve vaccines as we ship them around the world. The active components in the drug for instance, antibodies

have enemies like water and heat. Protein's intermolecular as well as intramolecular interaction changes as a function of temperature which further destabilize its structure. Besides protein structure, water is also not independent of the effect of temperature. It changes its structure as a function of temperature. Hence, different formulations are optimized to store antibodies. We in our study have tried to study the effect of Ionic liquids (ILs) on the conformational and colloidal stability of Immunoglobulin G (IgG) antibodies as a function of time at room temperature. ILs are salts which are salts (consist of cation and anion), but remain as liquids at room temperature. Unlike water they remain stable at higher temperatures too. We have performed Real-time studies using DLS, Far-UV Circular Dichroism spectroscopy and SDS- PAGE. Further thermal fluorescence has been performed to study the thermodynamic parameter of stability of IgG in presence of ILs. All the results obtained from thermal, colloidal and structural studies have demonstrated a great potential of cholinium based ILs as formulations in the area of storage and transportation of pharmaceuticals.

AO-CYSA-14 : Synthesis and Characterization of a Deep Eutectic Solvent with Tetrabutylammonium Bromide (TBAB) and Itaconic Acid

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A new class of deep eutectic solvents (DESs) which are composed of hydrogen bond acceptor (HBA) and hydrogen bond donor (HBD), appear as an auspicious substitute for ionic liquids and organic solvents. DESs are cheaper, safer, non-toxic, biodegradable, and bio-compatible and hence fall in the category of green solvents. DES synthesis is an example of a reaction with 100% atom economy. TBAB-itaconic acid-based DES was prepared by mixing Tetrabutylammonium bromide (TBAB) and itaconic acid at 88 °C until it formed a homogenous liquid. It was cooled to RT and used without any further purification. It was characterized by using TGA, FTIR, and NMR. In this synthesis, TBAB and itaconic acid in different molar ratios like 1:1,1:2,1:3,3:2,2:1 were taken as raw materials. The melting point measurement of all these DES samples was carried out and illustrated with the help of a phase diagram. The best alternative among the selected set is (1:1) as it remained a highly viscous liquid at RT. Physical properties such as density, viscosity, surface tension, refractive index, conductivity, and pH will be studied. Even computational chemistry will be used to predict thermodynamics properties of DES. Further investigation into

the applications of this newly synthesized DES as solvents in TLC, HPLC, and even in extraction processes is underway in our laboratory.

AO-CYSA-15 : Sonophotocatalytic Degradation of Acid Red by using ZnO and Fe Doped ZnO Nano Catalyst

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Abstract: Fe-doped ZnO nano catalyst was synthesized by co-precipitation method. The intrinsic characteristics of a prepared nano Fe-doped ZnO catalyst were studied using a variety of techniques including powder X-Ray diffraction (XRD), scanning electron microscope (SEM) Electron dispersive X-ray spectroscopy (EDS). In this study, degradation of Ponceau S as a dye pollutant was investigated in the presence of ZnO and Fe-doped ZnO nano catalyst using sonolysis, photocatalysis, sonocatalysis and sonophotocatalysis. The UV light and ultrasonic probsonicator at 20 kHz and 150 W powers were used as an irradiation source. The effect of H_2O_2 on sonocatalytic, photocatalytic and sonophotocatalytic degradation was investigated. At optimum conditions the dye degradation efficiency was influenced by addition of H_2O_2, the highest dye degradation was obtained as 98% by US+UV+Fe-doped ZnO+H_2O_2. The experimental kinetic data followed the pseudo-first order model in doped and undoped sonocatalytic, photocatalytic and sonophotocatalytic processes but the rate constant of sonophotocatalysis is higher than sonocatalysis and photocatalysis process. The sonophotocatalysis was always faster than the respective individual processes due to the more formation of reactive radicals as well as the increase of the active surface area of nano catalyst.

AO-CYSA-16 : Simple, Fast and Sensitive Detection of Mefenamic Acid on the CTAB Mediated Glucose Modified Sensor using a Voltammetric Approach

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In this study, a novel and robust glucose-modified carbon paste electrode (CPE) for the ultrasensitive detection of mefenamic acid (MA) is developed. MA, a non-steroidal anti-inflammatory drug used for its antipyretic and analgesic effects, is harmful to the patient in

higher doses. MA is also listed as a chemical pollutant that negatively affects the environment. From this point of view, a sensitive sensor to identify the MA was developed by using a glucose-modified carbon paste electrode in the presence of a cationic surfactant, cetyltrimethylammonium bromide (CTAB). The developed sensor probe was characterized using different electrochemical techniques and then used to study the electrochemical nature of MA. The sensor could detect MA with a linear dynamic range (LDR) of 0.025 to 500.0 µM and a limit of detection (D_L) of 1.01 nM. Interference from co-existing molecules was found to be negligible. The real sample analysis was performed in human urine samples and pharmaceutical tablets with SWV, and higher recoveries of 92.70-99.16% and 96.0-98.5%, respectively, were obtained. This demonstrates that the sensor can be further used in other biological, pharmaceutical, or environmental samples to detect MA.

AO-CYSA-17 : Direct and Sensitive Electrochemical Evaluation of Pramipexole using Graphitic Carbon Nitride Sensor

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Pramipexole (PMXL) belongs to the benzothiazole class and is used to treat Parkinson's disease; however, overdose leads to some abnormal effects that can trigger some severe side effects. As a consequence, it demands a sensitive analytical tool to track the trace level of PMXL. In this work, we have successfully developed a graphitic carbon nitride (gCN) sensor (gCN·CPE) for the trace-level detection of PMXL. The synthesis of gCN was done using the high-temperature thermal condensation method and employed for surface characterization using TEM, XRD, and AFM techniques. The electrochemical characterization was evaluated using the EIS and CV techniques. The cyclic voltammetry (CV) behavior of PMXL displayed an anodic peak in the forward scan indicating the electrooxidation PMXL. The influence of different parameters on the electrochemical behavior revealed the diffusion governing the electrode process with an equal number of hydronium ion and electron involvement. For the fabricated gCN·CPE good linearity range was noticed from 5.0×10^{-8} M to 5.0×10^{-4} M and a lower detection limit (L_D) of 1.2×10^{-8} M was achieved for the selected concentration range (5.0×10^{-7} M to 3.0×10^{-5} M). The selectivity of the electrode in PMXL detection was

investigated by conducting an interference study, while the tablet sample analysis demonstrates the sensitive and real-time application of the electrode. The good recovery values for the analysis illustrate the efficiency of the electrode for PMXL analysis.

AO-01 : Visible Light Water Splitting Over $MnCdSTiO_2$/Pt Composites Synthesized by Simple SILAR Technique

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The use of clean, renewable energy for human needs is one of the most challenging research areas. Sunlight is a clean energy source that can be stored and used. To this end, among various approaches, Quasi Artificial Leaf or solar water splitting via semiconductor materials are the best for collecting and storing abundant solar energy as clean, easily transportable hydrogen fuel. In this context, TiO_2 has been widely studied as one of the leading photocatalysts in recent decades due to its low cost, non-toxicity and high chemical stability. Recent studies have shown that the combination of wide-band gap photocatalysts and narrow-band gap semiconductors can collect visible light to facilitate charge separation and increase the efficiency of H_2 generation. Here we present the fabrication of $MnCdSTiO_2$/Pt composites on fluorine-doped tin oxide (FTO) plates. Titanium dioxide paste was coated on FTO (SnO_2 /F, TEC 15) substrate by doctor blade method. A titanium oxide electrode was sensitized with CdS grown by the method of Successive ionic layer adsorption and reaction (SILAR). The materials thus synthesized were characterized using various analytical techniques such as powder X-ray diffraction pattern (PXRD), HRTEM, XPS and Raman spectra. The morphology and microstructure of $MnCdSTiO_2$/Pt composites were investigated by scanning electron microscope (SEM). FTO coated with $MnCdSTiO_2$/Pt composites were used for water splitting and hydrogen generation under one sun condition using a solar simulator. FTO coated with $MnCdSTiO_2$/Pt composite shows excellent activity for hydrogen evolution (43 ìmol/h/g). Activity was found to be dependent on the number of SILAR cycles and the immersion time. Activity decreased when the CdS film thickness exceeded the optimal size (10–12 ìm). The detailed mechanism of solar water splitting on $MnCdSTiO_2$/Pt coated FTO was also studied.

AO-02 : Studies on Synthesis and Characterization of Biologically Significant Hetero Annulated Fused Pyrroles

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The importance of natural and synthetic pyrroles arises from their wide range of applications in various fields such as medicinal chemistry, catalysis, dyes, and materials science. The objective of this work is to design novel synthetic strategies for novel pyrrole fused scaffolds through the catalyst Cu (II)-(Acedoben)-Fe3O4. The core-shell structure and the characteristics of the prepared magnetic nano-catalysts were corroborated through powder X-ray Diffraction (PXRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDAX), and FT-IR techniques. Also, the structures of synthesized compounds were corroborated on the basis of FTIR, nuclear magnetic resonance (NMR), mass, and elemental analyses data. The biological screening of synthesized compound was done against pathogenic microorganisms. Staphylococcus Aureus (Gram positive bacteria) Klebsiella Pneumoniae (Gram negative bacteria) with a view to explore their anti-microbial action.

AO-03 : Microwave Assisted Synthesis of Fused Azepine Derivative via Intramolecular Cyclisation of Strained Alkyne

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In the diversified arena of heterocycles, the seven-member heterocyclic compounds have been less explored. Owning to the interesting structure, eclectic scope of natural properties and being an important pharmacophore fragment viz, aza ring systems in the structure of balanol, (-)-cobactin T etc and use in drug designing under heading of antifungal, antibacterial, antivirus agents, etc drag immense attention of chemists and made it exploited for the synthesis, reaction and biological properties. Among various reported cyclisation methods for azepine synthesis, for the first time an exquisite and accomplishable access to construct N-substituted aryl halides azepine fused derivatives was established via microwave radiations under mild conditions by incorporating a strained eight membered alkyne ring with electron withdrawing substituents attached to it, obtained with an appreciable yield. The structures of synthesized compounds were

corroborated on the basis of FTIR, nuclear magnetic resonance (NMR), mass, and elemental analyses data. Furthermore, a quantum computational study was computed to investigate the density functional theory-based chemical reactivity parameters of the synthesized derivatives.

AO-04 : Synthesis of Novel Polysubstituted Oxazole via Tandem Oxidative Cyclization Pathway Catalyzed by $CuNiFe_2O_4$@Lys-GO

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The pursuit for designing efficient heterogeneous catalytic systems for tandem oxidative cyclization reactions has provided a great impetus to research efforts, as it enables the step well as confers the benefits of a facile catalytic recovery. In the present study, we disclose a novel $CuNiFe_2O_4$@Lys-GO catalytic system which was successfully prepared by immobilization of copper substituted nickle ferrite nanoparticles on lysine-grafted graphene oxide nanosheets, in which ferrite moeity acts as an oxidation catalyst and lysine has the role of base catalyst. Also, lysine amino acid used to modify the surface of graphene oxide nanosheets which the prepared support can improve dispersion and uniform loading of nanoparticles for the tandem oxidative cyclization of amines and â-keto esters, leading to the production of biologically active, polysubstituted oxazole moeties.

AO-05 : Related Substances Method Development and Validation for the Identification, Quantification of Organic Impurities in Epirubicin Hydrochloride using RP-HPLC

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A rapid, simple, sensitive, and reliable analytical method was developed for a concurrent evaluation of Epirubicin and its impurities namely Doxorubicin, and Doxorubicinone. The present work is carried out with HPLC having Zorbax Eclipse XDB C_{18} column on Altima ODS 150mm X 4.6mm, 5 µm. The optimized parameters were maintained at a flow rate of 1.0 ml/min, detection wave length is 254nm, Mobile

phase used for the study is OPA Buffer: Acetonitrile (56:44 % v/v). The buffer pH was maintained at 2.5 and the temperature was ambient i.e., 25!. The retention times for Doxorubicinone, Doxorubicin, Epirubicin are 9.706, 7.924, and 2.527 respectively, Total run time is 45 min. % RSD precision in system suitability assay was found to be 0.3% and for related substances was 2.4%. The values of LOD and LOQ obtained from Epirubicin were 0.0144 and 0.0479, for Doxorubicin 0.0149 and 0.0496, and for Doxorubicinone 0.0142 and 0.0474. Linearity for assay was determined from 50% to 150%. Degradation studies were also carried out at acid, base, peroxide, thermal and photolytic conditions. The present analytical method was validated as per the defined protocol and it meets the specified acceptance criteria. Hence, the stability indicating validated method is suitable to identify the related substances in Epirubicin.

AO-06 : Estimation of Essential and Toxic Metals in Cord and Maternal Blood of the Women with or without Preeclampsia - A Case Study

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Preeclampsia appears to be a leading and strong worldwide cause of maternal and perinatal mortality and morbidity. The objective of this study is to evaluate the essential and toxic metals concentrations of cord and maternal blood of the women with or without preeclampsia. For this study, we have collected 10 mother child pairs blood samples maternal and cord for the measurement of essential and toxic metals by inductively coupled plasma- optical emission spectrometry (ICP-OES). Statistical analysis was performed with variables such as birth weight, birth height, head circumference, ponderal index and independent variable i.e., metals concentrations. Significant difference was found in number of children and height of the females. The results of this study support an association between environmental exposure to essential and toxic metals and preeclampsia, fetal anthropometric growth leading to a non-significant reduction in birth weight, height, head circumference and ponderal index. For some elements, there was a major relationship between metals and preeclampsia, with higher concentrations in preeclamptic women than control group women. Efforts should be made to reduce exposure of females of reproductive age in relation to long-term impact on health. To the best of our knowledge, this is the first study of its kind in the Agra region that measured multiple essential and toxic metals in delivering mothers and cord blood samples of the women with or without preeclampsia.

AO-07 : Effect of Various Environmental Pollutants on Human Life

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An environment pollutant is that substance which is present in the environment may produce abnormality in metabolism or alter the well-being of organism. Lead, mercury, arsenic, aluminum etc. are some heavy metals present in the environment that causes poisoning in human beings. We consider our homes as the safest place to live but various volatile organic compounds are found to be the major causative agents for the newly described "sick building syndrome". During food preparation toxins like monosodium glutamate also enters our body. There are some occupations in which persons are prone to get poisoning of these heavy metals. Some recent researches shows that woolen carpets could help in air pollution by absorbing harmful chemicals from cleaning fragrances , paints and furniture's. In the present work, study conducted on the effects of various kinds of environmental pollutants on human life.

AO-08 : Facile and Biogenic Synthesis of Cu2O-ZnO Nanocomposite using Callistemon Viminalis Leaf Extract and Antimicrobial Application

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The current article presents a green one-pot synthesis of Cu_2O-ZnO nanocomposite for their antimicrobial efficacy, prepared via Callistemon viminalis aqueous leaf extract. To confirm that the biomolecules in leaf extract are responsible for the bioreduction of copper and zinc ions, an FTIR spectroscopic investigation of Cu_2O-ZnO NCs was conducted. While powder XRD analysis of the bimetallic composite indicated nanosize and lattice interaction, energy dispersive X-ray spectrum analysis allowed for the identification of the elemental composition. SEM, TEM, and TGA/DTA methods were also used to screen biosynthesized Cu_2O-ZnO nanocomposite. The product's purity and the presence of copper and zinc oxides had been examined using X-ray photoelectron spectroscopy (XPS). By comparing the antibacterial properties of Cu_2O-ZnO nanocomposite with those of Cu_2O nanoparticles (against S. aureus, P. aeruginosa, and C. albicans), the synergistic

effect of copper and zinc was also investigated. The findings show that Cu_2O-ZnO nanocomposite have greater potential than Cu_2O nanoparticles.

AO-09 : Determination of Physico-Chemical Parameters of Groundwater of Agra and Firozabad Regions and its Possible Impact on Human Health

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"Water is the elixir of human life." It is quite important for living organisms. The main source of water is rain, rivers, Glaciers and groundwater. Groundwater is one of the chief sources of water supply over the world. Only 2.5% of the worlds water is fresh and it has been used for drinking for a long time and its purity has made it a well-known source of potable water.

In this study the physicochemical parameters were investigated to determine the water qualities of different groundwater samples of Agra and Firozabad regions. The physicochemical parameters were investigated such as TDS, pH, Turbidity, EC, BOD, COD, total hardness, temporary hardness and permanent hardness. The collection of samples was done in pre monsoon and post monsoon in the year of 2021-2022. Groundwater samples were taken from nine blocks of Agra (Barauli Ahir, Khandauli, Etmadpur, Fatehpur sikri, Bah, Saiyyan, Shamshabad, Bichpuri, Acchnera) and nine blocks of Firozabad (Araon, Eka, Jasrana, Khairgarh, Firozabad, Tundla, Madanpur, Narkhi, Shikohabad)

The problem of groundwater contamination due to heavy metals is one of the major concerns in major areas. Due to this contamination of heavy metals has been linked to developmental retardation, various cancers, kidney damages etc. The toxic trace metals, can affect the mental and central nervous system, blood composition, lungs, liver and other organs in the human body.

AO-10 : Analysis of Chemical Tracers for Biogenic Material in Inhalable Ambient Particulate Matter

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Endotoxin contamination is common problem with recombinant protein and nucleic acid purified from Gram -ve bacteria such as E.coli when bacterial cells are actively growing or when their

membrane disintegrates on death. The essential component of the cell wall known as lipo polysaccharide or LPS is released into the surrounding environment. This LPS component known as endotoxin create dangerous contamination and they can trigger inflammations or septic in animals and tissue culture. Endotoxin is heat stable molecules associated with outer membranes of certain gram negative bacteria. This endotoxin can be used as the biogenic tracer of gram negative bacteria. Endotoxin contamination is a typical concern with recombinant protein and nucleic acid isolated from gram negative like e coli. When bacterial cells are actively developing or when their membrane disintegrates on death, the key component of the cell wall known as lipo-polysaccharide or LPS are released into the surrounding environment. They are found as constituent of aerosol particle and act as tracers for Gram-ve bacteria. This dissertation reports the mass concentration of respirable suspended particulate matter (RSPM) in ambient matter and concentration of endotoxin in respirable suspended particulate matter. The concentration ($\mu g\text{-}m^{-3}$) of RSPM, known as inhalable suspended particulate matter are found to be quite high. The values are many fold higher than WHO, USEPA and NAAQs standards. The concentration of endotoxin ($EU\ m^{-3}$) is found to be in the reported range.

AO-11 : Importance of Personal Exposure Monitoring in Today's World

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In today's world researchers' and the general public's interest in indoor air quality in vulnerable settings like homes and indoor public spaces has grown. More people are becoming aware of this issue as they spend more time indoors than outside, especially those who are most susceptible to the effects of poor air quality, such as the elderly, the young, and those in poor health. Numerous epidemiological studies have shown that there are strong correlations between exposure to particulate matter, which have detrimental impacts on human health, including cardiac and respiratory diseases. The effect of this pollutant on the health of the inhabitants emphasises the significance of monitoring it in various indoor microenvironments. Humans' breathing and cardiovascular systems are seriously harmed by exposure to these small particles. Personal exposure monitoring can be considered for determining direct exposure to airborne environmental contaminants. We conducted a study for adults and children who spent most of their time in different indoor microenvironments like homes, schools, and

offices. The concentration of PM2.5 was measured using personal samplers from SKC and the medium volume sampler for recording the outdoor concentration of PM2.5 that may contribute to this indoor environment. From December to February 2013 to 2015 the sampling was conducted. The data obtained from this long-term study was compared to the standards of NAAQS and WHO, which were found to be significantly much higher. The outcomes from this study indicate that children have a higher rate of contaminant absorption than adults, and as a result, they are more likely to develop respiratory and asthma-like conditions.

AO-12 : Monitoring of Organochlorine Pesticide Residues in Apple (Melus domestica) Pomegranate (Punica granatum), Bottle Gourd (Lagenaria siceraria), Ridge Gourd (Luffa aegyptiaca) and Pointed Gourd (Trichosanthes dioica) by Gas Chromatography

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Twenty organochlorine pesticides including isomers of benzene hexachloride (α-BHC, β-BHC, γ-BHC and δ-BHC), heptachlor, aldrin, heptachlor epoxide, γ-chlordane, α-chlordane, endosulfan-I, 4,4'-DDE, dieldrin, endrin, 4, 4'-DDD, endosulfan II, endrin aldehyde, 4, 4'-DDT, endosulfan sulphate, methoxychlor, and endrin ketone were monitored in five samples two fruits (apple and pomegranate) and three vegetables (bottle gourd, ridge gourd and pointed gourd) by using gas chromatography coupled with electron capture detector (ECD). Apple was found contaminated with α-BHC and δ-BHC; Pomegranate was found contaminated with δ-BHC, heptachlor epoxide and dieldrin; Bottle gourd and Ridge gourd were found contaminated with heptachlor epoxide; Pointed gourd was found contaminated with d-BHC and heptachlor epoxide.

AO-13 : An Overview of Halogenated Polycyclic Aromatic Hydrocarbons in fine Particulate matter in Mumbai, India

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Environmentally harmful polycyclic aromatic hydrocarbons (PAHs)

are mostly created when organic resources like fossil fuels are burned inefficiently. The atmospheric sources of PAHs have been reported highest in China followed by India and then the United States, according to inventories that have been created and assessed. Numerous authors from across the world have looked into the prevalence of halogenated PAHs (HPAHs), such as chlorinated PAHs (ClPAHs) and brominated PAHs (BrPAHs), in different environmental media, including air, water, soils, and biota. The present study was conducted in Mumbai in the state of Maharstra for a week to study the concentration of haloginated PAHs during the month of December 2019 and was published in 2021. According to the study the possible origins from relationship with markers like hopanes, steranes, and trace elements are discussed. During the campaign, the mean concentrations of total ClPAHs and BrPAHs were 0.54 ng/m3 and 0.25 ng/m3 at the urban site, respectively, and 0.16 ng/m3 and 0.02 ng/m3 in the suburban site. While the composition profiles varied in each air sample, there was a comparable pattern in the differences in total Cl/BrPAH concentrations between urban and suburban sites. The detailed recent results will be presented in the conference.

AO-14 : Analysis of Nanoparticle (Toxic Metals) From Riverbed Sediments of Ganga River in Vaishali District (Bihar,) India

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The urbanization have significant impact on the heavy metal contamination. The River water quality has been deterioted due to the indiscriminate discharge of untreated sewage, industrial waste and other anthropogenic activities. Riverbed sediments act as sink for pollutants released from anthropogenic activities and gives surrogate information of water quality of river. Indo-Gangetic basin is hugely populated and Ganga River is life of people living in the region. Hence, the aim of the present research was to determine the water environment quality of Ganga River near Vaishali district of Bihar and identify sources of pollution. The sediments were collected from the different sites in in the period from July to October. The sediment samples were collected from different sites, transported to the laboratory and analyzed for metals viz., Zn, Cr, Pb, Cd and Cu. Analysis were carried out using flame absorption spectrometry method. The highest content of Zn, Pb and Cr were recorded in the sediments, which may be resulting from the city pollutant and dead body burning near the city. The research suggests anthropogenic activity and impact

of agricultural activity for slightly elevated Cd level. Water quality index were also determined. There is urgent need to take steps for control measures and to stop contamination of sediments of river near to highly populated and polluted areas.

AO-15 : S-doped g-C_3N_4 /g-C_3N_4 : A S-type Heterojunction for Enhanced Photocatalytic Water Splitting

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In situ calcination method was used for synthesis of the S-type heterosystem S-doped g-C_3N_4 /g-C_3N_4 using different precursors (urea, thiourea, melamine and urea-thiourea). As prepared samples were tested for water splitting for hydrogen generation in 20% CH_3OH under 300W Xe light source. The system made by urea and thiourea (1:1), exhibit the maximum rate for hydrogen generation via water splitting i.e. 485.51 $\mu molg^{-1}h^{-1}$ (with 1.75% apparent quantum efficiency(AQE)), which is 1.37 and 1.29 times higher than the g-C_3N_4 system made by urea 353.77 $\mu molg^{-1}h^{-1}$ and thiourea 376.07 $\mu molg^{-1}h^{-1}$. The cause of higher rate of hydrogen evolution is due the formation of the S-type hetero junction S-doped g-C_3N_4 /g-C_3N_4 that improved efficiency of the system than the normal type-II heterojunction due to the improved charge separation and the higher redox ability the oxidation SC and reduction SC sites of the system. Based on advance analyses techniques (XRD, UV-Vis, SEM, EDX, PLE, ESR, XPS, SPV, etc) photocatalytic electron transfer mechanism was also proposed for the studied system.

AO-16 : Heavy Metal Contamination in Yamuna River and its Impact on Aquatic Animals and Plants

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The Yamuna River, which is the lifeline of Delhi, is one of the most-polluted River in the country. About 85 percent of the pollution is caused by domestic and industrial sources. The quality of the river is severely affected by the discharge of untreated domestic and industrial effluents. For the study, Yamuna water samples were collected from Mathura, Agra, Firozabad and Etawah sites. The objective of this study is to assess the water quality of pre-monsoon and post-monsoon of Yamuna River. A wide range of contaminants are continuously

introduced into the river and their toxicity is a problem of increasing significance for ecological, evolutionary, and environmental reasons. Heavy metals viz., Lead (Pb), Copper (Cu), Cadmium (Cd), Chromium (Cr), Zinc (Zn), Nickel (Ni) and Arsenic (As) are very hazardous for aquatic as well as human life. By the process of bioaccumulation these heavy metals are deposited into the aquatic animals and plants and it may cause different diseases. The main aim of this paper is to provide prevailing condition of the river is a matter of grave concern, and there is an urgent need to take strict measures to ensure cleanliness of the river and prevent further contamination and supposed to be stop such type of water pollution to save aquatic life.

AO-17 : COVID-19 and Cigarette Smoking : A Complex Interaction and What Evidence Need Our Attention

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The COVID-19 pandemic has caused severe mortality and morbidity globally. The current data shows that the cigarette smoking rate of COVID-19 patients is relatively small, and the smoking status for these people cannot be precisely measured. Smoking can deteriorate a person's health and increases COVID-19 symptoms. The major objective of this research is to establish the correlation between smoking and the chance of transmission of COVID-19. During the Covid pandemic mass population stayed at home, which could have been stressful for them and for this reason they frequently used cigarettes and other tobacco products. The NPS positivity rate and covid hospital admissions were numerous for the people who regularly smoke than the individuals who don't smoke. The data acquired demonstrated that the health issues of frequent smokers were more chronic and at higher risk. By making some effective changes we can create a smoke-free world.

AO-18 : Development of Efficient and Selective Ultrasensitive Persimmon@AgNPs for Colorimetric Detection of Hg (II) Ions and Antibacterial Effects: A Real Water Analysis

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The formulation of eco-friendly silver nanoparticles (AgNPs) using persimmon leaves extract has been described. The presence of various

organic substituent in the persimmon leaves serve as reducing and stabilizing agents for the fabrication of AgNPs. They also provide a suitable binding site to the mercuric (Hg^{2+}) analyte in the colorimetric detection metal ion in the water sample. The biogenic fabrication of silver nanoparticles depends upon some of the basic parameters such as pH, time and concentration of leaf extract. Synthesized Persimmon@AgNPs desired for the colorimetric sensing were characterized by UV-Vis, FTIR, XRD, ZPA, EDX and HRTEM. Different dilutions of Hg^{2+} ions were also considered, and a detection limit (LOD) for Hg^{2+} ions of around 0.0001 ppm was observed. The sensing strategy was used to determine Hg^{2+} in real water samples. Furthermore, biogenic nanoparticles showed significant antibacterial activity against both strains of bacteria S. aureus and E. coli. The positive and effective response of the synthesized Hg^{2+} sensor, together with its antibacterial activities, makes Persimmon@AgNPs potentially applicable for the cheap, portable and colorimetric sensors in water remediation.

AO-19 : The Study in Variation of Gel Time of Surface Modified Kota Stone Slurry in KSS Reinforced Epoxy Composite

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The present research work focuses on the surface modification of the Kota stone slurry wherein the modification was done through Mechanical , Thermal and Chemical activation. The KSS was coated with the metastable phase (MSP) of polythene and was blended with polyethylene glycol 600(PEG 600). The study in the variation of the surface modified KSS reinforced epoxy composite by viscometer DV2T with gel timer and gel time can be summarised as the lowest gel time was noticed for NaOH activated KSS reinforced epoxy composite i.e 54 minutes and the highest gel time was noticed for KSS reinforced epoxy composite i.e 2 hours and 42 min (Experiments were conducted at 1 rpm speed with 2,083,000 cp viscosity built up, 93% torque). The criteria for the variation in the gel time is the Vanderwall force of attraction between the hydrocarbon part of the coated filler and the hydrocarbon part of polymer matrix was prominent and latter on when it was blended by PEG 600 with OH moiety then hydrogen bonding was significant between the filler particle and the epoxy matrix which fasten polymerisation and decrease gel time with early viscosity built up. So in this study it was very much cleared that if interaction

is there in between the filler and matrix that may be Vanderwall or may be ionic interaction. The effect in gel time was appreciable with reduction of size by Mechanical activation. The aim of the work is to understand the effects of inclusion of various modified fillers in the transition phenomena that occur during polymerisation.

AO-20 : Carbon Quantum Dots : Photoluminescence Properties and FRET Donor Efficiency for Sensing Applications

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Carbon quantum dots (CQDs) which are a new class of fluorescent carbon nanomaterials was discovery first time in 2004 during purification of single-walled carbon nanotubes (SWCNTs). It has received extensive attentions, and a large number of investigations on CQDs has been made in last two decades due to their strong and tunable fluorescence (FL) properties, which enable their applications in sensing, catalysis, biomedicine, optoelectronic, and bioimaging. The effect of heteroatom doping, enhanced quantum yields (QYs), and fluorescence mechanism such as quantum confinement, surface state and molecular fluorophores have largely been debated. The intrinsic properties of nitrogen dopped CQDs depends on the nature of doping of nitrogen atoms such as graphitic, pyridinic, pyrrolic and amine which plays significant roles in modulating the fluorescence QYs, energy levels and fluorescence decay life time of CQDs. The challenging task of synthesizing multicolor emissive CQDs can meet the current challenge of new LED materials. The fluorescence quenching (Turn-off) and fluorescence recovery (Turn-on) properties of CQDs can be used to design fluorescence-based optical sensors for large class of analytes of environmental and biological importance. The Foster/ fluorescence resonance energy transfer (FRET) based phenomena is most suitable technique for the development fluorescence-based sensors. We have investigated that the fluorescence tunability of CQDs make them suitable donors for fluorescence resonance energy transfer (FRET) with wide range of donor materials. Due to significant overlapping of FL spectra of CQDs with absorption spectra of gold nanoparticles (AuNPs) and mangnese dioxide (MnO_2) nanostructures, we enabled to develop FRET-based sensors for detection of pesticides and biomolecules such as glutathione, cholesterol and

acetylcholinesterase (AChE) enzyme. The FRET between carbon quantum dots (CQDs) and gold nanorods (AuNRs) may arise from distinctive overlap of transverse and longitudinal bands of AuNRs with fluorescence (FL) spectra of CQDs. In this context, we have developed successfully developed a FRET-based sensor for the detection of glucose, glutathione and acetylcholinestrase enzyme. Therefore, the intrinsic properties and FRET behavior of CQDs will be discussed.

AO-21 : Corrosion of Calciferous Animals in Marine Environments

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Molluscs families are snails, gastropods, bivalvia, unio, cephalopod, oysters, clam, cardiidae, whelk, ammonites and they are known as calciferous animals. Saline water is essential for the survival of their life. These animals outer layer are made of calcium carbonate. Ocean water is major absorber of carbon dioxide. It converts carbon dioxide into carbonic acid that acid develops corrosive medium for calciferous animals. The concentration of carbon dioxide increases in atmosphere day by day due to burning of coal, thermal power stations, metallurgy industries, cement industries, transport vehicles, infrastructure development works, burning of agricultural wastes, deforestation and decomposition of biowastes. These sources are major emitter of carbon dioxide. Carbonic acid decreases pH of ocean water and it starts corrosion reaction with calciferous species. This acid interacts with outer surface calciferous species to develop chemical, electrochemical and biochemical reaction. Corrosion reactions deteriorate outer layer of calciferous animals and finally destroy their life. The greenhouse gases are producing global warming and climate change to exhibit corroding effects on calciferous animals. Acids develop galvanic, pitting, stress, crevice and intergranular corrosion on the surface of calciferous animals. The physical, chemical and biological factors are also responsible for the corrosion of calciferous animals. They can change their physical, chemical, biological properties and tarnish facial appearances. Ocean water is alkaline in nature which is suitable for calciferous animals' growth and development. Corrosive substances reduce alkalinity of ocean water and enhance acidic character and create hostile environment of calciferous animals. Corrosive substances enter into rivers through drain and human activities make water acidic thus produce hostile environment for gastropods, unio and clam. Calciferous animal's essential components are proteins, carbohydrates, lipids, nucleic acids and materials. These essential components are

dissociated into carbon dioxide, ammonia, methythiol and water in acidic medium. Coral reefs or mounds are made of secretions of calciferous animals which are corroded in acidic medium. Keywords: Corrosion, Calciferous Animals, Molluscs, Ocean, Carbonic acid.

AO-22 : Management of Radioactive Contaminated Solid Waste using various Chemical Leachents and Ultrasonic Technique

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India is exploring options other than fossil fuels to meet the current requirement of energy and it is mainly nuclear power. India's three stage nuclear programme and closed fuel cycle consists of reprocessing of SNM at various stages. Handling of SNM is carried out in leak tight glove boxes provided with gauntlets for various operations. During this process lots solid wastes are generated mainly neoprene gauntlets, PVC materials and process equipment and its spare parts. All these solid wastes are alpha contaminated and are not qualifying for disposal as non alpha waste and require special methodology of disposal. If SNM is recovered from these solid wastes, it will come in category of non alpha and waste disposal become easier. An effort was made to treat such type of waste in laboratory using various leachents viz. Nitric acid, Na_2CO_3, HF, oxalic acid, mixture of oxalic acid & nitric acid in ultrasonic system. Ultrasonic systems were designed, fabricated and installed in glove boxes for the recovery of SNM from these solid waste. Results were highly encouraging and procedure is scaled up to treat bulk solid waste and its safe disposal.

AO-23 : Monitoring of Pesticidal Contamination Level of Organochlorine Pesticides in Summer Season Fruits and Vegetables

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Fruits and vegetables have nutritional value, but they can also be source of toxic contaminants such as pesticide residues. Pesticides used for fruits and vegetables production results in increased health risks and health costs, humiliation of the environment and productivity loss. The aim of this study was to estimate presence of pesticide

residues in summer season fruit and vegetable purchase from local market. The constant use of pesticides contaminated fruits and vegetables pose a leading threat to public health. Gas chromatography equipped with electron capture detector (GC-ECD) was used to monitor 20 organochlorine pesticides including isomers of benzene hexachloride (α-BHC, β-BHC, γ-BHC and δ-BHC), heptachlor, aldrin, heptachlor epoxide, γ-chlordane, α-chlordane, endosulfan-I, 4,4′-DDE, dieldrin, endrin, 4,4′-DDD, endosulfan II, endrin aldehyde, 4,4′-DDT, endosulfan sulfate, methoxychlor and endrin ketone in six summer season fruits and vegetables (bottle gourd, sponge gourd, brinjal, plum, kiwi fruit and pineapple). All fruits and vegetables were found to be contaminated with pesticides. Only plum and pineapple was found contaminated with one pesticide, rest of the vegetables was found contaminated with two or more than two pesticides. The concentrations of estimated pesticides were less than the maximum residue limit values but the regular eating of pesticide infected fruits and vegetables may create serious health problems. The results of study indicated the need for strict guideline and regular monitoring of banned pesticide residues in fruits and vegetables to protect consumer's health.

AO-24 : Synthesis, Characterization and Application of Graphene/Zr Composite Supported on Activated Carbon for Efficient Removal of Fluoride from Drinking Water

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Fluoride is a serious public health issue in many regions of the world because of its elevated concentration in water resources. Defluoridation of drinking water requires cost-effective adsorbents. Graphene/zirconium/activated carbon (G/Zr/AC) nanocomposite has been synthesised and characterised via field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectrometry (EDX analysis), N_2 physisorption (BET analysis), Fourier transform-infrared spectroscopy (FTIR), and X-ray diffraction (XRD). In addition, the point of zero charge (pHpzc) was determined. The result showed that graphene/Zr nanoparticles have been successfully anchored onto the activated carbon, which plays a significant role in the defluoridation of water. The G/Zr/AC adsorbent study for the removal of fluoride from water was investigated in a batch system under various conditions. The adsorption studies were carried out by optimizing various parameters such as initial pH, adsorbent dose,

adsorption time, agitation, and initial fluoride concentration. The results showed that at low pH values, the G/Zr/AC composite was more effective at adsorbing fluoride, with a maximum adsorption of 74.6%. Among the conditions of temperature and agitation evaluated, the best results were achieved at 30°C and 200 rpm. The system proved equilibrium after 4 h of operation. While the Langmuir isotherm (linear/non-linear) best represented the equilibrium data, with a maximal adsorption capacity of 81.47 mg/g, the pseudo second order kinetic model best described the kinetic data. In other words, the findings we got prove that the material produced is effective adsorbent and can be used in the removal of fluoride from drinking water.

AO-25 : Sensitive, Cost Effective and User-Friendly Method for Determination of Active Ingredient Content in Penthiopyrad: A Complete Development and Validation Study

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A cost effective, sensitive and user friendly method was developed and validated to determine active ingredient content in penthiopyrad by using LC-MS. Penthiopyrad (1-methyl-N-[2-(4-methylpentan-2-yl)thiophen-3-yl]-3-(trifluoromethyl)pyrazole-4-carboxamide) is a novel succinate dehydrogenase inhibitor (SDHI) fungicide which inhibits fungal respiration and effectively controls a wide range of diseases caused by basidiomycetes, ascomycetes and deuteromycetes . A reverse phase chromatographic technique was used for the analysis. 0.1% formic acid in water: acetonitrile (5:95 v/v) was used as mobile phase and C18 column was used as stationary phase. Mass spectrometric detector was fine-tuned and maximum abundance was obtained at capillary (kV) 2.0, cone voltage 50. Ionization mode was kept ES+ and scanning was done for m/z ratio 360. Parameters like LOD, LOQ, specificity, method precision, linearity and accuracy were studied by following various international guidelines. Correlation coefficient for linearity falls within the limit ≥ 0.99. Lower values of LOD and LOQ 0.0120 and 0.0363 ppm respectively were obtained which makes the method sensitive enough. A mean recovery of 100.55% was obtained. The method was found reliable, sensitive, specific, and fit for intended use.

AO-26 : Adsorption Characteristics of CNT Intercalated Moringa Leaves

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In this contribution adsorption characteristics of CNT functionalized Moringa leaves as compared to pristine moringa leaves (1%,3%,5%)have been studied to remove methylene blue dye more efficiently. The amount of MB dye adsorbed was sensitive to initial concentration ,amount of CNT functionalized moringa leaves powder ,pH and temperature. All these factors were studied by UV visible spectrophotometer. The adsorption capacity of MOLP and functionalized CNT was estimated for MB at different adsorption variables like pH 4 to 9, MB initial concentration (.05ppm -1ppm),time (0-60 min),temperature (20-50^{0}C).The internal porous structure of CNT functionalized Moringa leaves was explored using SEM and FT-IR techniques. FT-IR showed the presence of carboxylic carbonyl and phenolic groups which greatly enhance adsorption capacity and play an important role in the fixation of cationic dye molecule.

AO-27 : An Amalgamation of Ecological, Analytical and Practical Attributes to Develop Extension to Greener Analytical Methods using the Concept of White Analytical Chemistry

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In developing Greener analytical methods the other parameters affecting the quality attributes of the method needs to be given consideration. Along with the Greener concept (green), the Analytical (red) and the Practical feasibility (blue) factors together contribute to derive the whiter analytical methods driven by the White Analytical Chemistry principles. The RGB colour model is an additive colour model in which red, green and blue colours are mixed together in various proportions to form a different array of colours. In this process of the RGB colour model, if the three colours are added with the full intensity of light, then the white colour is formed. The white analytical method similarly is an amalgamation of the ecological, analytical and

practical attributes. The Whiteness of the analytical method can be enumerated considering the individual parameters in developing an appropriate method. The White Analytical Chemistry concept is nearby to the notion of ecological development due to a more all-inclusive view, as it endeavours for a concession that avoids a categorical increase in greenness at the expense of suitability and attainability.

AO-28 : Bio-Fuels Future and Challenges: India's No Fossil Fuel Policy of 2070

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Biofuels are a new type of renewable transportation fuels produced from biomass-based renewable resources such as plants, animal by-products, or microorganisms. The production of biofuels is also an innovative field that is rapidly evolving, particularly in the arena of producing renewable fuels with hydrocarbon structures already found within the matrix of existing petroleum fuels. Biofuels play a particularly important role in decarbonising transport by providing a low-carbon solution for existing technologies, such as light-duty vehicles in the near term and heavy-duty trucks, ships and aircraft with few alternative solutions in the long term. By 2030 under the Net Zero Scenario biofuel production reaches 24,00,000 million liters, requiring average growth of around 16% per year. India at the 26th session of the Conference of the Parties (COP26) to the United Nations Framework Convention on Climate Change (UNFCCC) held in Glasgow, United Kingdom, expressed to intensify its climate action by presenting to the world five nectar elements (Panchamrit) of India's climate action. A significant increase in biofuel production is needed to get on track with the Net Zero Emissions by 2050 Scenario and deliver the associated emission reductions. a step towards achieving India's long term goal of reaching net-zero by 2070.

AO-29 : Comparison of Variation in Atmospheric Pollutant Concentration during the Episodic Haze Event at a Downwind it of Indo-Gangetic Plain

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Air pollution has affected the air quality as well as human health due to rapid urbanization and industrialization. From December 2019

to January 2020, Agra encountered an episodic event, Haze, related to poor visibility. During the haze event, the daily average $PM_{2.5}$ and ΣBTEX concentration reached 153.1 µg/m^3 and 257.6 µg/m^3, however, visibility reduced by ~2.2 times. However, concentrations of secondary aerosols species, NO_3^-, SO_4^{2-}, and NH_4^+, were 21.0, 16.8, and 11.5 µg/m^3 respectively during haze which were higher than the non-haze (14.1, 5.0 and 6.2 ìg/m^3). $PM_{2.5}$ and BTEX were found to be 2-3 times higher as compared to non-haze. Similarly, 23%, 13% and 22 % increment was observed in trace gases (CO, NOx and O_3) during the haze. Toluene showed the higher ozone forming potential (143.2 ìg/m^3) during the haze period. Meteorological parameters show that temperature was lower in haze (6 °C < T < 15 °C) as compared to non-haze (12 °C < T < 21 °C). RH during haze period was always > 90% and reached a maximum value of over 98% during the night. SEM-EDX images of the $PM_{2.5}$ showed spherical shaped particles enriched with K which may be attributed to the biomass burning.

AO-30 : Climate Change - Its Impact on Indian Society and Rural Women

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Climate change refers to the long-term shifts in temperatures and weather patterns. But Climate change is threat multiplier and it has affecting every minute thing present on the Earth. But while making reports generally we ignore the background impacts of Climate Change. Like impact on Women- their Health, Economic conditions, Human rights, participations etc. Because of climate change and accumulation of GHG's women are going anaemic (National Family Health Survey-5). We have already achieved 1^0C rise in global mean surface temperature and going to achieve 1.5^0C upto 2050. It will completely change the life of women, more burden and pressure on women. Less nutrition because of lack of food security for women and girls, already 400million females of India are dependent on PDS system. We have already outlined SDG's but topic of Climate change creating rift between developed and Developing countries and women are one of most sufferer of this pass–n-pass concept. World already agreed on 1.5^0 C concept so now question is about the life of women of Thar, Assam, Coastal areas, Odisha and central India. Water scarcity, Heavy rainfall, rise in water level, frequent natural disasters and heavy deforestation already affected the life of 47percent native womens. So it's need of hour to include women in main decision making policies because 70percent peoples suffer from climate change induced events are Women.

AO-31 : Status of Wetlands of District Mainpuri U.P.

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District Mainpuri has many water bodies and wetlands, and many of them emerges during rainy season, but they are in endangered status. Their conservation is important. These wetlands gives shelter to several plants and animals. Wetlands are habitats for plants and animals and they hold definite place in ecosystem. Wetlands of District Mainpuri U.P. contributes to large population of Saras Crane and other wetland birds. Physiochemical status of five wetlands were studied viz, Markandeshwar, Saman Bird sanctuary,Sauj, Kirithua and Bhamwat Canal. Saman and Sauj are IBS (bird life Data Zone) under bird area programs of BNHS and bird life international while Saman was declared Ramsar Site in 2019 . As, wetlands play an important role in maintenance of fauna and flora, critical balance of physical, chemical and biological factors is very important for the inhabitants. Conservation of wetlands should be considered while taking up developmental programs by human beings. In this paper the physiochemical status of these wetlands has been discussed along with their conservation strategies.

AO-32 : Sugar Mill Effluent and Its Impact on the Environment

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Development is a natural and continuous process. Industrial development is the major factor causing environmental pollution. India is a fast growing country. The increase in industrialisation is not only consuming a large area of agricultural lands but simultaneously causing environmental degradation. The sugar industry ranks second among the major agro based industries in our country. Nowadays sugar industries are involved in the production of sugar, electricity and ethanol. It has a significant role in the national economy. However the effluent coming out from such industries are toxic in nature and bear a high degree of pollution load. In India the sugar industry generates about 1000 L of waste water for 1 ton of sugarcane crushed. If the effluent discharged without treatment poses pollution problems in both aquatic and terrestrial ecosystems. Proper treatment of effluent must be followed before discharging into the natural source. In this review the recent advancement in the aerobic, anaerobic and physico - chemical treatment technologies and further research possibilities

have been explored. The reuse of treated wastewater was also investigated.

AO-33 : Potential Health Risk Assessment and Source Apportionment using Receptor Modeling Technique of Selected Trace and Toxic Elements in Groundwater of Bastar Division, India

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An inclusive assessment of groundwater was carried out in the Southern part of Chhattisgarh in the Bastar region which is an intensively cultivated zone to ascertain the quality of water. Using pooled research design, about 160 groundwater samples were obtained during the pre-monsoon (PRM) and post-monsoon (POM) periods. Groundwater samples were analyzed for selected trace elements (Al, B, As, Be, Cd, Ba, Co, Cu, Fe, Cr, Sb, Ni, Li, Sn, Mn, Zn, V and Se) using inductively coupled plasma mass spectrometry (ICP-MS; Thermofischer, Model iCAP RQ.ASX-560) and major ions (Cl^-, NO_3^-, SO_4^{2-}, F^-, Na^+, K^+, Ca^{2+} and Mg^{2+}) using the ion chromatography instrument (DIONEX ICS -1100). Principal component analysis (PCA) and positive matrix factorization (PMF) receptor models were applied to samples collected during PRM and POM to identify probable pollution sources. Both PCA and PMF results revealed that the natural, geogenic and agricultural were the three major sources of groundwater contamination in the study area. Further carcinogenic and non-carcinogenic risks related to the exposure of heavy metals/metalloids in groundwater were estimated to know the extent of the risk posed by the pollutants. Among the measured elements, arsenic has shown relatively higher non-carcinogenic and carcinogenic risk in children as well as adults.

AP-CYSA-01 : Are Electric Vehicles Really Safe for Environment ?

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Electric vehicles have attracted widespread interest because of their ability to reduce energy consumption and emissions. Governments

and manufacturers continue to make new commitments for electric vehicle sales, and the cost of manufacturing electric vehicles continues to fall, making them more competitive with internal combustion vehicles. Advances in lithium-ion battery technologies have been key to the growing success of electric vehicles, and a continued transition to electric drive will necessitate far greater battery production. The scientific understanding of the exact environmental impacts of electric vehicles continues to evolve, and the impacts of battery production on electric vehicles' overall emissions are an especially complex topic. Recent studies have investigated the greenhouse gas emissions from battery production, finding a wide range of results and implications. Meanwhile, governments also have begun to consider this issue, and questions have even arisen regarding whether battery life-cycle impacts could be integrated into vehicle policy. In this briefing, we review the research literature, analyse the overall life-cycle greenhouse gas emissions impact of electric vehicles, and discuss key related trends into the future.

AP-CYSA-02 : Heavy Metals in Drinking Water and their Impact on Human Health

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The term "heavy metal" refers to any metal or metalloid element that has a relatively high density ranging from 3.5 to 7 g/cm, and is toxic or poisonous at low concentrations. These metals are non – biodegradable in nature and due to this nature they become a serious threat to human health. Humans are exposed to heavy metals mainly through water consumption. Metals like Thallium (Tl), Arsenic (As), Selenium (Se), Mercury (Hg) can bio accumulate in human body (e.g., in lipids and gastrointestinal systems) and may cause cancer, alopecia and many other health related problems. . The main sources for drinking water pollution are improper dumping of domestic and industrial wastes. Determination of these metals in drinking water can be done with the help of Inductive Coupled Plasma (ICP) or Atomic Absorption Spectroscopy (AAS). This paper deals with heavy metals in drinking water, their types, sources, diseases, metals responsible for these diseases. The methods of reduction of heavy metals and their removal in drinking water will also be discussed during my presentation.

AP-CYSA-03 : Handling of E-Waste by Metal Extraction from Electronic Waste

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Every year electronic waste of 50 million tones is generated due to devices like mobiles, computers, digital machines etc. These devices contain various metals, some are also precious, so to reuse them we need to extract them from batteries, motherboards, chips, ICs outdated old processor etc. This is a very major issue and challenge for waste management. Waste generation is the main cause of pollution. Some wastes are recyclable but are tedious to be made able to reuse. Over 50% of the e-waste consists of ferrous materials and it can be processed and extracted by mechanical shredding hydrometallurgical methods, and bioleaching etc. In this study the methods which extract valuable metals like Cu, Al, Ag, Au converting e-waste pollutions threats into metal resources those who increase economy of the country will be discussed. These include handling of e-waste including combustion in incinerators, disposing in landfill or exporting overseas. Additionally, the presence of precious metals (PMs) which make e- waste recycling attractive economically will be presented like pyrometallurgical routes.

AP-CYSA-04 : Bioplastic A Facile Solution for A Sustainable Environment

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Plastic usage is increasing the number of pollutants in the environment. Plastic particles and other plastic-based pollutants are found in our environment and food chain, posing a threat to human health. From this perspective, the biodegradable plastics material focuses on creating a more sustainable and greener world with a smaller environmental imprint. Bioplastics made from renewable resources can be naturally recycled by biological processes, thus limiting the use of fossil fuels and protecting the environment. Therefore, bioplastics are sustainable, largely biodegradable, and biocompatible. Today, bioplastics have become a necessity in many industrial applications such as food packaging, agriculture and horticulture, composting bags, and hygiene. From this point, bio-based plastic research is taking attention for a sustainable and greener environment with a lower footprint on the environment. This paper will give a new idea of bioplastics in material, processing, and applications

AP-01 : Elimination of Hexavalent Chromium Cr (VI) with Activated Carbon Prepared from H_3PO_4 Activation of Withania somnifera

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Chromium metal is found in industrial wastewater at a much higher concentration than the prescribed limit set by different regulatory authorities. Since chromium (VI) is very toxic and carcinogenic, it requires removal at source, that is, before its discharge to the water bodies. The present work is carried out for removal of Cr (VI) from aqueous solution by using activated carbon prepared from locally available Withania somnifera as a low-cost adsorbent in batch mode. Characterization of prepared activated carbon was done by FTIR, SEM-EDX. The effects of pH, adsorbent dose, contact time and initial metal ion concentration on removal of Cr (VI) were studied in batch process. Different kinetic and isotherm models were examined and the model parameters were determined.

AP-02 : Experimental and Statistical Analysis of Domestic Wastewater using Water Quality Parameters

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One of the major challenges facing people in the twenty-first century is the supply of quality and affordable water. Water availability struggles to keep up with the rapidly increasing demand around the world which is made worse by increment in population, a changing climate, and water quality degradation. Environmental monitoring includes testing for water quality. Poor water quality has an impact on the ecosystem around it as well as aquatic life. These sections deal over all indicators that affects the water quality in the surroundings. Physical, chemical, or biological factors can make up these characteristics. Temperature and turbidity are examples of physical characteristics of water quality and parameters like pH and dissolved oxygen are examples of chemical properties. These water quality parameters are explained in terms of data interpretation on the basis of locality. In this paper, we will analyse grey water. Domestic wastewater which is generated by toilets, bathrooms and kitchens are commonly called as grey water. According to the analysis, systems for treating grey water should include procedures that can trap

contaminants with small particle sizes and change organic waste into minerals, regardless of the quality of the water.

AP-03 : Effect of Pesticides on Enzyme Activity of β-glucosidase and Cellulase Enzyme in Soil of Farrukhabad Region (UP) India

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In the present study, modern agriculture depends upon the chemical pesticides are frequently used in agriculture fields to increase crop production. Effect of pesticides on enzyme activity of β-glucosidase and cellulase enzymes in soil of Farrukhabad region. Soil were collected in rainy season from Farrukhabad region viz., Kaimganj, Amritpur and Farrukhabad tahsil. Soil microbial diversification is indispensible to maintain functional diversity and enzyme mediated critical soil process that detoxify soil from environmental pollutants like pesticides, due to excessive use of pesticides viz., Cypermethrin, Endosulfan and Mancozeb controlling the insects. In India the present study was carried out to assess the effect of different concentration of the pesticides. Results shown that the effect of pesticides on soil enzyme activity slightly decreases while with out pesticides enzyme activity of β-glucosidase and cellulase increases in selected soil.

AP-04 : Global Warming and Natural Disasters

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Global warming refers to the phenomenon that the earth's atmosphere and ocean temperature rise during a certain period of time mainly due to the temperature rise caused by human factors. Since the industrial revolution, humans have burned fossil fuels in large quantities, and the concentration of carbon dioxide in the atmosphere has risen rapidly. At the same time, deforestation has led to a decrease in the absorption of carbon dioxide by the earth and an increase in the amount carbon dioxide in the atmosphere. Because these green house gases are highly permeable to visible light from solar radiation and are highly absorptive to long wave radiation reflected from the earth, they can strongly absorb infrared rays from ground radiation, resulting in Global warming. Climate warming will redistribute Global precipitation, melt glaciers and frozen soils and raise sea levels. It not only harms the natural ecosystems balance, but it also threatens mankind's food supply and living environment.

Global warming is the long term heating of Earth's surface observed since the pre industrial period (between 1850 and 1900) due to human activities, primarily fossil fuel burning, which increases heat trapping green house gas levels in Earth's atmosphere. This term is not interchangeable with the term climate change .

Since pre industrial period, human activities are estimated to have increased Earth's Global average temperature by about 1 degree Celsius (1.8 degree Fahrenheit) , a number that is currently increasing by more than 0.2 degree Celsius (0.36 degree Fahrenheit) per decade. The current warming trend is unequivocably the result of human activity since the 1950s and is proceeding at an unprecedented rate over millennia.

AP-05 : Effects of Pesticides on Enzyme Activity of Dehydrogenase and Urease Enzymes in Soil of Aligarh Region (U.P.) India

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The use of pesticides in agriculture has highly increase crop yield, However, today most pesticides are polluting water , soil atmosphere and food. Pesticides are also impact soil enzymes . Which are essential catalyst rulings the quality of soil life. In the present study, the role of pesticides viz; acephate and two pyridyl methyl amine class insecticide acetamiprid and imidacloprid in soil collected in rainy season from different region of Aligarh (Atrauli, Khair and Iglas). On analysis than the effects of pesticides on enzyme activity of dehydrogenase and urease enzymes feable decrease while without pesticides enzyme activity of dehydrogenase and urease enzyme feably increase

AP-06 : Ground Water Quality Assessment of Nursing Homes Area of Agra City, U.P. (India)

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Water is one of the most important natural resources which provide drinking water for more than one half of the nation's population. In the present study we report the ground water quality of nursing homes area of Agra city. The water samples were collected from four sampling sites of nursing homes areas and their physico chemical parameters such as pH, conductivity, chloride, total alkalinity, Fluoride,

Hardness, temperature, turbidity etc were analysed as per standard methods. The results reveals that the water quality of most of the sites of nursing homes areas of Agra city is not suitable for drinking purpose which recommends the use of indigenous technologies, to make water fit for drinking purpose.

AP-07 : Photo Sensitized Degradation Of 4-Methylaniline Using TiO_2 as Photocatalyst

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The photocatalytic action of the TiO_2 has been studied on 4-methylaniline. Photocatalytic degradation of 4-methylaniline solution in a suspension of titanium dioxide was carried with the use of artificial light sources (UVA). The effects of various process variables on degradation performance such as concentration of substrate, catalyst concentration, pH and intensity of light have been investigated. Photoproduct was characterized by physical, chemical and spectral methods. A tentative mechanism has been proposed with overall reaction. The results show that the degradation of the substrate can be carried out conveniently and efficiently using TiO_2 semiconductor as photocatalyst.

AP-08 : Catalytic and Biochemical Study of Derivative of Benzoxazole of some Lanthanides

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Lanthanide ions are possessing typical characteristics for example, lanthanide contraction, unique magnetic properties etc. The product of lanthanide ions with 2-(1,3-benzoxazole -2-yl - sulfanyl)-N-phenyl acetamide 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 (expressed as BSPA) ligand is allowed to react with solution of lanthanide perchlorates and attempt has been made to synthesize solid BSPA complexes. These complexes are subjected to U.V visible spectroscopy, IR spectroscopy, TGA analysis, mass spectroscopy, elemental analysis etc. For structure elucidation and then antimicrobial activity studies by standard methods. Catalytic effects of these complexes are studied for different types of chemical reactions. Attempts have been made to correlate structural characteristics with properties of these complexes.

AP-09 : Analytical and Biochemically Characterization 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.

AP-10 : Synthesis and Characterisation of Poly Hydroxyethylmethacrylate-Co-Acrylamide Containing Nanocomposites

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The present work focuses on the synthesis of co-polymer Hydroxyethyl methacrylate (HEMA) and Acrylamide (AAm) by bulk polymerisation and further mixes with the two different nanoparticles ZnO and NiO.The prepared co-polymer nanocomposites were also characterized by using FTIR, UV, TGA- DTA/DSC, SEM, Antibacterial activity, Anticorrosive property and Swelling behaviour of the hydrogel. The thermal study was performed to study the interaction of components used in the hydrogel and also to study the thermal stabilities of the material. The analytical techniques such as TGA, DTA and DTG were used for the characterization of HEMA-co- AAm nanocomposites. TGA curve shows the thermal stability of HEMA-co-AAm nanocomposites was improved and the thermal stability higher than the stability of virgin HEMA and AAm in inert (N_2) atmosphere. The co-polymer containing HEMA and AAm plays a significant role in TGA/DTA curve, the addition of nanocomposites improved the thermal stability of co-polymer nanocomposites. The co-polymer nanocomposites were fully decomposed above the 450 ^{0}C but due to the nanoparticles the shifting in the graph clearly shows correlation with the enhanced

tensile and stiffness properties. The FTIR -ATR shows characterised peak in the region from 4000-600 cm^{-1} which shows the bonding between HEMA and AAm nanocomposites. The ester group, amine group and hydroxyl group were present in all the samples which indicated the bonding between HEMA-co-AAm. The UV-Visible analysis shows that most of the samples shows absorbance in the ultraviolet region. The co-polymer nanocomposites were good UV absorber, wavelength decreases as nanoparticle concentration increased which indicated that the nanoparticles and co-polymer are good thermal resistance than pure polymer. SEM image of co-polymers nanocomposites clearly shows the irregular size and homogeneously dispersion of co-polymer whereas the shiny portion indicated the deposition of nanoparticles. The Antibacterial property clearly shows that the co-polymer nanocomposites shows a good antibacterial activity in all the sample due to adding of a nanoparticle in it. The anticorrosive activity of co-polymer nanocomposites also shows a good corrosion inhibitor due to the positive shift in the graph by adding the binder to the co-polymer nanocomposites. The hydrogel of HEMA-co-AAm also shows a high swelling property which can easily use in the many application purposes.

AP-11 : C-Dots as Impending Nanoprobe and Potent Alternative to Metal-based Quantum Dots

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Carbon dots (C-Dots) are a class of zero-dimensional fluorescent quasi-spherical nanoparticles with a size below 10 nm and have the potential to replace semiconductor quantum dots. Carbon quantum dots are emerging as a rising star of carbon nanomaterials, C-dots have the same excellent optical properties as traditional quantum dots such as good photostability and wide excitation however in comparison with quantum dots they possess lower or no toxicity and better biocompatibility without toxic heavy metal elements Hence we can say that C-dots are evolving as a potent alternative to classical metal-based semiconductor quantum dots. C-dots by their unique physicochemical, optical, and electronic properties were explored as biosensors [1], drug carriers 3], and bioimaging probes. The favorable fluorescence properties of C-dots exhibit great potential for applications in analytical chemistry, especially in environment and biological sensing and imaging [2]. There is the various method by which C-dots can be synthesized like the synthetic method, hydrothermal method, laser ablation method, and arc discharge method. Top-down and bottom-up

approaches are used for the fabrication of C-dots. Thus the preparation, properties, and applications of C-dots have drawn great attention. Green chemistry synthesis of C-dots has received great attention, which reduces both cost and time, and results in the high-yield formation of environment-friendly material.

AP-12 : Impact Of Vehicular Emission on $PM_{2.5}$ And Associated Chemical Contents From National Highway At Urban And Semi Urban Location

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The current study was an attempt to measure ambient air quality in term of $PM_{2.5}$ and associated heavy metals at two different sites i.e. Agra (Urban site) and Tundla (Semi-Urban site) near very busy crossing on NH-19 (old NH-2) and characterised in term of heavy metals via ICP-OES. From the outcomes it was determined that the influence of $PM_{2.5}$ concentration was greater at the suburban site (77.59ìg/m^3) as compared to the urban site (72.86ìg/m^3). Concentrations of $PM_{2.5}$ have been compared with prescribed WHO standards and NAAQS given by CPCB India and had been observed to be higher. Ten metals had been subsequently determined, among which, Ca (11.65231/ µg/m3), showed the highest concentration, accompanied by Al (1.397µg/m^3) and Fe (0.97325/ µg/m3). The concentration of metals followed the vogue >Al >Fe > K > Pb > Mn > Co > Cr > Cu > Ni and Ca>Al >Fe > K > Mn > Pb > Cr > Ni > Cu > Co at both the sites (semi urban and urban). The Enrichment factor (EF) values concluded that Al, K, Fe, and Mn had been graded the soils as less enriched (EF< 10) while Co and Pb had been classified as very highly enriched (EF>100). Hazard Quotient (HQ) for Al, Cr, Mn, and Ni is lower than the safe level (HQ= 1) Whereas Excess Lifetime Cancer Risk (ELCR) of Cr(VI) and Ni exceeded the respective safer limit ELCR $\geq 10^{-6}$. This work will assist to attain the interest of the government and different environmentalists in the direction of the chemical composition in the form of metal associated with fine PM from transportation near highways in this area.

AP-13 : An Analysis for Future Impacts of Electrical Vehicles to the Environment

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Electrical vehicles technology has been identified as being key technology in reducing future emissions and energy consumption in

the mobility sector. The 90s have brought us to an era of environmental crisis. We are faced with the problems of air pollution, both indoor and outdoor acid rain, water pollution, hazardous wastes, toxic landfills and leaking storage tanks in our soil, to name a few. Our rapid advances into the industrial and technological age have contributed to these problems. However, energy tools have been analyzed and verified in providing significant contribution in terms of environmental clean-up and a healthier World.

AP-14 : Effects of Pesticides on Enzyme Activity of Amylase and Phosphatase Enzaymes in Soil of Kannauj Region (U.P.) India

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Enzymes are the vital activators in life processes, likewise in the soil they are known to Play a Substantial role in maintaining soil health and its environment. The laboratory studies were conducted to resolute the effects of pesticides (such as atrazine, paraquat and fluridone) on enzyme activities of amylase and phosphatse soil enzymes in selected soil from different region of Kannauj U.P (Teh: Tirwa, Chhibramau and Kannauj) in rainy season. In the present study, It was observed that an effect of pesticides on enzyme activity of amylase and phosphatase feably decreased as compared to control soil in selected region of Kannauj (U.P).

AP-15 : Evaluation of the Physicochemical Characteristics of Industrial Wastewater

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Since the industrial revolution, new causes of pollution have been detected almost daily. As a result, there is a risk of water contamination everywhere. The increasing population density in urban areas adds significantly the amount of wastes in the environment. The toxic materials present in these wastes potentially harm aquatic flora and fauna throughout the process of industrial effluent discharge into water bodies, upsetting the entire system and posing either direct or indirect risks to human health. It is unclear how pollutant rates can change. The rise in illnesses linked to the water supply makes a precise assessment of the degree of environmental contamination possible. In this paper, the water quality index has been calculated using measurements of physicochemical parameters. Water samples

were collected to evaluate temperature, total dissolve solids (TDS), pH, acidity, alkalinity, biochemical oxygen demand (BOD), chemical oxygen demand (COD), and using standard methods. The Water Quality Index values indicate that the water is highly polluted and unfit for drinking, household use, or the healthy survival of aquatic life and that immediate management is required.

AP-16 : Spectroscopic and Calorimetric Investigation of High Fluoride Contaminated Soil

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The collection of fluorine contaminated soil and its sampling was carried out in Remuna area of Balasore district of Odisha, Inida. The IR spectrum indicates the presence of fluoride of various inorganic metals such as aluminium, iron and silicon. The ^{19}F NMR spectrum of soil confirms the presence fluorine in soil. The thermal analysis such as TG-DTA and DTG graphs are used for the determination of moisture, soil organic carbon (SOC) and soil organic matter (SOM) present in soil. The SOC content in contaminated soil varies from 0.13% to 0.38%, while SOM content is ~ 0.76%. The DSC was carried out at the heating rate 5K min^{-1} with sapphire standard. The DSC indicates that fluorine contaminated soil behaves exothermically in the temperature range 296.80 K to 351.80 K. The negative specific heat capacity, C_p, decreases in magnitude with increase of temperature and increases after 339.30 K. The minimum value of C_p is -0.30 $Jg^{-1}K^{-1}$ at 339.30 K and maximum C_p is -0.62 $Jg^{-1}K^{-1}$ at 299.30K. The negative specific heat capacity of soil is explained using thermodynamics. All thermal analysis was carried out in presence of N_2 atmosphere.

AP-17 : Impact of Heavy Metals Present In E-Waste on Environment

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Electronic waste or E-waste comprises old, end-of-life electronic appliances such as computers, laptops, TVs, DVD players, refrigerators, freezers, mobile phones, MP3 players, etc., disposed of by their original users. the categories of E-waste materials, major pollutants including

ferrous/non-ferrous metals, plastics, glass, printed circuit boards, cement, ceramic, and rubber side, and some valuable metals (such as Cu, Ag, Au, Pt, Cd, Cr, Al, Li, Hg, Ni, etc.) Toxic elements from E-waste materials, released in the air, water, and soil, include As, Cd, Cr, Cd, Hg, and Pb, causing pollution. It contains many hazardous constituents that may negatively impact the environment and affect human health if not properly managed. Various organizations, bodies, and governments of many countries have adopted and developed environmentally sound options and strategies for E-waste management to tackle the ever-growing threat of E-waste to the environment and human health. This review presents E-waste composition, categorization, Global and Indian E-waste scenarios, prospects of recoverable, recyclable, and hazardous materials found in the E-waste, Best Available Practices, recycling, and recovery processes followed, and their environmental and occupational hazards. Based on the discussion, various challenges for E-waste management particularly in India are delineated, and needed policy interventions were discussed.

AP-18 : Low-Cost Synthesis of Waste Tea-Mediated CuO Nanoparticles for Visible-Light-Driven Photocatalytic Degradation of Rhodamine B Dye

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This work presents entirely a new, green, and non-expensive route of synthesis of copper nanoparticles (NPs) using waste tea. The crystalline nature of waste tea-mediated Cu NPs (WT-CuO NPs) was confirmed by XRD and SAED analyses. Further characterizations of WT-CuO NPs were done using UV-vis spectroscopy, FTIR spectroscopy, FE-SEM, EDX, and HR-TEM. The WT-CuO NPs when applied as visible light-driven photo catalyst for degradation of Rhodamine B dye. Adsorptions of Rhodamine B (RhB) dye follow pseudo-first-order kinetics. It was found that the dye degradation showed best results in the presence of sunlight at a pH of 8, Rhodamine B dye (RhB) Dye concentration 50 ppm with 50 mg of WT-CuO NPs. At room temperature, the maximum removal of dye was achieved in 90 min by stirring. Rhodamine B dye (RhB) showed that degradation was 98.90 % within the experimental time. The WT-CuO NPs could be reused at least for three times without any significant loss in degradation efficiency.

AP-19 : Adsorption and Photocatalytic Performance of Activated Carbon and Activated Carbon-La_2O_3 Nanoparticles Composites for Malachite Green

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In present study, the removal of Malachite Green (MG) dye by Activated Carbon and Activated Carbon-Lanthanum Oxide nanoparticles composites were investigated. La_2O_3 nanoparticles were prepared by Precipitation method and Activated Carbon-La_2O_3 nanoparticles composites were prepared by impregnation method. Activated Carbon and synthesized Activated Carbon-Lanthanum Oxide nanoparticles composites were characterized by FTIR spectroscopy, X-ray diffraction (XRD), Field emission gun scanning electron microscopy (FEG-SEM) and High resolution transmission electron microscopy (HR-TEM) for surface morphological and crystalline size determination. The X-ray diffraction patterns revealed that the particles exhibited a crystal structure at the suitable temperature. The average particle size of the nanocomposites from the X-ray diffraction is about 33-44nm and also scanning electron microscopy shows good morphology and exhibited clearly cubic and hexagonal shape. The Transmission electron microscopy (TEM) shows the crystalline size of structures is 34-43 nm. Further, the photocatalytic degradation of Malachite Green dye was measured by visible absorption spectroscopy using Activated Carbon and Activated Carbon-La_2O_3 nanoparticles composites. To obtain the optimal conditions for the dye degradation, the effect of various experimental parameters, like amount of adsorbents, pH, concentration of dye, contact time and light intensity on the rate of reaction was studied. A tentative mechanism for the photocatalytic degradation of Malachite Green was proposed. Photocatalytic degradation of Malachite Green dye followed pseudo first-order kinetics. It was found that the dye degradation gave the best results at a pH of 8, MG Dye concentration 200 ppm and using 70 $mWcm^{-2}$ light intensity with 0.080 g of adsorbent. At room temperature, the maximum removal of dye was achieved in 60 min. It was found that the percentage of dye removal was improved from 90.24% for Activated Carbon to reach 98.11% for Activated Carbon-La_2O_3 nanoparticles composites.

AP-20 : The Synthesis and Characterization of 21iro(Fluorene-9,9'-xanthene) and Carbazole based Poly(Arylene Ether)s.

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In this study, we synthesised a series of poly(arylene ether)s having fluorine and carbazole moieties. These light emitting polymers are synthesised by catalytic polymerization between Spiro[dibenzo xanthene-fluorene] and bisphenol carbazols in high yield. Alkyl/Cyclo-alkyl substituted diphenyl carbazole unit is covalently linked into polymeric system in the main chain. These spirofluoene based building blocks could increase the thermal and oxidative stability of organic optoelectronic materials which are highly promising for the development of single polymer layer light emitting diodes. These copolymers were well characterised by different spectroscopic techniques such as UV/Vis, FTIR, Fluorescence and NMR (^{1}H, ^{13}C).Molecular weight is determined by GPC.

AP-21 : Impact of Pollution from Harduaganj Thermal Power Plant on Health of Population and Environment : A Study

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Harduaganj Thermal Power Station, consists of the three major thermal power plant of U.P., is located in Kasimpur of district Aligarh on the bank of Uppar Ganga canal which is running in the NW to SE direction. This study was aimed to study the phyico-chemical and heavy metal status of Harduaganj thermal power station discharged wastewater used by local farmers for growing seasona crops.

As these twin wastes may contain heavy metals, their release in surrounding environment will have potential negative impact on soil, water and air along with human health. The thermal power plant wastewater possessed a high BOD and COD. The concentration of some essential inorganic ions was higher in thermal power plant discharged wastewater as compared to ground water. Of these Phosphate, Sulphate, Calcium, Magnesium and Potassium could considered beneficial as these are essential for the normal growth of a plant.It may be pointed out that high concentration of sodium and chloride are known to cause specific ion toxicity to plants. The thermal power plant complex of Kasimpur has been selected as source of pollution in this case study. The huge amount of coal, burned in the

thermal power plant daily average 38 metric tone result releasing a huge amount of smoke and other poisonous gases i.e. SO_2, NO_2 and CO_2 to the atmosphere.

AP-22 : Heavy Metal Toxicity Found in Some Higher Plants Around the Taj Trapezium Zone (TTZ) : A Comparative Study

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The concentrations of some heavy metals (iron, lead, zinc and copper) in the leaves of Azardirachta indica, Delbergia sissoo and Mangifera indica were determined around the "polluted (near highways)" and "non-polluted area (far from highways)" sites near Agra region during summer of the year 2009. Heavy metal concentrations in leaves were determined by Atomic Absorption Spectrophotometer (AAS) instrument and XRD. Significant differences were found for heavy metals between "polluted" and "non-polluted" areas. Overall, according to our findings plants such as Azardirachta indica, Delbergia sissoo and Mangifera indica are a good bioindicators and can be used in elemental air pollution monitoring studies in urban-industrial conurbations.

AP-23 : A Review on Fluoride Consumption and its Remedies in Groundwater in Endemic Villages of Hathras District, U.P. (India)

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Water being pumped up from underground sources and used for domestic as well as irrigation purposes in several parts of Hathras division is high on fluoride content and is alkaline besides containing a high volume of heavy metals. Samples of ground water collected from different villages of Hathras district have recorded more content of fluoride in the ground water. The water also contains a large volume of TDS (total dissolved solids), high degree of PH level (alkaline) and excess quantity of iron ore. Today, it is a known fact that the groundwater quality is degrading day by day, which is a serious matter of concern, as poor quality water causes threats to health and hygiene of living beings. Presence of large amount of fluoride in ground water is associated with dental and skeletal fluorosis (>1.5 mg/l) and inadequate amount with dental caries[1] (<1 g/l).The permissible consumption of fluoride is recommended to be 0.05 /day/kg of body

weight for maintaining good health. The average weight of villagers of Hathras district is about 50 to 60 kg. Thus per day permissible consumption of fluoride is about 2.5 to 3mg. The scientific data on fluoride contents in food indicates that about 2 to 3 mg fluoride is consumed from food, milk and tea alone leaving very little scope for the consumption through water. As it is very difficult to isolate the food having high fluoride content in the daily food chain, it was therefore decided to install reverse osmosis plants for water defluoridation. Within one year of installation of Reverse Osmosis (RO) plants, the interaction with the communities started giving positive signs of general improvement in health and wellbeing due to reduction in incidences of waterborne diseases and other health related problems of the villagers. Hence, on the basis of above facts, it was decided to give a review article on the content of fluoride consumptions and its remedies in ground water of different endemic villages of Hathras district, UttarPradesh, India.

AP-24 : Ambient Air Quality Monitoring of Nandurbar City : A Case Study

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The ambient air quality monitoring was carried out at three different locations in Nandurbar city during the period of 1st January 2022 to 1st June 2022. The parameters likes Respirable suspended particulate matter (RSPM) i.e. PM_{10}- (particulate matter having diameter or equal to 10µm), $PM_{2.5}$ (particulate matter having diameter or equal to 2.5 µm), SPM (suspended particulate matter having size greater than 10 µm were estimated by gravimetrically. Also, the gases concentration presence in air such as Sulphur dioxide (SO_{2-}), Nitrogen dioxide (NO_2), was estimated with help of air gas sampler machine. The eight and four hour continuous air sampling was done for the collection of RSPM and gas samples at each location respectively. The result shows that, the value of PM10 cross the permissible limit laid down by the National Ambient Air Quality Standard (NAAQS). While the gases i.e SO_2 and NO_2 are as per the NAAQS.

AP-25 : A Physico-Chemical Assessment of Water Quality at Two Locations of Chambal River in Dholpur (Rajasthan)

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Over the past several years deterioration in water quality has gradually rendered the chambal river water unsuitable for various beneficial purposes and the maintain and restore the wholesomeness of river water in terms of the ecological sustainability is the logical necessity of today. The present study deals with physico-chemical characteristic of chambal river water in national sanctuary area of Rajasthan at Dholplur district, India. The main purpose of study to evaluate the various physico- chemical parameters as well as seasonal effects on water quality parameters like, BOD, COD, pH Hardness, DO, Calcium, Potassium, chloride, Fluoride, Sulphate etc. along with some heavy and trace metals within the sanctuary region. The analyzed water quality data indicate that the chambal river water at two locations is pollution free except exceeding value of lead i.e. 0.04 mg/L. Thus the chambal river water can be serve as good habitat for many aquatic life such as Flora and Fauna.

AP-26 : A Review on Human Health Effect of Heavy Metals

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These metals have been extensively studied and their effects on human health regularly reviewed by the international bodies such as the WHO. The heavy metals have been used by humans for thousands of years. Although several adverse health effects of the heavy metals have been known for a long time, exposure to heavy metals continues, and is even increasing in some parts of the world, in particular in less developed countries, though emission have declined in most developed countries over the last 100 years. The recent data indicate that adverse health effects of cadmium exposure may occur at lower exposure levels than previously anticipated, primarily in the form of kidney damage but possible also bone effects and fractures. The general population is exposed to lead from air and food in roughly equal proportions. Exposure to the arsenic is mainly via intake of the food,

drinking water and food being the most important source in most populations.

AP-27 : Waste Water Management and Water Quality of River Yamuna in Agra, Ancient Capital of India

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River Yamuna is treated as twin sister of River Ganges. But it is one of most polluted river of India because it crosses from nearby the megacities. Agra,an ancient capital of India during Mughal period now famous for Leather products and Petha sweet. But the environmental impact of Petha sweet is very bitter for river Yamuna and its aquatic species. Conductivity, salinity and sodium content were within the permissible categories. Chloride concentration exceeded acceptable levels of drinking water guidelines. Water quality was poor at all locations with respect to heavy metal contamination, especially along the lower section of the Agra stretch. Heavy metal concentrations were manifold higher than the acceptable limits of drinking water according to the BIS guidelines and reached ~29, 4.9, 10, 31, 27, 83, 7.3 and 27 times higher, respectively, for metals Aluminum, Copper, Chromium, Cadmium, Iron, Lead, Manganese and Nickel. The Waterworks Bridge and the Poiya Ghat are major point sources. Low oxidation–reduction potential reflected high organic loads and traces of Eutrophication together with significant levels of Nitrate and total Phosphate. Discharges from agriculture, sewage, leather industries and Petha manufacturing units could be important sources of high metal concentration. This calls for urgent measures to be taken for prevention of metal contamination in the river, through both, technology as well as implementation of regulations in order to sustain huge populations in megacities like Agra. Waste water treatment from point sources needs tremendous improvement on the city. Treatment of the entire waste generated up to the tertiary level is required for minimizing dissolved solids, especially toxic metals, and rendering reuse in agriculture suitable. Treatment plants need proper operation, maintenance, uninterrupted power supply and regular monitoring. Various measure and programmes need to be undertaken to ensure safe reuse of wastewater.

AP-28 : Light Absorbing Carbonaceous Aerosols Over Himalayan Glacier Regions

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Light-absorbing carbonaceous aerosol is a major concern these days. They are capable of absorbing a wide range of solar radiation, which can disrupt earth radiation budget. This study was carried out at the Himalayan glacier region [Thajiwas glacier, 2799 m asl, Gomukh glacier, 3415 m asl, and Zemu glacier, 2700 m asl], which is located in the western Himalayan region (WHR), the central Himalayan region (CHR), and the eastern Himalayan region (EHR). The sampling was conducted during the summer ending with the onset of monsoon and winter (2019 – 2020). Ambient $PM_{2.5}$ samples were taken on quartz filters with a low volume sampler followed by OC and EC quantification using IMPROVE_A thermal optical reflectance protocol. Light absorption properties such as absorption coefficient (b_{abs}, Mm^{-1}), mass absorption efficiency (MAE, m^2g^{-1}), absorption angstrom exponent (AAE) and single scattering albedo (SSA) were calculated using UV-Visible spectrophotometer equipped with integrating sphere.

INORGANIC CHEMISTRY SECTION

Sectional President's Address

Ruthenium Complexes as Anticancer Drugs

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For the last four decades anticancer chemotherapy has concentrated on cisplatin derivates. In spite of their consistent side effects, cisplatin derivates have a central part in most anticancer treatments. In the search for drugs with fewer side effects other metal complexes have been examined over the past few years. Like all metal drugs, the activity of the ruthenium compounds depends on both the oxidation state and the ligands. Ruthenium as a substitute for the toxic platinum metal has received a lot of attention recently. Organometallic compounds such as half-sandwich ruthenium–arene complexes are very versatile and have proven to be active against cancer cells due to their wide and diverse structural types and varied ligand bonding modes which offers considerable potential in fine tuning their biological properties. Activity tuning of arene complexes have been discussed by varying, amines, phosphines and other chelating ligands.

IL-01 : Recent Advances in Organic-Inorganic Hybrid Complexes of Organotin (IV) : New Perspectives and Applications

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The chemistry of organic-inorganic hybrid complexes of organotin(IV)has been extensively studied due to the synthetic, structural , technological and biological applications of these complexes. Various potential organic ligands such as heterocyclic â-diketones, Schiff bases, N-protected amino acids, oximes have been employed for the synthesis of these complexes. The structures of these complexes have been characterised with the assistance of elemental analysis, molecular weight measurements, mass spectral studies and spectroscopic evidences. Some of these complexes have also been studied with the help of single crystal X-ray analysis and density functional theory (DFT/B3LYP method).There was a synergy in the experimental data and theoretical data of these complexes. These newly synthesised complexes demonstrated a wide range of biological applications. The optimised molecular structures, geometries, dipole moments, energy gap and electronegativity of some of these complexes have also been studied by computational analysis. The lower values of energy of organotin(IV) complexes as compared to the corresponding ligands suggest higher stability of the complexes.

IL-02 : Metal Chelates : Biomedicinal Aspects

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The Pandemic Covid-19, forced medicinal scientists to view and review the chemotherapeutic search including use of Purposed and Re-purposed drugs. Could metallodrugs or metal-chelates be an Alternative or Supplementary medicines? The Challenges and Possibilities, are before us to answer by making intensive researches. The interfacial studies overlapping Inorganic chemistry and Biomedical sciences , have attracted the attention of bioinorganic scientists in search of novel pharmacophores and metallodrugs. Inorganic chemistry applied to biology and medical sciences, has emerged as a recent offshoot of bioinorganic/medicinal-inorganic chemistry, which includes also, the metal-based drugs, metal sequestering or mobilizing agents, metal containing diagnostic aids and the medicinal recruitment of endogenous metal ions. There are references in indigenous Indian

medicinal system Ayurveda, on the same. The metal complexes are amenable to combinatorial synthetic methods and an immense diversity of structural scaffolds can be achieved. Metal centers are capable of organizing surrounding molecules to achieve pharmacophoric geometries that are not readily achieved by other means. Understanding these interactions can lead the way towards rational design of metallopharmaceuticals implementations of new co-therapies. The design and synthesis of a suitable ligand perhaps is the key step in the development of coordination complexes with unique properties and novel reactivity. *Principle of Reverse Pharmacology* may help substantially in restoring the concept and therapeutic use practices of *Traditional Medicinal systems*, on issues to prevent and minimize the prevalent attacks of mutating and resisting microbes including viruses and fungi.

Metal complexes derived from Schiff bases and its derivatives have been studied extensively due to their facile synthesis, unusual configurations, and structural labiality. The insertion of designed Schiff bases as ligands in metal coordination sphere produces specific functionalities and exciting features with interesting theoretical and practical applications. Related issues shall be discussed in this lecture.

IO-CYSA-01 : $LaMnO_3$/rGO Composite: Synthesis, Characterization and its Application for Supercapacitor

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The pure $LaMnO_3$ and $LaMnO_3$/rGO (25,50,75 wt%) composites are synthesized by using citrate gel auto-combustion route and mechanical mixing method respectively. The well intense peaks of rGO in $LaMnO_3$ XRD pattern confirmed the perfect formation of $LaMnO_3$/rGO (25,50,75 wt%) composite materials. The presence of various functional groups, stretching and vibrational modes were analyzed by the Fourier Transform Infra-Red (FTIR) technique. The scanning electron microscopy (SEM) confirmed the porous surface morphology of the compounds and it reveals that $LaMnO_3$ is embedded between the sheet of rGO. $LaMnO_3$/rGO75 (wt%) composite exhibits excellent capacitance at a current density 1 Ag^{-1}, it also reveals the electrochemical GCD process, the specific capacitance of $LaMnO_3$/rGO75 (wt%) is nearly double when compared with pure $LaMnO_3$. Owing to excellent electrochemical performance of LMO/rGO75 (wt%) electrode can be used as a promising candidate for high performance supercapacitor application.

IO-CYSA-02 : Effect of Montmorillonite Clay on the Properties of Chitosan/poly (Vinyl Alcohol) Films

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Eco-friendly polymer films have drawn much attention in antimicrobial coatings, drug delivery systems, wound healing, tissue engineering, and wastewater treatment due to their biocompatibility and biodegradability. The blended chitosan/polyvinyl alcohol (CS/PVA) films incorporated with montmorillonite (MMT) were prepared using a solution blending-casting method. The effect of MMT concentrations of 0%, 0.5%, 1%, 3%, 5%, and 7% on the structural, thermal stability, and surface properties of blended CS/PVA film was investigated using various characteristics methods like Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Scanning electron microscopy and energy dispersive X-ray spectroscopy (EDS), and Differential scanning calorimetry (DSC) measurements. It was found that the properties of the films changed as the MMT content varied. FT-IR results showed the interaction between chitosan and PVA through hydrogen bonding. CS/PVA film SEM-EDS and XRD results revealed that the MMT was well dispersed and predominantly exfoliated inside the CS/PVA matrix. Moreover, partial aggregation of MMT in the film structure was observed with increasing MMT content from 5% to 7%. DSC analysis reveals that thermal stability was enhanced with the increasing amount of MMT. It showed that adding an appropriate amount of MMT to the film could further improve the properties and enlarge the potential applications of blended films.

IO-CYSA-03 : Health Risk Assessment of Potentially Toxic Metals in Settled Dust in Schools of Agra Region (India)

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Indoor air pollution is 2-3 times more harmful than that of ambient and as per State of Global Air (2019) report, the pollution has contributed to 1.6 million deaths worldwide in 2017. The concern increases when the exposed population is delicate and they expend their second highest time in a critical microenvironment like schools which have high population density improper ventilation. Among other pollutants indoor settled dust settled onto objects, surfaces, floors and their re-suspension may be an important source of exposure to pollutants. Settled dust can be a clump of various contaminants

including heavy metals which have high persistent nature in environment, high toxicity, and detrimental health effects. The study was carried out in winter season (2021) to examine metals concentration and associated children's health risk from school dust samples of urban and semi-urban schools located in residential and roadside areas of Agra, India. Dust samples were collected by softly brushing windows, floors, tables and chairs of classrooms with soft paint brush and collected in dust pan. Geo-accumulation (Igeo), pollution (PI), integrated pollution (IPI) and pollution load (PLI) indexes were used to determine metals contamination while USEPA health risk assessment models were utilized to assess the health risks in children. The result indicated that Ca (48.06%) was abundant while Cd (0.005%) had lowest concentration in dust samples of all schools. The result from pollution indices revealed that school dust were extremely contaminated with Fe and Cr while moderately contaminated with Mn, Pb, Ni, Cu. Moreover, the health risk model results showed no significant non cancerous risk in children with primarily highest hazardous index (HI) of Pb at residential (8.7E-02) and roadside (4E-02) urban schools whereas Cr at residential (7.0E-02) and roadside (6.9E-02) semi-urban schools. It was also inferred that posed risk by metals was highest through ingestion pathway than others. The cumulative HI of all metals and exposure route, the schools were in the order as urban residential > semi-urban residential > semi-urban roadside > urban roadside. Pb posed highest carcinogenic risk (CR) in all exposure at all schools and the value of CR ranged from 4.64E-07 to 3.53E-02. The findings of the study indicate that more investigations should be spend on potentially toxic metal contaminations in schools of Agra, especially for Pb, Cd and Cr.

IO-CYSA-04 : Surfactant Assisted Synthesis of Cu Doped ZnO for Catalytic Diselenide Bond Formation

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Recently, there has been an increasing demand for efficient methods to synthesize disulfides and diselenides owing to their important roles as structural motifs in a wide range of biologically and pharmaceutically active compounds.In the present work,bare and Cu-doped ZnOnanocrystallites are synthesized by surfactant-assisted hydrothermal method and thoroughly characterized by IR, XRD, FE-SEM and UV- Visible techniques. XRD showed that the diffraction peaks of all the products were in good agreement with the crystallite size ranging from 18nm - 20nm for Cu-ZnO. FE-SEM images explored

different morphologies.From UV-Visible band gap energy for SDS assisted synthesized Cu-ZnO was 3.31eV - 3.35eV. The effective one pot procedure is developed for direct synthesis of diselenidesfrom aryl halide and selenium in DMF. All the diselenide derivatives were thoroughly characterized by IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy.The important feature of this method is using Cu doped ZnO as a reusable and chemoselective catalyst. This protocol has several advantages such as ambient conditions, the use of a small amount of catalyst, ligand free system and an easily available and low-cost reagents.

IO-CYSA-05 : Synthesis of Biologically Active Ternary Metal Complexes Derived from Isatin Derivative and 1,10-Phenanthroline

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Two novel ternary metal complexes of Ni(II) and Co(II) were prepared by conventional thermal method using Schiff base(primary ligand, derived from isatin and phenylhydrazine) and 1,10-phenanthroline as secondary ligand. The structure of compounds was characterized by using various techniqueslike elemental analysis, FTIR, ^{1}H NMR, melting point determination, molar conductance measurement, magnetic moment measurement etc., and their biological evaluation was conducted against Staphylococcus aureus and E. coli bacterial strains and two fungal strains, i.e.Aspergillus niger and Candida albicans. Co(II) metal complex exhibited good antibacterial activity against both strains. Among these synthesized compounds Co(II) metal complex is most potent for selected bacterial and fungal strains.

IO-CYSA-06 : Synthesis and Characterization of a Deep Eutectic Solvent with Tetrabutylammonium bromide (TBAB) and Itaconic Acid

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A new class of deep eutectic solvents (DESs) which are composed of hydrogen bond acceptor (HBA) and hydrogen bond donor (HBD), appear as an auspicious substitute for ionic liquids and organic solvents. DESs are cheaper, safer, non-toxic, biodegradable, and bio-compatible and hence fall in the category of green solvents. DES synthesis is an

example of a reaction with 100% atom economy. TBAB-itaconic acid-based DES was prepared by mixing Tetrabutylammonium bromide (TBAB) and itaconic acid at 88 °C until it formed a homogenous liquid. It was cooled to RT and used without any further purification. It was characterized by using TGA, FTIR, and NMR. In this synthesis, TBAB and itaconic acid in different molar ratios like 1:1,1:2,1:3,3:2,2:1 were taken as raw materials. The melting point measurement of all these DES samples was carried out and illustrated with the help of a phase diagram. The best alternative among the selected set is (1:1) as it remained a highly viscous liquid at RT. Physical properties such as density, viscosity, surface tension, refractive index, conductivity, and pH will be studied. Even computational chemistry will be used to predict thermodynamics properties of DES. Further investigation into the applications of this newly synthesized DES as solvents in TLC, HPLC, and even in extraction processes is underway in our laboratory.

IO-CYSA-07 : Synthesis of Zn(II) and Hg(II) Complex with Schiff Base of Anthracene and Phenothiazine Derivative and their Spectroscopic Study

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Schiff bases are an immense group of compounds specified by the presence of C=N linkage. The versatility of Schiff base may be created by combining a variety of alkyl or aryl substitutes. These types of compounds are found in nature as well as may be synthesized in laboratories. Recently, Schiff bases have been an electrifying and encouraging topic to many biochemists and researchers.[1] Schiff bases are an important part of the study in the area of medicine and material sciences. There are several progressions and evolutions towards smooth synthesis and bio applications. Schiff bases as organic molecules and complexes play an important role in medicine or drug synthesis.[2] A Schiff base was prepared by 2-aminoanthracene and 2-acetylphenothiazine by condensation. This synthesized Schiff base and glycine ligand participated in the synthesis of complexes of 3d(Zn) and 4d(Hg) metal salt. All the synthesized compounds were characterized by spectroscopic techniques (UV-Vis, FTIR, NMR, Mass spectra, etc.) as well as physicochemical analytic techniques (magnetic moment, conductance, elemental contribution, etc.). Biological studies were also employed for all synthesized compounds and a comparison of their activities was established in this article.

IO-CYSA-08 : Particulate Matter concentration and Ion Contamination in different Indoor Microenvironments of Schools in Agra, India

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Indoor air pollution has been recognized as a serious health concern especially for school children. An investigation of concentrations of Particulate Matter ($PM_{2.5}$ and $PM_{1.0}$) was carried out along with the measurement of anion concentrations (F^-, Cl^-, NO_3^- and SO_4^{2-}), in the indoor microenvironments of schools at two different locations namely Urban and Semi-Urban which were further classified into Roadside and Residential location. The study was carried out in the winter season, using a low volume sampler to collect PM. The collected samples were then extracted for anions which were analysed on Ion Chromatography. The average concentration of PM was found out to be 48.932 ± 12.89 µg/m^3 and 32.161 ± 13.46 µg/m^3, for $PM_{2.5}$ and $PM_{1.0}$ respectively. The total ionic concentration associated with aerosol particles was higher for $PM_{2.5}$ (6.67 ± 2.88 µg/m^3) than in $PM_{1.0}$ (3.74 ± 2.72 µg/m^3), showing approximately 2% higher concentration in the former. The results indicate the dominance of NO_3^- (55.17%) species in $PM_{2.5}$ particles while the SO_4^{2-} (57.37%) species dominated the $PM_{1.0}$ particles. F^- and Cl^- were found in relatively low concentrations in both sizes. Ionic concentration for Roadside sites were higher (19.83% - 11.85% of total PM concentration) than for Residential sites (13.25% - 5.42% of total PM concentration). The trend for ion concentration follows $NO_3^- > SO_4^{2-} > Cl^- > F^-$ for $PM_{2.5}$ and $SO_4^{2-} > NO_3^- > F^- > Cl^-$ for $PM_{1.0}$ respectively.

IO-CYSA-09 : Mixed Ligand Complexes of Trivalent Chromium with histidine, Chromone and Quinoline Derivatives : Synthesis, Characterization and Antimicrobial Studies

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Schiff bases metal complexes are versatile compounds due to their broad spectrum of biological applications. There was a lots of development took place in recent years in the field of Schiff bases compounds with a series of applications, from synthetic to biological to technological spheres. Two new Schiff bases (E)-6-methyl-3-(1-(2-phenylhydrazineylidene) ethyl)-4H-chromen-4-one [L_1], and (E)-2-((2-

phenylhydrazineylidene) methyl) quinoline Schiff base[L_2] were synthesized as a result of the condensation of phenyl hydrazine with 3-formyl-6-methylchromone [L_1] and 2-Quilnolinecarboxaldehyde [L_2] respectively in 1:1 molar ratio. Two mixed ligand complexes were synthesized by reaction of Cr (III) metal ion with histidine and newly synthesized ligands L_1, L_2 respectively. Elemental analysis, FTIR, mass spectroscopy, and ^{1}H NMR have been used to justify their proposed chemical structures. The antimicrobial activities of the chromium (III) complexes and the free ligands against bacterial strains, S. aureus, E. coli, and fungal pathogens, C. albicans were determined.

IO-CYSA-10 : Designing and Spectral Studies of Zn(II) Complex of S-benzyl β-(N-2-methyl-3-phenylallylidene)dithiocarbazate as a Potential 2019-nCoV main Protease Inhibitor

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Antimicrobial resistance is fast growing global concern with swift increases in multidrug-resistant bacteria. This gives the researchers the task of looking for a solution. New coordination compounds could be considered as best solution. Based on this, we report S-benzyl β-(N-2-methyl-3-phenylallylidene) dithiocarbazate (L) formed novel complex Bis[S-benzyl-β-(N-2-methyl-3-phenylallylidene) dithiocarbazate] zinc(II) having general formula [$Zn(L)_2$] with Zn(II)-acetate, its bio-efficacy has been examined against the growth of bacterial strains namely gram-positive S. aureus and gram-negative E. coli to evaluate their anti-microbial potential, the inhibition diameter results obtained by mean deviation of E. coli and S. aureus against standard drug (Erythromycin) were 28.13, 42.09, 62.3 & 27.27, 39.11, 58.11 mm and 26.03, 40.18, 59.12 & 26.5, 36.3, 57.06 mm. Structural perlustrated by UV-Vis, FT-IR, Raman, ^{1}H-NMR, ^{13}C-NMR, Mass spectroscopy revealed that [$Zn(L)_2$] complex has distorted square planner geometry around the metal ion, coordinated through N_{imine} and $S_{thiolate}$ atoms. Density functional calculations of [$Zn(L)_2$] in gas phase were performed by using DFT (RB3LYP) with LanL2DZ basis set and the results are: chemical hardness (η) 0.007915 eV, chemical potential (μ) 0.11643 eV, electron afûnity (A) -0.10852 eV, softness (S) 7.855 eV, ionization energy (I) -0.12435 eV, electronegativity (χ) -0.11643eV, dipole moment (D) 4.0690 Debye and having comparative stabilization energy -1718.1753 eV. VEDA-4 software was employed for theoretical FT-IR spectrum perlustration, which yielded 237 fundamental vibrational modes along with potential energy distribution percentage (PED%) showing non-

linearity of $[Zn(L)_2]$. Theoretically calculated parameters like UV-Vis, FT-IR, ^{1}H-NMR, ^{13}C-NMR, Raman, HOMO-LUMO energy gap and electrostatic potential were in conformity with calculated results, along with thermal analysis up to 800 ^{0}C in nitrogen atmosphere. The compound was docked with 2 different receptors 1HT0, 1U3T, 1U3V and 3S7S to find the best ligand protein interactions.

IO-CYSA-11 : Synthesis, Spectrochemical Characterization, Antifungal, DNA Binding and Antioxidant Screening of Novel Schiff base Ligand and its Ni(II) & Cu(II) Metal complexes

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To explore effective bioactive compounds, a novel Schiff base ligand 4-chloro-2-(2,5-dimethoxybenzylideneamino)-5-nitrophenol derived from 2,5-dimethoxybenzaldehyde and 2-amino-4-chloro-5-nitrophenol along with their Ni(II) and Cu(II) metal complexes were synthesized. These compounds were characterized spectrochemically by molar conductance, FT-IR, UV-Vis, mass spectra, P-XRD; the TGA analysis was used to determined the thermal stability of synthesized compounds. The coordination sites of the synthesized ligand are azomethine nitrogen and phenolic oxygen, which makes the ligand monobasic - bidentate. The metal complexes showed distorted octahedral geometry having two water molecules. The antifungal activity was tested against the fungi Aspergillus Niger and Fusarium Oxysporum, which depicts that the Cu(II) gives better antifungal activity. The DNA binding 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 than the Ni(II) complex and Schiff base ligand. Furthermore, testing of the compounds have been done for radical scavenging potency by using DPPH, the Cu(II) complex gives better antioxidant activity than the others.

IO-CYSA-12 : Functionalized Graphene Oxide Loaded Ionic Tolfenamate Complexes as Rationally Designed Vehicle for Cancer-Targeted Drug Delivery

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This study focused to demonstrate the impact of the anticancer activity of nanoparticles of ionic tolfenamate copper complex 1 by

using graphene oxide as a drug carrier. Complex 1 crystallized in the triclinic P-1 space group possessing the lattice parameters, a = 7.6964(11) Å, b = 14.775(2) Å, c = 19.213(3) Å, α = 108°, β = 93º, γ = 97º per unit cell. The complex was loaded on GO, which was prepared by the simple ultrasonication method. The successful loading of complexes on GO depicted that the encapsulation of complexes on GO occurred via π–π stacking and electrostatic mode of interaction. The corroborative results of all the techniques along with molecular docking suggested the electrostatic mode of interaction of complexes-GO towards the preferential target RNA. Cleavage activity was performed by gel electrophoretic assays which indicated that complexes-GO cleaves tRNA molecule. The cytotoxic studies of complexes-GO were evaluated against human lung cancer (A549) cell lines and triple negative breast cancer (MDA-MB-231) cell lines. These experiment results revealed significant cytotoxic activity against the treated cancer cell lines. The kinetic results provide clear evidence of endocytosis of complexes, revealing that the released drug complexes from carrier (GO) has specifically entered into the cell nucleus.

IO-01 : Spectral, Magnetic and Biocidal Studies of Mn(II), Ni (II), Co(II) and Cu(II) Mixed Ligand Complexes

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The M (II) transition metal have been prepare mixed ligand complexes with tinidazole & 4-amino benzoic acid under reflux for several hours in an ethanolic medium. The crystalline complexes were subjected to spectral, magnetic and comparative fungicidal behavior of both ligands with their M(II) complexes have also been studies against A. niger and A. flavus.

IO-02 : Synthesis and Spectral Characterization of Ni(II) Complexes of 13-membered dioxa-diazamacrocycles Derived from β-diketones and 1,8-diamino-3,6-dioxaoctane

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Ni(II) complexes of the type [$NiLCl_2$] (where L= 13-membered N_2O_2 macrocycle) have been synthesized by [1+1] cyclocondensation of 1,8-diamino-3,6-dioxaoctane with β-diketones such as 2,4-pentanedione, 1-phenyl-1,3-butanedione and 1,3-diphenyl-1,3-propanedione in the

presence of Ni(II)chloride . These complexes have been characterized by elemental analyses, molar conductances, electronic, IR and FAB mass spectra. On the basis of the above studies, a six coordinate distorted octahedral geometry has been proposed for all the complexes.

IO-03 : Structural Improvement of $CaFe_2O_4$ by Ni Metal Substitution toward Enhanced Magnetic, Optical and Electrical Properties

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Ni^{+2} substituted Calcium ($CaFe_2O_4$) ferrites with various compositions ($Ni_xCa_{1-x}Fe_2O_4$; x=0.0, 0.2, 0.4, 0.6, 0.8, 1.0) is prepared by citric acid gel method. The effect of incorporation of Ni^{+2} ion on structural, morphological, magnetic, optical and DC electrical properties of $CaFe_2O_4$ is investigated by various techniques. An attempt is made to improve the distorted orthorhombic crystal structure of $CaFe_2O_4$. FT-IR spectra revealed the formation of spinel structure. Structural analysis by XRD pattern asserts the transition of Pnma orthorhombic symmetry to Fd-3m cubic crystal structure. The decreasing trend in volume due to lattice compression with the addition of Ni^{2+} in $CaFe_2O_4$ is observed. Raman spectra attributed relaxation in distortion of crystal structure. The variation of magnetic parameters as a function of substitution is studied from hysteresis loop. UV-DRS spectra demonstrated the substitution of Ni^{+2} ion decreases the band gap energy. DC electrical conductivity inferred improvement of the charge carrier mobility due to Ni^{2+} substitution.

IO-04 : 2/3 D Zinc Oxide Nanostructures for Environmental Remediation

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The zinc oxide (ZnO) nanostructures were synthesized using hydrothermal reaction technique at 180°C with varying reaction time viz., 2, 4, 8 and 12 h. The prepared ZnO nanostructures were characterized with different spectroscopic and microscopic techniques. The XRD indicate the formation of 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 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 photocatalytic activities of prepared ZnO nanostructures were investigated by following degradation of 100 mL, 10 ppm methylene blue (MB) dye. Among the prepared ZnO nanostructures, the ZnO prepared at 8 h of reaction time shows highest MB degradation rate, the observed apparent rate constant value is $3.3 \times 10^{-2} \pm 0.1 \times 10^{-2}$ min^{-1}, which is five times more than 4 h reaction time.

IO-05 : Potentiometric Studies on Binary Complex of some Lanthanide Metal(lll) Ions

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The thermal decomposition of Lanthanide metal complexes has attracted the attention of several workers. Many metals were developed for deriving kinetic data from TG curves. But it is difficult to find a suitable equation to describe the kinetics of all the reactions. Particularly in case when kinetics varies the process. The thermal decomposition rate of a complex is determined by the rate at one or more of the states.

The kinetic parameters like activation energy (Ea) , order ofof reaction (n), frequency factor (log Z) and activation entropy (S^0) were calculated by applying Doyle's method modified by Zsako and Coat's and Redfernmethods.

The binary solid complexes of Sm(lll) with Quinaldic Acid and Eu(lll) with L- Serine were isolated from the mixture of equimolarsolutions of metal nitrates and ligands. The pH of the solution was adjusted to 7.0. The mixture was refluxed in ethanol for 3-4 hours on waterbath. The solid mass obtained, on cooling, was filtered, washed,recrystallized and dried at 60 -70 ^{0}C. The complex was subjected to elemental analysis and the metal contents were estimated by conventional standard methods. The probable formulae of the complexs were assigned on the basis of elemental analysis and are well supported by TG curves.

IO-06 : Fabrication of An Efficient Amino substituted 1,4-naphthoquinones Sensitized TiO_2 Photoanode based DSSCs.

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The amino-substituted 1,4-naphthoquinone as photosensitizers, viz; BrA5; 2-bromo-3-(pentylamino)naphthalene-1,4-dione, BrA6; 2-bromo-3-(hexylamino)naphthalene-1,4-dione, BrA7; 2-bromo-3-(heptylamino) naphthalene-1,4-dione, BrA8; 2-bromo-3-(octylamino)naphthalene-1,4-dione, have been synthesized from 2,3-dibromonaphthalene-1,4-dione and primary amines. The TiO_2 photoanodes have been prepared by chemical bath deposition and doctor blade method followed by calcination at 450 ^oC. After sensitization of photosensitizers (BrA5, BrA6, BrA7, and BrA8) on the TiO_2 photoanodes, the Fourier-transform Infrared Spectroscopy (FT-IR) analysis of photosensitizers showed the existence of N-H bands. The scanning electron micrograph (FE-SEM) indicates the morphologies of TiO_2 and ZnO photoanodes. The optical properties of photoanodes show the broad band each in the visible region, which are assigned to $n \rightarrow \pi^*$ charge-transfer transition. The XRD pattern of TiO_2 photoanodes confirmed the anatase and rutile mixed phases. The dye-sensitized solar cell (DSSC) system was formed by the sensitization of photosensitizers on TiO_2 photoanodes. The photosensitizer's photovoltaic performances in TiO_2-based photoanodes were studied through electrochemical impedance analysis. The TiO_2/BrA8-based DSSC is due to the higher photosensitizer loading and fast electron injection. The power conversion efficiencies of the DSSCs fabricated using BrA8 photosensitizer on TiO_2 photoanode are higher than other photosensitizers (BrA5, BrA6, and BrA7). The present study will open a new route to fabricate highly efficient DSSCs using amino substituted 1,4-naphthoquinone photosensitizers.

IO-07 : Carbon Dioxide into Formic Acid in the Presence of Copper Complex as Catalyst : Synthesis, Characterization and Catalytic Study

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The synthesis and characterization of metal complexes with 1,10-Phenanthroline derivative was attempted and summarized. The

electrocatalytic behaviour of metal complexes for the hydrogenation of carbon dioxide was performed through cyclic voltammetry, XPS, UV-Visible spectroscopy, controlled potential electrolysis and IR-SEC. Among the metal complexes, the copper complexes with 1,10-Phenanthroline derivative was tested as an efficient and selective catalyst for the hydrogenation of CO_2 to formic acid under 70 bar total pressure, 75°C. The experimental outcomes indicated that the higher efficiency of copper complex for the hydrogenation of CO_2 into formic acid was achieved with 92% yield & 58000 TON. This reaction system exhibited high stability and reusability. Here, the conjugated 1,10-Phenanthroline ligand system which lower the reduction potentials as well as to lower the over potentials for the CO_2 reduction. Further, the destabilization of the copper-bound formate accelerates product extrusion, the rate-limiting step in catalysis. Here, the ligand core containing azomethine and electron withdrawing substituent makes metal complex as effective catalytic performance with higher turnover number as compared to existing cobaloxime and metal glyoximate. Further, the anionic acetate group in the metal complex effectively catalyses the hydrogenation of CO_2 at relatively modest overpotentials (400 mV at pH 3), with a turnover number of 40,000. (12 hrs). As a result, the copper complex serves as an active and strong catalyst, reducing overpotential and so increasing the efficiency of energy conversion. In place of artificial photosynthesis, CO_2 hydrogenation can be used to create fuels with great selectivity and efficiency, such as formate/formic acid.

IO-08 : Abnormal Synergistic behavior of Metal Chelates of 1,10-Phenanthroline Scaffold for Enhancing Hydrogen Evolution from Water

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The design and development of metal complex architecture with a multidenate heterocyclic organic compound that modulates hydrogen evolution from water. To achieve effective hydrogen evolution efficiencies of metal chelates bearing Phenanthroline scaffold, [ML].2(OAc) (L:1,10-Phenanthroline analogous contains aromatic core; M=Co, Zn, Cu & Ni ions) were designed and synthesised. A square-planar arrangement with moderate distortion was attributed to the above metal chelates based on spectroscopic data and analytical studies. The experimental observations highlighted that metal chelates were effective towards hydrogen evolution under photochemical and

electrocatalytic condition. During the photochemical process, the metal chelate was combined with fluorescein (photosensitizer) and triethylamine (sacrificial e donor) showed enhanced hydrogen evolution under photochemical irradiation that correlates with electronic and conjugation of ligand. Copper complexes with the highest TON and TOF values (11,500 and 7800) had the best catalytic activity at pH 10.6 in CH_3CN:H_2O (1:1 ratio). All of the promising findings offers novel paths for hydrogen production with chromophores and metal catalysts. Due to its abnormal synergistic behaviour imparts the potential of redox characteristics, metal ions with highly conjugated ligands showed hydrogen production with impressive results. This research could pave the way for the growth of metal complex as hydrogen generation catalysts.

IO-09 : Synthesis, Spectroscopic Characterization, Thermal and in vitro Antimicrobial Studies of bis(N,N-diethyldithiocarbamato-S,S') Antimony(III) derivatives with some Oxygen and Sulfur Donor Ligands

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Replacement reactions of bis(N,N-diethyldithiocarbamato-S,S')antimony(III) chloride have been carried out with oxygen and sulphur donor ligands like thiosalicylic acid, mercapto succinic acid, disodium oxalate, sodium phenolate, benzoic acid, thiobenzoic acid, thioglycolic acid, propionic acid, thioacetic acid, thiphenol, 2-aminothiophenol to give mixed bis(diethyldithiocarbamato)antimony(III) derivatives of the corresponding ligands in refluxing benzene. These newly synthesized complexes have been characterized by elemental analysis (C, H, N, Sb and S), melting point, molecular weight determinations, spectral [UV, IR and NMR (^1H and ^{13}C)] and thermal studies. All these newly synthesized complexes are yellow and brown colored solids and are soluble in common organic solvents.

These complexes have been also screened for their antimicrobial activities using the well diffusion method. The free ligands as well as their mixed metal complexes were tested in vitro against four bacterial strains two Gram-positive 1. Staphylococcus aureus, 2. Bacillus subtilis and two Gram-negative 3. Escherichia coli and 4. Klebsiella pneumoniae and two fungal strains 1. Aspergillus niger and 2. Candida Albicans to assess their antimicrobial properties. The results are indeed positive and exhibited good antibacterial effects. Chloroamphenicol

and Terbinafine were used as standard antibacterial and antifungal drug respectively for comparison. On the basis of all above studies these synthesized complexes help to understand different structural and biological properties of main group elements with sulfur donor ligands.

IO-10 : Synthesis, Characterization and Application of Functionalized Magnetite Nanoparticles in Microplastic Removal

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Magnetite nanoparticles (MNPs) with their distinctive properties is pacing into diverse fields. It is their super-magnetic phenomenon that attracted researchers to apply these MNPs in environmental applications apart from other fields as these aid in easy separation process. There are various synthesis methods reported, while co-precipitation method is preferred here to synthesize the magnetite nanoparticles. Further, as MNPs aggregate, these are functionalized with functional groups such as SiO_2, PEI (Polyethylene imine), APTES (3-Aminopropyl tri-ethoxy silane), specific imines and amide. The functionalized MNPs are taken for characterization with instruments such as FTIR (Fourier Transform Infrared Spectroscopy), SEM-EDX (Scanning Electron Microscopy), Zeta analyzer to study and confirm the MNP synthesis, functional group and their morphology. These functionalized MNPs are taken for environmental application specially to remove microplastics.

IO-11 : Chemoselective Aerobic Oxidation of Alcohols Catalyzed by Copper-quinoneoxime Complex - A Biomimetic Approach

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Two redox active quinoneoxime-based $[N_2O_2]$ donor ligands viz. 3-hydroxy-4-(hydroxyimino)naphthalen-1(4H)-one (A) and 3-hydroxy-4-(methoxyimino)naphthalen-1(4H)-one (B) and their corresponding copper complexes $[Cu(A)_2]$ and $[Cu(B)_2]$ have been synthesized. The structures of all synthesized compounds were characterized by NMR, FTIR, UV-VIS, and mass spectroscopy. The electrochemical behavior of ligands and their complexes were studied using Cyclic Voltammetry. Further, both complexes were screened as a catalyst for the aerobic oxidation

of alcohols. Complex [$Cu(A)_2$] act as an efficient catalyst for the selective oxidation of primary alcohols to corresponding aldehydes with a good % yield under mild conditions. Catalyzed products were isolated and characterized by ^1H NMR spectroscopy. Whereas complex [$Cu(B)_2$] does not demonstrate any catalytic activity, this variation in the catalytic activity of the copper complexes may be due to the presence of intramolecular H-bonding interactions between two ligand scaffolds of complex [$Cu(A)_2$].

IO-12 : Synthesis, Characterization, and Study of Anti-Microbial Activity of Metal Complexes of Isonicotinohydrazide Schiff Base Ligand

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New Schiff base N'-(1-(p-tolyl)ethylidene)isonicotinohydrazidehas been synthesized by condensation reaction of isonicotinohydrazide with 4-methylacetophenone and itsCu(II), Ni(II), Mn(II), and Fe(III)complexes were prepared. Complexes were characterized on the basis of various spectroscopic techniques like IR, ^1H and^{13}C NMR studies, elemental analysis and magnetic studies. Synthesized Schiff base ligand and metal complexes were screenedagainstanti-microbial activity. Interestingly, all Schiff base metalcomplexes showed a higher antibacterialactivity than their parenthydrazone Schiff base ligand.

IO-13 : Preparation of Schiff Base and Complex of Fe(iii) Derived from Hydroxylamine and 4-methylacetophenone and their Characterization

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A Schiff base was prepared from hydroxylamine-hydrochloride and 4-methylacetophenone and worked as a primary ligand in the synthesis of a complex of Fe(III) with L-valine. Amino acid participated as a secondary ligand. Acetophenone derivatives have great significance in antimicrobial[1], anticancerous, anticonvulsant, anti-inflammatory, etc. arenas. Schiff bases have specific chemistry in themselves which play important role in medicines/drug design, and treatment of some chronic diseases. Acetophenone plays important role in human metabolism too. Acetophenones are mainly used in pharmaceuticals[2] and cosmetic products. L- valine containing complexes can be used in drugs that participate in DNA binding and cancer treatment.[3] All the synthesized compounds were passed through the next steps- elemental

investigation, conductivity check, magnetic moment measurement, and structural analysis through spectral techniques(UV-Vis, FTIR, NMR, etc.). The prepared compounds will be further passed through biological screening to get the direction of use.

IO-14 : Synthesis of Novel Polysubstituted Oxazole via Tandem Oxidative Cyclization Pathway Catalyzed by $CuNiFe_2O_4$@Lys-GO

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The pursuit for designing efficient heterogeneous catalytic systems for tandem oxidative cyclization reactions has provided a great impetus to research efforts, as it enables the step well as confers the benefits of a facile catalytic recovery. In the present study, we disclose a novel $CuNiFe_2O_4$@Lys-GO catalytic system which was successfully prepared by immobilization of copper substituted nickle ferrite nanoparticles on lysine-grafted graphene oxide nanosheets, in which ferrite moeity acts as an oxidation catalyst and lysine has the role of base catalyst. Also, lysine amino acid used to modify the surface of graphene oxide nanosheets which the prepared support can improve dispersion and uniform loading of nanoparticles for the tandem oxidative cyclization of amines and â-keto esters, leading to the production of biologically active, polysubstituted oxazole moeties.

IO-15 : Study of Chelating Behaviour of Thiosemicarbazone Ligand to Fe (II), Co (II) and Ni (II) Metal Ions

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As a consequence of the bioinorganic importance of carbazones and their transition metal complexes, their chemistry has invited a wide attention. Thiosemicarbazones are multidentate ligands containing several coordination sites with supper ability to form chelated complexes. It is very interesting to study the chelating behaviour of multidentate ligands. For the present study 2-acetylfluorenethiosemicarbazone has been synthesized by the condensation of 2-acetylfluorene and thiosemicarbazide.The ligand has been used for complexation with Fe(II),Co(II) and Ni(II).The percentage composition of complexes and Molar Conductivity predict the formulation of complexes as ML_2X_2 (Where L is 2-

acetylfluorenethiosemicarbazone and X is Cl^- or CH_3COO^-).The comparison of FTIR spectra of complexes with that of free ligand indicates the coordination of ligand through azomethine and thione Sulphur. The NH and NH_2 group of the ligands don't participate in coordination. Thus, the ligands act as neutral bidentate forming five membered chelates with metal ions. The magnetic moment of these complexes is well in accordance with number of unpaired electrons. The electronic spectra of complexes have been studied elucidation of complexes. The number of electronic bands and derivation the value of various crystal field parameters clearly predicts the distorted octahedral geometry around the metal ions.

IO-16 : Combinatorial Approach to Fabricate Silica Doped Polyvinyl Alcohol / Hydroxyapatite / Carrageenan Nanocomposite for Bone Regeneration Applications

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Bone tissue engineering is a fascinating approach for the development of an ideal nanocomposite implants which infer superior biocompatibility and causeminimal toxicity to the surrounding tissues. Herein, this work aims to synthesized ternary nanocomposites integrating nanohydroxyapatite/ κ-carrageenan/ silica doped polyvinyl alcohol in three different ratios (HCP1, HCP2 and HCP3) and a binary system comprised of nanohydroxyapatite and κ-carrageenan (HC). The developed nanocomposite samples were analyzed and compared via different physio-chemical and biological approaches to explore their potency to regenerate bone tissues. Thermogravimetric analysis, differential temperature analysis, x-ray diffraction analysis, infra-red spectroscopy providesinformationregarding phase and structure of nanocomposites, complex formation, thermal stability, etc. Scanning electron microscopy revealed relatively rougher surface morphology of HCP3 nanocomposite than other prepared nanocomposites which assist better mineral deposition over HCP3 nanocomposite. HCP3 nanocomposite manifested higher osteogenic differentiation and lesser cytotoxicity than other developed nanocomposites which was corroborated by in vitro biomineralization, ARS, ALP, protein adsorption, cell viability and hemolysis. HCP3 also exhibited optimum swelling ability and improved biodegradability and anti-bacterial activity predicting it as a promising nanocomposite implant for future orthopedic applications.

IO-17 : Enhanced Electrochemical Performance of Polyaniline (PANI) /Nickel Ferrite nanoparticles ($NiFe_2O_4$) as supercapacitor electrode material

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The electrochemical performance of PANI can be significantly improved by incorporation of spinel-type transition metal oxide, i.e., nickel ferrite ($NiFe_2O_4$) into the PANI matrix. The synthesised sample were physically characterised by SEM, UV-vis, FTIR and XRD, which confirmed the synthesis of all prepared materials. The PANI/$NiFe_2O_4$ nanocomposite showed good interaction with uniformly porous and agglomerated globular morphology. Electrochemical measurements, such as cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), and electrochemical impedance spectroscopy (EIS), were used to analyse the electrochemical performance of electrodes for supercapacitor application. The PANI/$NiFe_2O_4$ composite exhibited enhanced specific capacitance value of 758 Fg^{-1} compared to bare PANI1:1 (677 Fg^{-1}), at 10 mV/s scan rate in a two-electrode system. This may be due to nickel ferrite nanoparticles filling the vacant places beneficial for efficient ion migration and fast electron transfer rate. It was therefore confirmed that the PANI1:1/ $NiFe_2O_4$ composite electrode material showed enhanced supercapacitive performance than pure PANI and nickel ferrite electrode material.

IO-18 : Investigation of Morphology and Optical Properties of Nano-Cellulose Film of $AgNO_3$

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Flexible cellulose nanofibrils film substrates with high smooth surface and high transparency are attractive for next- generation flexible transparent electrical device applications. In recent years, tuning optical properties of the substrates has become more and more important for the fabrication of the transparent electronic devices. There are extensive studies on the development of composite solutions involving various types of materials. Consequently, this works aims to incorporate polymers of nanocrystalline cellulose a composite thin film via the spin-coating method. Then, Fourier transform infrared (FTIR) spectroscopy is employed to confirm the functional groups of

the NCC thin film. The atomic force microscopy (AFM) results revealed a relatively homogeneous surface with the roughness of the NCC thin film being slightly higher compared with individual thin films. Meanwhile, the ultraviolet/visible (UV/visible) spectrometer evaluated the optical properties of synthesized thin films, where the absorbance peaks observed around a wavelength of 220 to 700 nm conforming incorporation of nanometal. An optical band gap of 4.082 eV was obtained for the composite thin film, which is slightly lower as compared with a single material thin film. In conclusion, this work has successfully developed a new sensing layer in fabricating an effective and potential heavy metal ions sensor.

IO-19 : Thermal Analysis of Some Transition Metal Complexes of Dithiocarbamates

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The some selected transition metal copper(ll), nickel(ll), cobalt(ll) and manganese(ll) complexes have been synthesised and characterised with the help of IR , elemental, magnetic , NMR and thermogravimetric analysis.

After characterisation and structural determination, the detailed thermogravimetric analysis of these complexes for stability, activation energy(E) frequency factor(Z), entropy of activation(S),free energy of activation (G) have also been investigated, with the help of conventional and Freeman and Caroll's equation and discussed in the present work.

IO-20 : Study of Structural, Optical, Morphological and Photoluminescence Properties of Hydrothermally Synthesized YVO_4 : Dy^{+3} Codoped with K^+

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In this study, the luminescence properties of YVO_4:Dy^{3+} are modified by co-doping of potassium ion and the materials were prepared by hydrothermal technique followed by its calcination at 500°C. By analysing Powder X-ray Diffraction (P-XRD), SEM and TEM, Fourier transform infrared (FTIR), UV-DRS and photoluminescence techniques of the as-prepared products, it was determined that co-doping of potassium ion affects the properties of crystal phase and

photoluminescence. The P-XRD pattern reveals the formation of the tetragonal crystalline phase. On the other hand, morphological studies show that samples have regular bipyramidal structures. Functional group analysis shows the band near 500 cm^{-1} attributed to Y-O absorption. An intense band around 781 cm^{-1} corresponds to symmetrical stretching due to the V-O vibration of the VO_4^{3-} group. Furthermore, in PL emission spectra, the most intense emission peak was observed at 571 nm, due to the $^4F_{9/2} \rightarrow {}^6H_{13/2}$ transition of Dy^{3+} on excitation at 320nm. The optimum concentration of K^+ ion co-doping for improvement in the photoluminescence properties of yttrium vanadate doped with Dy^{3+} phosphor was found to be 10 at.%. The calculated band gaps of YVO_4:5 at. % Dy^{3+}: x at. % K^+(x=0,1,3,5,7,10 and 15) samples were found to be 3.62, 3.61, 3.63, 3.62, 3.61, 3.60 and 3.62 eV respectively.

IO-21 : Synthesis, Structural Characterization and In Vitro Cytotoxicity Assessment of New Mononuclear Cu(II)/Co(II) Schiff base Complexes

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In this work, report synthesis, structural characterization and in vitro biological evaluation of four mononuclear Cu(II) and Co(II) complexes (1"4) derived from Schiff base ligand scaffolds L1 and L2. The synthesized complexes 1"4 were thoroughly characterized by various analytical and spectroscopic techniques. The DFT calculations were performed to determine the structural and electronic of complexes 1 4 based on their respective HOMO and LUMO energy values. Hirshfeld surface analysis were carried out to examine numerous intermolecular interactions which define the stability of crystal lattice structures. Furthermore, comparative in vitro DNA/ BSA binding studies were carried out by employing various biophysical methods which revealed higher binding propensity of copper analogues. The antioxidant activity of complexes 1–4 was also evaluated against the free radical DPPH which demonstrated better radical scavenging activity by copper analogues. In addition, the cytotoxicity of the complexes was evaluated against MDA–MB–231/HCC1806 (triple negative breast cancer cell lines) and HT–29 (colorectal cancer cell lines) which revealed remarkable cytotoxicity of Cu(II) complex 3 against the tested cancer cell lines. The toxicity profile of the complexes was also evaluated against VERO (normal kidney epithelial) cells which validated their low toxicity behaviour.

IO-22 : Photoelectrochemical Water Splitting Study on $BiVO_4$ Thin Films Irradiated with 600 keV N^{2+} Ion

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The requirement of primary energy source is fulfilled by the combustion of fossil fuels which is also related to emission of greenhouse gases. Hydrogen generation by using photoelectrochemical (PEC) water splitting route is one of the most promising methods for solar to chemical energy conversion and for the use of hydrogen as future fuel. The scientists world over are pursuing research on design and synthesis of the most efficient electrode but so far desired results have not been achieved.

Present work is focused on studying $BiVO_4$ thin films irradiated with 600 keV Ar^{2+} ion for photoelectrochemical water splitting. All the samples were characterized by XRD, SEM, EDX, UV-Visible spectroscopy. The influence of ion irradiation on $BiVO_4$ thin films for photoelectrochemical performance has been studied by current voltage characteristics, Nyquist plots, Mott-Schottky analysis and efficiency measurements. Maximum photocurrent density was obtained at optimum irradiation fluence.

IO-23 : 18-Membered Macrocyclic Complexes of Mn(III) Containing Diazatrioxa Donors Synthesis And Demonstration by their Spectral and Biological Studies

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Present work emphasis the synthesis of macrocyclic complexes of Mn(III) containing di-aza and tri-oxa donor moieties within the eighteen-membered cyclic ring via template synthesis routes. Reaction of various â-diketones namely 2,4-pentanedione, 1-phenyl-1,3-butanedione and 1,3-diphenyl-1,3-propanedione with 4,7,10-trioxadiaza-1,13-diamine carried out in presence of Mn(III) metal salt in [1:1:1] molar ratios. Elemental analyses, H^1NMR, infrared, mass spectrometry, magnetic susceptibility, and molar conductance measurement methods have been used for characterization of synthesized complexes and based on these studies a six coordinate distorted octahedral geometry for all these complexes has been proposed. In-vitro antibacterial activities of

these complexes were checked against Streptomyces griseus (gram-positive), Escherichia coli (gram-negative), Staphylococcus aureus (gram-positive) and Pseudomonas aeruginosa (gram-negative) bacterial strains and for antifungal studies Trichoderma Reesei (MTCC-164), Aspergillus niger (MTCC-282), Penicillium funicolusum (MTCC-1013) and Fusarium oxysporium (MTCC-2480) fungal strains were used. Standard known antibiotics such as Streptomycin and Ketakenazole were used for comparison of both antibacterial and antifungal studies respectively. All these synthesized macrocyclic complexes showed good antimicrobial activity.

IP-CYSA-01 : Ru(II)(η^6-p-cymene) Conjugates Loaded Onto Graphene Oxide : An Effective pH-Responsive Anticancer Drug Delivery System

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Graphene oxide based nano drug delivery system is considered one of the promising platforms to deliver therapeutic drugs at the target site. In this study, Ru(II)(•^{6}-p-cymene) complexes containing the benzothiazole ligand were covalently anchored on graphene oxide using the ultrasonication method. The nano conjugates GO-NCD-1 and GO-NCD-2 were characterized by FT-IR, UV-visible, ^{1}H NMR, TGA, SEM and TEM techniques, which confirmed the successful loading of both the complexes (NCD 1 and NCD 2) on the carrier with the average particle diameter size of 17±6.9 nm and 25±6.5 nm. In vitro DNA binding studies of the nano-conjugates were carried out by employing various biophysical methods to investigate the binding interaction with the therapeutic target. Our results suggest (i) high K_b and K_{sv} values of the graphene-loaded conjugates (ii) effective cleavage of plasmid DNA at a lower concentration of 7.5 and 10 µM via an oxidative pathway(iii) fast release of NCD 2 at acidic pH, that could have good impact on the controlled delivery of drug. Molecular docking, DFT studies, and cytotoxicity activity against three cancer cell lines by SRB assay were also performed.

IP-CYSA-02 : A Chromone based Colorimetric Fluorescence Sensor for Selective Detection of Cu^{2+} Ions and its Application for In-Situ Imaging

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A chromone-based chemosensor Probe 1 was designed, synthesized, and characterized by FTIR, UV-vis, ^{1}H NMR, ^{13}C NMR, and mass

spectrometric studies. Probe 1 exhibited high selectivity and sensitivity for the Cu^{2+} ions over various metal ions (Al^{3+}, Cr^{3+}, Co^{2+}, Cd^{2+}, Mn^{2+}, Fe^{3+}, Ni^{2+}, Zn^{2+}) that was investigated by colorimetric, absorption, and fluorescence titrations. The binding mode of Probe 1 with the Cu^{2+} ion was derived from Job's plot measurements, and it showed 2:1 stoichiometry. Probe 1 revealed an association constant value of 8.48×10^{8} $M^{"2}$ as determined by employing non-linear least square fit data. The detection limit of Probe 1 for the Cu^{2+} ion was found to be $0.273 \times 10^{"6}$ mol $L^{"1}$. Furthermore, the experimental utility of Probe 1 was examined in different biological samples viz., healthy liver tissues, F. gigantica infected liver tissues, and the adult F. gigantica worms to detect the presence of copper-containing biomolecules. DFT studies were performed to support the sensing mechanism. The results of these experiments demonstrate that Probe 1 could be a promising chemosensor for the instant naked eye and fluorescence detection of Cu^{2+} ions in different biological samples.

IP-01 : Comparative Study of Photoluminescence Properties of Samarium Vanadate and Dy Doped Samarium Vanadate

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In this study, $SmVO_4$ and Dy^{3+} doped $SmVO_4$ have been synthesized by hydrothermal method. The formation of the tetragonal crystalline phase is demonstrated by the P-XRD graph. Morphological findings reveal that the samples contain regular bipyramidal structures. From FTIR analysis, Sm-O absorption is associated with the band at 529 cm^{-1}. The symmetrical stretching caused by the V-O vibration of the VO_4^{3-}group corresponds to a strong band near 775 cm^{-1}. Furthermore, from PL emission spectra, it can be seen that the most intense emission peaks were noticed at 550 nm (caused by $^4F_{9/2} \rightarrow {}^6H_{13/2}$ transition of Dy^{3+} and $^4G_{5/2} \rightarrow {}^6H_{5/2}$ of Sm^{3+}) and at 663 nm (due to $^4F_{9/2} \rightarrow H_{11/2}$) on excitation at 405 nm. The optimal concentration of Dy^{3+} ion doping for improving the photoluminescence properties of samarium vanadate phosphor was determined to be 5at.%. The energy band gaps of $SmVO_4$ and $SmVO_4$: x at.% Dy^{3+} (x = 1,3,5,7,10, and 15) were calculated using the Tauc relation and found to be between 3.73 eV- 3.81 eV.

IP-02 : Spectral and Antibacterial Activities of Co (II) Complexes with Heterocyclic Schiff Bases

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Coordination compounds are found in many places on the earth's surface. Every living system includes many coordination compounds. The metal complexes of Schiff bases are also of prime importance in analytical chemistry and chemotherapy. Co (II) complexes of Schiff bases are of great interest in studying the effect structural changes in the ligand system on heterocyclic coordination. vitamin B_{12} is a large complex of cobalt. Heterocyclic compounds are well known for their antifungal, Anti inflammatory, herbicidal, antiamebic, antifertility antiparkison.

In Co (II) 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 benzaldehydle with 2 amino thiazole/2- amino – 6 methyl pyridine have been synthesized and characterized with the help of elemental analysis, IR and electronic spectral data. Comparative bacterial behavior of Schiff bases with their Co (II) complexes have also been studied against E coli and S Aureus.

IP-03 : Synthesis, Physicochemical Characterization, DFT Studies and Biological Screening of a Novel Schiff Base Ligand and its Cu(II) and Zn(II) Metal Complexes

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The two effective bioactive Schiff base metal(M: Cu(II) and Zn(II)) complexes were designed by condensing the novel Schiff base ligand (E)-5-(diethylamino)-2-((5-methylthiazol-2-ylimino)methyl)phenol(4DEA) with respective metal salts. These compounds were physicochemically characterized by molar conductance, FT-IR, UV-Vis, thermal analysis, P-XRD and electrochemical studies. The coordination sites of the synthesized ligand are phenolic oxygen, azomethine nitrogen and thiazole nitrogen which makes the ligand monobasic - tridentate. 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 metal complexes showed

distorted octahedral geometry. The antifungal activity of the synthesized compounds was screened against the two fungal species i.e. Aspergillus Niger and Fusarium Oxysporum ,in which the Cu(II) complex gives better antifungal activity than the Zn(II) complex and Schiff base ligand(4DEA). On the other hand the DNA binding and cleaving activity was screened against circular plasmid 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 activity than the Zn(II) complex and Schiff base ligand (4DEA).

IP-04 : Mixed Ni(II)/Co(II) Complexes of Nalidixic Acid Drug : Synthesis, Structural Characterization, DNA/BSA Dinding Profile and Cytotoxicity Assessment

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In this work, herein we report synthesis, structural characterization and in vitro cytotoxic evaluation of two mixed Co(II)/ Ni(II)-nalidixic acid-bipyridyl complexes (1&2). The structural analysis of metal complexes 1 and 2 was carried out by analytical and multispectroscopic techniques. The crystallographic details of complexes 1 & 2 revealed a monoclinic crystal system with P21/c space group. DFT studies of complexes were performed to get electronic structure and localization of HOMO and LUMO electron densities. Hirshfeld surface analysis was employed to understand the various intermolecular interactions. The comparative interaction studies of complex 1&2with DNA/BSA were performed by diverse multispectroscopic and analytical techniques to evaluate their chemotherapeutic potential. Furthermore, the cytotoxic assessment of complexes 1&2 was examined against MDA-MB-231 (triple negative human breast cancer cell line) and HepG2 (liver carcinoma cell line) employing MTT assay which revealed remarkably effecient and specific cytotoxic activity of complex 2.

Sectional President's Address

Enantioselective Synthesis of Statins

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Cholesterol is necessary for the proper functioning of all human organs, although it is also the cause of coronary heart disease which is a leading cause of death worldwide. Scientists and the pharmaceutical industry have discovered a remarkable class of drugs known as statins, which lower cholesterol levels with excellent efficiency in the blood and reduce the prevalence of heart attacks. Statins precisely inhibit HMG-CoA reductase, which is involved in the rate-controlling step in the biosynthesis of cholesterol. Statins are well-proven front-line drugs for the treatment of coronary heart disease and have been for several decades in the clinical practice because of their promising competence, protection profiles, and long-term benefits in lowering the risk of cardiovascular events. In this regard, our research group has a long-standing interest in the development of an efficient and concise asymmetric synthesis of statins from commercially available cheap sugars.

The existing methods for the preparation of the statin side chain framework were based on the Chiron approach, asymmetric catalysis, and chemo-enzymatic resolutions. The major drawbacks of these synthetic methods are the use of Narasaka-Prasad reduction, which involved the diastereoselective reduction of carbonyl group using pyrophoric diethyl-methoxy-borane, cryogenic conditions for a high degree of stereo control. The loss of half the unwanted isomers in the case of resolution methods, the cost burden of enzymes, asymmetric catalysts, and column chromatography are the main drawbacks of the

existing synthetic methods. Therefore, terse and efficient strategies for the asymmetric synthesis of statins are developed from our group. The developed synthetic routes have potential for scale-up and could be used to produce statins on industrial scale.

OIL-01 : Chemistry of Amino Acids and Peptides Containing Selenium

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Peptides are ubiquitous in nature and wealth of methodologies are available for chemical synthesis of peptides in solution and solid phase. Peptides can be prepared in sufficient quantities for pharmacological and clinical assays, drugs. Peptide drugs, however, can be applied therapeutically only to a limited extent because of their chemical and enzymatic liabilities. The field of peptide backbone modification has grown tremendously over the last decade owing to the improved biological and structural properties possessed by the resulting unnatural analogs. One of the major research interests of our group is to design and develop novel intermediates through C- or N-terminal modification and demonstrate their utility for the synthesis of peptidomimetics. Selenium containing compounds have gained prominence with the identification of various selenoproteins where selenium is predominantly present in the primary structure as selenocysteine (Sec, U). We have developed novel selenium building blocks namely isoselenocyanates at both N- & C- termini of amino acids and their utilty in selenoureido peptidomimetics. Further PCl 5 / LiAlSeH reagent system has been employed for efficient synthesis of selenoxo peptides from native peptides and their N-terminal chain extension to yield peptide-selenoxo peptide hybrids. Solution phase synthesis of cyclosporine O by step-by-step linear condensation approach mediated by zinc dust and solid phase synthesis of human catestatin has also been demonstrated in our lab.

OIL-02 : Click Chemistry - A Nobel Prize Reaction for the Year 2022 : The Growing Impact in Glycoscience

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Just after the discovery of 'Click Chemistry' by K B Sharpless and Morten Meldal in 2002, this modular reaction is considered as one of

the most reliable protocols and has been widely explored in various emerging fields. 1 It just says 'click' and the molecules are coupled together through triazole as biologically imperative linker. The protocol is reached to a highest recognition i.e. 'Nobel Prize in Chemistry for the Year-2022' awarded to Carolyn R. Bertozzi, Karl B Sharpless, and Morten J Meldal for 'the development of click chemistry and biorthogonal chemistry". Both Sharpless and Meldal have laid the foundation for the functional form – Click Chemistry – where two different molecular building blocks linked together quickly, efficiently and with excellent regioselectively. This Nobel Prize in Chemistry is actually about making difficult processes easier, a truly inspiring concept. Carolyn R Bertozzi has engaged this modular tool to a new dimension through using it in living organisms, 2 a perception widely explored in chemical biology and great impact in drug development. A clear understanding of the role of carbohydrate in a number of important biological events has led to an increased demand for the sugar-based molecules for their complete chemical, biological, and pharmacological investigations. Through utilizing this regioselective triazole forming CuAAC 'Click Chemistry', tremendous efforts have been made during the last 21 years to furnish diverse range of the desired triazole-appended molecular architectures. In this context, synthesis of a broad range of simple to complex glycoconjugates achieved in my laboratory 3-10 will be presented in great detail.

OIL-03 : Synthetic Approach and in Silico Molecular Modelling of Different Heterocycles Fused Ring System : Their in Vitro Antimicrobial, Anti-Mycobacterium, Anti-Malerial Anti-Oxidant and Anti-Protozoal Evaluations

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The lack of efficacy, development of resistance and tolerance, unexpected toxic side-effects and incompatibility with other drugs has 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 of heterocyclic hybrids has been recognized in the field of medicinal chemistry because of their wide applicability. 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 cruzi has 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-04 : Bond Formations between Two Nucleophiles : Construction of Biologically Interesting N-Heterocycles

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The development of efficient methods for construction of C-C and C-X (X = N, O, S, etc) bonds under mild conditions is one of the great challenges in organic chemistry. Transition-metal catalyzed classical coupling reactions have been proven to be powerful tools for the construction of various C-C and C-X bonds, and reactions of this type have been widely applied in the areas of pharmaceuticals, agriculture, food industries, and so on. Generally, in those classical coupling reactions, bond formations occur between an electrophile and a nucleophile in the presence of a transition-metal catalyst. Both the electrophiles and the organometallic nucleophiles are usually obtained from pre-functionalization of their corresponding hydrocarbons. However, with the development of modern synthetic methodology and the urgent demand for green and economical synthesis, traditional couplings face big challenges on account of their inevitable drawbacks such as low atom economy and considerable generation of harmful by-products. At this point, direct bond formation between two or more

nucleophiles, especially hydrocarbons, would be an ideal alternative. As for the coupling between two nucleophiles requires an extra oxidant to promote bond formation, this type of reactions are designated as oxidative couplings. We have recently investigated several oxidative annulation reactions for the construction of nitrogen heterocycles such as quinoxalines, quinazolines, bis(indolyl)methanes, 2,4,6-triarylpyridines, 3 alkylideneindolin 2 ones, and 1,3-benazoles using amines as reaction partners. Sustainable metal catalysts such as iron or copper salts, and abundant oxidants viz., air or molecular oxygen were used for conducting the oxidative annulation reactions. The results of these studies will be presented in the conference.

OIL-05 : Organic Materials for Emerging Applications : Design, Synthesis, Characterization and Device Fabrication

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Organic materials are becoming more popular because of their increasing applications. Organic materials are light weight (low density) compared to inorganic materials, less expensive, easy to make them, easy to get them in pure form, versatile & have high structural diversity. One can modulate the organic material properties like UV-Vis-NIR absorption, luminescence, solubility, thermal properties (T_m, T_d & T_g), and electrochemical properties using various substituents/ groups/ appendages. Further organic materials can be layered by adopting techniques like spin coating or thermal vacuum evaporation. Initially we worked on a "highly polarized excited state" hypothesis and informed that optically excitation of an organic molecule experiences charge polarization in the excited state. The polarization in the excited state has pivotal role in many applications of organic molecules as materials. We at Indian Institute of Chemical Technology initiated research on these organic materials having various applications. We have designed, synthesized, characterized various organic materials and further taken to fabricate the devices with collaborations to evaluate these organic materials towards their suitability for the proposed applications. We have made organic materials having applications in (i) Photoresists; (ii) Molecular Switches; (iii) Non Linear Optics (NLO); (iv) Organic Light Emitting Devices (OLEDs) and (v) Solar Cells. The results obtained on these aspects will be discussed.

OIL-06 : From Waste to Wealth – Relooking at Some Commonly Synthesized Bromoorganic Compounds for their Pharmaceutical Properties

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The endless effort to design and develop new synthetic methodologies in research laboratories leads to the synthesis of different types of chemical compounds. Unfortunately, these synthesized compounds do not usually find any use after they are synthesized and accumulate in the laboratories, going on to become what is sometimes termed as 'Academic Chemical Waste'. Our group has been working on the development of synthetic protocols for bromo organic compounds and over time a number of different types of bromoorganic compounds have been synthesized. While it is known that bromoorganic compounds have various biological properties like antimicrobial, anti-oxidant, anticancer, etc, the compounds which had been synthesized through our methodologies were not tested for their intrinsic activities as they were considered 'products of routine test substrates'. However, in recent years studies are being carried out to assess the pharmaceutical properties of these earlier synthesized bromoorganic compounds and interestingly they were found to possess different important pharmaceutical properties ranging from anticancer, antioxidant, antibacterial and antifungal. The properties that were discovered and the in silico and in vitro techniques that were used for the pharmaceutical assessment of the compounds will be presented in this paper.

OIL-07 : Versatility of Heteroallenes for the Syntheses of Biologically Potent Scaffolds

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In recent years, development of novel synthetic methodologies have been attracted a great deal of attention for organic chemists around the globe, for the synthesis of structurally diverse biologically potent molecules. The advantages associated with these synthetic methodologies are lesser synthetic steps, use of cheaper and safer new alternatives, involves overall lesser reaction time, milder reaction conditions, and afforded high yields. Extensive efforts have been made by organic chemists around the globe and thus developed several kinds of new and highly efficient methods for the generation of various kinds of structurally diverse molecules of biological significance.

In recent years, carbon dioxide/carbon disulfide/carbonyl sulfide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and $COCl_2$. Recently, carbon dioxide/carbon disulfide/carbonyl sulfide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, we will focus some of our novel and efficient methods for the synthesis of biologically potent scaffolds.

OO-CYSA-01 : {Cu(II)[Cs-DABA-HACP]Cl} : A New Heterogeneous Catalyst for the Oxidation of Olefins

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We have developed a new heterogeneous catalyst, chitosan based Cu(II) catalyst, {Cu(II)[Cs-DABA-HACP]Cl} by treating Cu(II) Schiff base metal complex with chitosan. The newly prepared heterogeneous catalyst, {Cu(II)[Cs-DABA-HACP]Cl} was analyzed by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray analysis (EDX), Fourier transform infrared spectroscopy (FTIR), Thermo gravimetric analysis (TGA), X-ray powder diffraction (XRD) etc.

The catalytic performance of prepared heterogeneous Cu(II) catalyst was tested for the oxidation of olefins using 70% tert-butylhydroperoxide (TBHP) as an oxidant. The different products are obtained by the oxidation of olefins {Cu(II)[Cs-DABA-HACP]Cl}, which are very useful for industrial background. The prepared catalyst was highly recoverable and easy to handle, easy to separate

OO-CYSA-02 : Functionalisation of Graphene Oxide with Synthetic Polymer for Enhanced Mechanical Properties

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Graphene and graphene oxide (GO) represents an emerging field of interdisciplinary science spanning a variety of disciplines including chemistry, physics, materials science, device fabrication and nanotechnology. Polyethylene (PE)/functionalised graphene oxide as a nanocomposite of synthetic polymer with GO. Initial results showed

that Young's modulus, yielding strength and tensile strength of PE can be improved by incorporation of the PE graft-graphene oxide at very low loadings. GO samples confirmed by other characterization techniques such as TGA, FT-IR, TEM. This provides the possibility to prepare water soluble and biocompatibility GO based materials with better performance for enhanced mechanical property.

OO-CYSA-03 : Synthesis, In-Silico & In-Vitro Anti-Cancer Studies of Thieno(2,3-d)Pyrimidine based Pyrazole Derivatives

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The goal of our research was to create a new thienopyrimidine based pyrazole derivatives (6a–j), analyze their pharmacokinetic study, molecular docking studies and anti-cancer activity against MCF-7 breast cancer cell line with MTT assay. The Aza-Michael addition reaction was used to synthesize a unique series of thieno[2,3-d]pyrimidine-based pyrazole derivatives (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 Pharmacokinetics parameters such as Absorption, Distribution, Metabolism, Excretion and Toxicity have been performed. Docking studies of all the synthesized compounds were carried out against EGFR tyrosine kinase domains (4HJO) protein with the help of Schrodinger suites software. The docking study showed that compound 6a has good binding affinities. Further the in-vitro anti-cancer activity was observed with various concentrations of compound 6a and Fluorouracil.

OO-CYSA-04 : 'Turn On' Detection of Spermine and Spermidine in NIR Region by Pyridine Dipod∩SDS Ensemble

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Spermine and spermidine are water soluble and exist as tetra and tri cationic polyamines (pK_a = 11.50, 10.95, 9.79, 8.90) under physiological conditions (pH 7.4, water) and are found in all eukaryotic cells including humans. These are important for protein and nucleic acid synthesis, protection from oxidative damage, activity of ion channels, cell proliferation and differentiation. A high level of spermine / spermidine in urine is regarded as a biomarker for the timely diagnosis of cancer in certain tumors.

The ionic self-assemblies of DMPY-DO and CIPY-DO with SDS emit at 630 and 720 nm, respectively (λ_{ex} 490 nm) and undergo highly selective (40-80 times) increase in fluorescence intensity with spermine and spermidine (100 µM) in aqueous medium (HEPES buffer, 0.1% DMSO, pH 7.40). The limit of detection for spermine is 34 nM with CIPY-DO which is less than the concentration of spermine in human urine. The other amines, amino acids, proteins or biothiols do not interfere in the detection of spermine. The DLS and AFM studies reveal that the aggregates of CIPY-DO and SDS undergo further increase in size.

OO-CYSA-05 : Conjugated Azomethine-Based Optical Biosensing Platform for Ultrasensitive and Rapid Detection of Biomarker Glutathione in Human Blood Serum Samples

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A new approach for visual and colorimetric detection of glutathione (GSH) in an aqueous solution has been developed that is extremely simple and rapid. The designed biosensor conjugated azomethine (SL 1) used is simple to make and utilize, with the additional benefit of being cost-effective. By changes in absorption intensity as well as spectrophotometrically, it shows superb selectivity and ultra-sensitivity towards GSH over other amino acids and biomolecules. Based on the information provided above, we developed an approach to determine GSH qualitatively and quantitatively using a UV spectrophotometer, paper-based test strips, and visually, respectively. A satisfactory linear relationship may be achieved from 0.26 to 52 ìM with a detection limit (LOD) of 63 nM and detection quantitation (LOQ) of 210 nM. Moreover, the high recovery rates for human blood serum samples demonstrated that the proposed colorimetric technique is practicable, straightforward, and ultrasensitive, with a prominent application in regular biosample analysis.

OO-01 : Current Integrated Approach Toward the Discovery of Therapeutic Agents from Medicinal Plants

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Medicinal plants have been well documented for their medicinal

used since the ancient time for different ailments and have provided valuable drugs. The first ever isolation of a natural plant alkaloid introduced for therapeutic use is morphine marketed by Merck in 1827, and the first semi-synthetic pure drug aspirin, based on a natural product salicin, isolated from Salix alba was introduced by Bayer in 1899. This led to the isolation of many drugs such as antitussives(codeine), antihypertensives (reserpine), cardiotonics (digoxin), antineoplastics (vinblastine and taxol) and antimalarials (quinine and artemisinin). An analysis into the sources of new drugs from 1981 to 2007 reveals that almost half of the drugs approved since 1994 were based on natural products. During the years 2005–2007, 13 natural product related drugs were approved. Medicinal plants are continued to be an important source of new drugs or new lead molecules. In the twenty-first century, the pharmacological effects of medicinal plants have been considered for the discovery of promising future drugs/medicines for the management of health care in the various therapeutic areas. An integrative approach by combining the various modern discovery techniques and the new disciplines of integrative biology will positively provide the key to discover many new and novel drugs from plants in the near future. Keeping in view the importance of medicinal plants in the discovery new or novel drugs and our continuous work and effort 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. In this presentation, current integrated approach toward the discovery of novel therapeutic agents from medicinal plants will be discussed in detailed.

OO-02 : Efficient Utilization of Morita-Baylis-Hilmann Reaction to Construct Oxindole Derivatives

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Nitrogen or Oxygen containing heterocyclic compounds shows great impact in medicinal chemistry due to their biological importance, these are good intermediates in the construction of hetero aromatic substances such as oxindole derivatives, which are mostly synthesized with isatin components. We developed a newer method to construct oxindole derivatives through Morita-Baylis-Hillman reaction in one-pot synthesis. N-substituted isatins reacts with alkyl propiolates in presence of diisobutylaluminium hydride (DIBAL-H) at -78 º C with

excellent yield in 30 minutes. Initially, alkyl propiolates are treated with DIBAL-H and produces allene intermediate, which upon nucleophilic addition with N-substituted isatin produces 3-hydroxy oxindole derivatives.

OO-03 : Pd-catalysed C-H activation, its Mechanistic Aspects and Application for Synthesis of FDA Approved Selpercatinib and Erdafitinib Drugs

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Fenton first delivered his major article on transition metal catalysed C-H activation and functionalization reactions in 1894. Although the 1970s saw the renewed discussion on the topic with platinum chemistry. However, one of the most promising catalysts for organic synthesis that has a considerable impact on pharmaceutical and medical chemistry is palladium. The palladium catalysis is made feasible due to its high selectivities, milder reaction conditions, efficient, and cost-effective protocols. The Pd-mediated coupling reactions involve a catalytic cycle having the mechanistic steps such as oxidative addition, insertion, trans-metallation, reductive elimination, â-hydride elimination and â-group elimination. The C-C bond is reflected in Suzuki-Miyaura coupling reaction, the Sonogashira, the Heck, the Stille and Negishi cross- coupling reactions. While C-N bond formation is exemplified by the Buchwald-Hartwig amination reaction. In the present presentation the synthesis of some of the FDA approved drugs, which entails the abovementioned coupling reactions, will be highlighted. For example, the synthesis of selpercatinib, a prescription medicine against lung cancer that utilises Suzuki coupling will be highlighted. Likewise, synthesis of erdafitinib, a potent fibroblast growth factor receptor (FGFR) inhibitor against bladder cancer, via Suzuki and Buchwald–Hartwig cross-coupling reactions will be highlighted.

OO-04 : Green Synthesis of Zinc Oxide Nanoparticles using Sapindus Mukorossi Fruit Extact, Characterization and their Antioxidant Acitivity

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The present investigation covered a biogenic method for the synthesis of zinc oxide nanoparticles (ZnONPs) using Sapindus mukorossi fruit extract. Currently, green synthesis route is most

promising route for the synthesis of metallic nanoparticles in which various plant parts are being used. Nanomedicine utilizes biocompatible nanomaterials for diagnostic and therapeutic purposes. The synthesized zinc oxide nanoparticles were initially noticed through visual colour change from dark brown to yellow and further confirmed by surface plasmonic resonance band at 341 nm using UV-Visible spectrophotometer. Morphology and size were determined by TEM, XRD analysis revealed the crystalline nature and spherical shape with less than 16 nm average size of synthesized ZnONPs. The stability of ZnONPs was due to capping of oxidized polyphenols which was established by Fourier transform infrared spectroscopical study. It could be concluded that S. mukorossi can be used efficiently in the production of potential antioxidant ZnONPs for commercial application. The antioxidant activity of plant mediated zinc oxide nanoparticles was determined using a DPPH free radical scavenging assay. Results indicated that synthesized zinc oxide nanoparticles of S. mukorossi fruit could effectively scavenge the free radical which shows effective antioxidant activity.

OO-05 : Molecular Docking Studies of GC-MS Analyzed Bioactive Compounds from the Rhizome of Hedychium Rubrum with Four Protein Target

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Hedychium rubrum, a traditional medicinal plant of Manipur belonging to the family Zingeberaceae was screened for its biological activity. The methanolic extract of its rhizome was prepared by Soxhlet extraction method and was further subjected to GC-MS to know its bioactive compounds. The in vitro antimicrobial activity assay was tested against five bacteria causing UTI. Klebseilla pneumoniae showed most sensitive inhibition zone than that of the standard control. According to the higher quality of compounds from the GCMS results, nine compounds were selected for further in silico studies with GOLD software against four protein targets namely EGFR (PDB ID: 1M17), DNA gyrase (PDB ID: 5L3J), Uromucoid (PDB ID: 5FBH) and Caspase 3V266F (PDB ID: 5IAE). Among the 9 compounds, compounds HM4. HM7and HM8 have the ability to bind at the receptor site of all four targeted proteins. All compounds undergo ADMET and TOPKAT studies.

OO-06 : Synthesis and Computational Studies of 1,3,4-thiadiazole and Benzothiazole Clubbed Benzimidazole Analogous as Anti-Tubercular and Anti-Protozoal Agent

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The present article deals with the synthesis of newer N-Mannich bases (2a-j) of 2-(pyridin-4-yl)-1H-benzo[d]imidazole clubbed with benzothiazole (2a-e) and 1,3,5-thiadiazol (2f-j) under microwave irradiation. The synthesized scaffold has been well characterized by spectroscopic methods. They were evaluated for their in vitro leishmanicidal, trypanocidal, anti-mycobacterial and anti-bacterial potency. Benzo[d]imidazole bearing 1,3,5-thiadiazol 2i showed micromolar potency against L. mexicana and T. cruzi respectively with IC 50 value1.35 and 1.89 µg/mL. Whereas penta fluoro substituted 1,3,5-thiadiazol unit bearing final compound 2h were found to be active against M. tuberculosis in the primary screening. N- Mannich bases of benzimidazole with 1,3,5-thiadiazole had proven more potent than that of benzothiazole in their in vitro biological evaluation. Compound 2h showed good binding energy in the active pocket of the receptor (PDB ID: 4cod) with -8.517 docking score. The molecular dynamics (MD) simulation study for 2h validates the stability of a ligand-protein complex. In silico toxicity prediction result of active compounds ranges from 1000 < LD 50 d" 2000 mg/kg of body weight and hence predicted to be mildly toxic.

OO-07 : A Convenient One Pot Synthesis and Evaluation of Biological Activities of 2-Amino-4-Methylsulfanyl-6-(2-oxo-2H-chromen-3-yl)-2H-pyran-3-Carbonitrile and their Derivatives

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Heterocyclic compounds are abundant in nature and are of great significance to life because their structural subunits exist in many natural products such as vitamins, hormones, antibiotics etc. A practical method for the synthesis of such compounds is of great interest in synthetic organic chemistry. Coumarines have been established as

well-known naturally occurring heterocyclic compounds isolated from various plants they belong to family of lactones, coumarine is versatile pharmacophore which exhibits a wide variety of biological activities like antibacterial and antimicrobial.

The synthesis of coumarin derivatives has attracted considerable attention of organic and medicinal chemist due to its wide range in food additives fragrances, pharmaceutical and biochemical properties as well as theruptic application of coumarin depend upon the pattern of substitution. coumarin derivatives have been reported for anticoagulant, antiinflametry and antimicrobial.

The compound was prepared by the oxidative cyclisation of salicylic acid and 3-oxo- butyric acid ethyl ester to form 3-acetyl chromen and 2-(Bis-methylsulfanyl-methylene)-malononitrile by using anhydrous K_2CO_3 as a catalyst and DMF as a solvent. By using suitable solvent, the product was re-crystallized and separated out. The method of conversion of reactants into product is explained briefly.

OO-08 : Microwave Assisted Synthesis of Fused Azepine Derivative via Intramolecular Cyclisation of Strained Alkyne

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In the diversified arena of heterocycles, the seven-member heterocyclic compounds have been less explored. Owning to the interesting structure, eclectic scope of natural properties and being an important pharmacophore fragment viz, aza ring systems in the structure of balanol, (-)-cobactin T etc and use in drug designing under heading of antifungal, antibacterial, antivirus agents, etc drag immense attention of chemists and made it exploited for the synthesis, reaction and biological properties. Among various reported cyclisation methods for azepine synthesis, for the first time an exquisite and accomplishable access to construct N-substituted aryl halides azepine fused derivatives was established via microwave radiations under mild conditions by incorporating a strained eight membered alkyne ring with electron withdrawing substituents attached to it, obtained with an appreciable yield. The structures of synthesized compounds were corroborated on the basis of FTIR, nuclear magnetic resonance (NMR), mass, and elemental analyses data. Furthermore, a quantum computational study was computed to investigate the density functional theory-based chemical reactivity parameters of the synthesized derivatives.

OO-09 : Nanocellulose Reinforced with Chitosan for Biological Application as Wound Dressing

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In this study, green composite films based on cellulose nanocrystal/chitosan (CNC/CS) were fabricated by solution casting method. CS is antibacterial in nature, non-toxic, and biodegradable thus it can be used for the production of biodegradable film which is a green alternative to commercially available synthetic counterparts. Consequently, to improve these properties, CNC and/or inorganic nanoparticles had been used. FTIR, XRD, SEM, and TEM characterizations were conducted to determine the structure and morphology of the prepared films. Chitosan based composites have wide applicability and potential in the field of biomedical, packaging and water treatment. The mechanical properties of wet nanocellulose and chitosan nanocomposite films matched well with those of human skin, which demonstrate potential for uses as artificial skin and wound dressings.

OO-10 : Studies on Synthesis and Characterization of Biologically Significant Hetero Annulated Fused Pyrroles

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The importance of natural and synthetic pyrroles arises from their wide range of applications in various fields such as medicinal chemistry, catalysis, dyes, and materials science. The objective of this work is to design novel synthetic strategies for novel pyrrole fused scaffolds through the catalyst Cu (II)-(Acedoben)-Fe3O4. The core-shell structure and the characteristics of the prepared magnetic nano-catalysts were corroborated through powder X-ray Diffraction (PXRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDAX), and FT-IR techniques. Also, the structures of synthesized compounds were corroborated on the basis of FTIR, nuclear magnetic resonance (NMR), mass, and elemental analyses data. The biological screening of synthesized compound was done against pathogenic microorganisms. Staphylococcus Aureus (Gram positive bacteria) Klebsiella Pneumoniae (Gram negative bacteria) with a view to explore their anti-microbial action.

OO-11 : Synthesis of Novel Polysubstituted Oxazole via Tandem Oxidative Cyclization Pathway Catalyzed by $CuNiFe_2O_4$@Lys-GO

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The pursuit for designing efficient heterogeneous catalytic systems for tandem oxidative cyclization reactions has provided a great impetus to research efforts, as it enables the step well as confers the benefits of a facile catalytic recovery. In the present study, we disclose a novel $CuNiFe_2O_4$@Lys-GO catalytic system which was successfully prepared by immobilization of copper substituted nickle ferrite nanoparticles on lysine-grafted graphene oxide nanosheets, in which ferrite moeity acts as an oxidation catalyst and lysine has the role of base catalyst. Also, lysine amino acid used to modify the surface of graphene oxide nanosheets which the prepared support can improve dispersion and uniform loading of nanoparticles for the tandem oxidative cyclization of amines and â-keto esters, leading to the production of biologically active, polysubstituted oxazole moeties.

OO-12 : Withania Somnifera Dunal Plant uses in the Indian Traditional System of Medicine to Cure for Various Human Diseases

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Withania somnifera Dunal plant belongs to the family-solanaceae and commonly called as , Ashwagandha, Indian ginsing, winter cherry and cultivated in drier parts of India. It grows as a short shrub/herbs upto 35-75cm in height. Plant has long been considered as an excellent rejuvenator, a health tonic and cure for a number of health complaints. It is a sedative, diuretic, anti-inflammatory, increasing energy and act as an adaptogen that exerts a strong immunostimulatory and anti-stress agent. It is taken for treating cold and coughs, ulcers, diabetes, leprosy, nervous disorders, rheumatism, arthiritis, intestinal infections, bronchitis, asthma, anticancer and a suppressant in HIV and AIDS patients. According to Indian herbal system of medicine, it is considered as one of the most important herbs with better adaptogenic properties. Plant contains cuseohygrine, anahygrine, tropine, anaferine, aglycosides, withanolids, starch and amino acids. Withanolids from roots consists of steroidal molecules to fight inflammation. It stimulates

the immune system, increases memory and helps maintain general health and wellness. Ashwagandha is known to increase the production of bone marrow and acts anti-aging, anti-tumour and anti-inflammatory agents. Its steroidal is much higher than that of hydrocarisone which is common treatment in cancer cases, TB, HIV and AIDS activity and it is recognised as a blood tonic in gynaecological disorders including anaemia and irregular menstruation. Anxiety patients can also benefit from Ashwagandha plant extracts.

OO-13 : Periodate Oxidation Method used for the Confirmation of Seeds Polysaccharide Structure from Cassia Auriculata Linn. Plant

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Cassia auriculata Linn plant belongs to Caesalpiniaceae family and called as Avaram or Tarwar, is a small perennial shrub and occurs in Northern India and Western Peninsula. Water soluble seeds yielded polysaccharide on hydrolysis as D-galactose and D-mannose in 13 molar ratio by TLC. Column and Paper Chromatographic analysis. Present investigation mainly deals with the periodate oxidation method for the confirmation of seeds polysaccharide structure which was obtained by methylation studies. Periodate oxidation was carried out with sodiummetaperiodate and it consumed 1.25 moles of periodate with simultaneous liberation of 0.35 moles of formic acid per mole of anhydrohexose sugar unit after 50 hrs. The main polymer linkages are linked with ()—type with non-reducing linkages are linked with ()—type. On the basis of methylation results the proposed seeds polysaccharide structure of Cassia auriculata Linn. plant has been confirmed by periodate oxidation method.

OO-14 : Microwave Induced Synthesis and Antibacterial Screening of Some Novel Halogenated Isoxazoline Derivatives

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Isoxazoline, a five membered heterocyclic compound has emerged as an important molecule which plays a significant role in the field of

medicinal chemistry. Isoxazoline derivatives have played a vital role in the history of heterocyclic chemistry and received much attention owing to their diverse biological activities such as antifungal, antibacterial, anti-inflammatory, antiviral, analgesic, antioxidant, antituberculosis, anticonvulsant and anticancer. In present work a series of some novel halogenated isoxazoline derivatives were synthesized from condensation of substituted chalcone derivatives with hydroxylamine hydrochloride by microwave induced method. The synthesized compounds confirmed by IR, NMR, and Mass spectroscopic analysis. All compounds were screened for their antibacterial activity against E.Coli and S. Aureus. The result suggested that all compounds are more effective against S. aureus as compared to E. coli

OP-CYSA-01 : Synthesis and Biological Evaluation of Some New Chromenopyrimidine based Benzodiazepine Derivatives

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There has been a significant development in the synthesis and application of fused heterocyclic system in drug chemistry. Chromenopyrimidine derivatives have received a considerable attention due to their diverse range of therapeutic and pharmacological properties. 4-(4'-(2'-(substituted phenyl)-1H-benzo[b][1,4]diazepin-4'-yl)phenyl)amino-9-methoxy-5H-chromeno[2,3-d]pyrimidine derivatives were synthesized by reacting 4-(substituted phenyl chalcone-4'-yl)amino-9-methoxy-5H-chromeno[2,3-d]pyrimidine derivatives with ortho-phenylene diamine in presence of catalytic amount of sulphuric acid. All the synthesized compounds were characterized by their spectral analysis. Moreover, the synthesized compounds were evaluated for their anticancer activity by molecular docking studies and in-vitro cytotoxicity assay.

OP-CYSA-02 : Rose Flower – A Delicate Perfume or a Natural Healer

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The cultivation of roses as an ornamental plant has a long history. Apart from floricultural purposes, roses also have an economic importance as a source of natural fragrance in perfume and cosmetic industry and for medical applications. Rose hips, flowers, and their

extracts are used for tea infusions and for flavouring of a broad variety of foods. In the scent of roses, more than 400 volatiles compound have been identified and this review focuses on the key classes of these compounds. There are several possibilities to classify rose volatile compounds, for example by their biosynthetic pathways or their chemical structures. Beginning with cellular compartmentalization, we summarize the recent findings of volatiles derived from the methylerythritol phosphate- and mevalonic acid pathways, the shikimate pathway, and the formation of fatty acid and carotenoid derived volatiles. Additionally, we review recent knowledge about the enzymes involved in these pathways, i.e. methyltransferases, decarboxylases, reductases, carotenoid cleavage enzymes, and â-glycosidases. In the light of recent findings, we also summarize the rhythmic release of volatile compounds. Finally, the evolution of scent metabolic pathways of roses and future research aspects are discussed. Some side effects will also be discussed including contact dermatitis, urticaria, photoallergy and dyschromia.

OP-CYSA-03 : Novel AIE+ESIPT Coupled Benzothiazole based Materials and their Applications

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The 2-(2-Hydroxyphenyl) benzothiazole (HBT) fluorophore shows many salient features such as dual emission via the excited-state intramolecular proton transfer (ESIPT), ease of synthetic modification, and good photostability. HBT seems to be an ideal platform for constructing an efficient functional dual probe.

In the present work, a new aggregation-induced emission (AIE) based benzothiazole derivative (1), (2) and (3) were prepared. The studies revealed that probe 2 exhibits aggregation-induced emission enhancement characteristics in 80-99% aqueous media. These fluorescent aggregates of derivatives can specifically detect Cu^{2+} ions over different other metal ions with high sensitivity and selectivity in an aqueous medium. The aggregation–deaggregation behaviour of the probe was further confirmed by UV, Fluorescence, DLS, and AFM techniques. Due to the high fluorescence of $1@SiO_2$ and $2@SiO_2$ powder, fluorescence imaging of LFPs (Latent fingerprints) on a variety of porous and non-porous substrates including glove prints, up to level 3, without any post-treatment has been achieved. The derivative '3' were prepared for the selective sensing of H_2S in solid, liquid and gas phase in comparison to other biothiols.

OP-CYSA-04 : Green Chemistry : A New Trend in the Synthesis of Organic Compounds

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Organic chemistry has played a vital role in the development of diverse molecules which are used in medicines, agrochemicals and polymers. These molecules are synthesized in laboratories who adopt a process of synthesis but no attention is paid towards cost, energy efficient and release of harmful chemicals. But in the last few years special importance has been made towards green synthesis which avoids the above problem. It emphasis the trends in greener and sustainable process development during using alternate energy inputs (ultrasound- or microwave irradiation), photochemistry, and greener reaction media as applied to synthesis of organic compounds. It also provides a detailed literature review on green synthesis. The different tools of green chemistry used in synthesis of different molecules will be discussed in detail.

OP-CYSA-05 : Density Functional Theory Approach for Cellulose: Intermolecular Forces, Dissolution Mechanism and Crystal Structure

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Cellulose being the most abundant natural polymer, is a vital resource for multiple organic synthesis routes. Its importance is increasing in green chemistry rapidly but unfortunately some parts of cellulose chemistry are rather obscure till date. We use density functional theory, a quantum mechanical modelling method, to uncover parts of cellulose chemistry, specifically intramolecular structure, dissolution mechanism and crystal structure. Density functional theory model works on the axiom that everything there is to know about a material (a multi electron system), can be determined by a many body wave function, which in turn is related to density of multi electron system. This study focuses on finding the ground state crystal structure of cellulose and cell parameters, intramolecular forces at play at different chain size of polymer, energy calculations for glucose (monomer) release from cellulose chain, and dissolution mechanism with extent of hydrogen bonding. We have also correlated the results from computational study from existing experimental findings for some of the above-mentioned parameters; to validate density functional theory as a model for computational chemistry.

OP-CYSA-06 : Novel AIE+ESIPT Coupled Benzothiazole based Materials and their Applications

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Department of Chemistry, Guru Nanak Dev University, Amritsar

The 2-(2-Hydroxyphenyl) benzothiazole (HBT) fluorophore shows many salient features such as dual emission via the excited-state intramolecular proton transfer (ESIPT), ease of synthetic modification, and good photostability. HBT seems to be an ideal platform for constructing an efficient functional dual probe 1-4. In the present work, a new aggregation-induced emission (AIE) based benzothiazole derivative (1), (2) and (3) were prepared. The studies revealed that probe 2 exhibits aggregation- induced emission enhancement characteristics in 80-99% aqueous media. These fluorescent aggregates of derivatives can specifically detect Cu^{2+} ions over different other metal ions with high sensitivity and selectivity in an aqueous medium. The aggregation–deaggregation behaviour of the probe was further confirmed by UV, Fluorescence, DLS, and AFM techniques. Due to the high fluorescence of $1@SiO_2$ and $2@SiO_2$ powder, fluorescence imaging of LFPs (Latent fingerprints) on a variety of porous and non-porous substrates including glove prints, up to level 3, without any post-treatment has been achieved. The derivative '3' were prepared for the selective sensing of H_2S in solid, liquid and gas phase in comparison to other biothiols.

OP-CYSA-07 : Synthesis and Applications of Polyamide Nanocomposites

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Polyamides are renewable substance that has good processability and outstanding thermal properties. Polyamides and its composites are known as high performance polymer because of its various applications. We have discussed various synthesis and properties of PAs, the properties of PAs can be enhanced by using different 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.

OP-01 : Synthesis and Characterization of Reactive Dyes based on 4-Amino-N-(5-methylisoxazol-3-yl)-Benzenesulfonamide and their Dyeing Application on Various Fibres

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A new series of cold brand reactive dyes (D_1 to D_{12}) were synthesized by the coupling of diazotized 4-Amino-N-(5-methylisoxazol-3-yl)-benzenesulfonamide with various cyanurated coupling components in good yield. These reactive dyes were confirmed by H^1 NMR analysis, FTIR. The synthesized dyes have been applied out on cotton, silk and wool fibres. They were exhibit variety of colour shades with good dept and informality on the fibres. % exhaustion and % fixation of dyes were determined by using Glauber salt as fixing agent at various temperature condition.

OP-02 : Synthesis of Various Acid Dyes from Hydroquinone Derivative

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Synthesis of 1,4-phenylene bis(3-aminobenzenesulfonate) was synthesized by reduction of condense product of hydroquinone and m-nitrobenzenesulfonyl chloride. The compound was used as a bifunctional middle component in the preparation of tetra azo acid dyes. This di amino compound was tetra azotized and coupled with naphthalene based acid coupling component to give various tetra azo acid dyes. The obtained dyes were characterized by spectroscopic technique (IR, NMR) and the dyeing assessment of all dyes was evaluated on wool, silk and nylon fabrics. These dyes gave brown, violet, yellow, orange and pink shades on each fibers with good to very good fastness properties. The percentage dye bath exhaustion, fixation have studied.

OP-03 : Microwave Assisted Synthesis of 1-thia-4-Azaspiro[4.5]Decan-3-one Derivatives : Their Biological Evaluation and in Silico Study

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Microwave-assisted knovenagel condensation process using DBU base as catalyst yields 1-thia-4-azaspiro[4.5]decan-3-one derivatives in a simple and environmentally friendly manner. When this process is compared to the traditional method, it is discovered that the microwave method is more efficient in terms of time, yield percentages, and environmental impact. Compounds 2a, 2b, 2d, and 2h produce outstanding yield percentages. Spectral analysis, including IR, 1 H NMR, 13 C NMR, and Mass, is used to characterise all synthesised compounds. In vitro antibacterial and antitubercular evaluation is carried out for all derivatives. Compound 2a is found elevated active as antibacterial agent with MIC=50 µg/ml and compound 2l has towering antitubercular activity with MIC=0.47 µg/ml. Results of molecular docking analysis support the results of in vitro evaluation as, against antibacterial protein compound 2a has lowest binding energy and against antitubercular protein 2l is highly attached. Idealistic of synthesized compounds are checked using ADMET study and all of them are found copybook.

OP-04 : Newer 7-Chloroquinoline Derivatives: Synthesis and In Silico-In Vitro Study of Antimalarial and Antimicrobial

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In this work, new series of 7-chloroquinolines (M5a-o) were synthesized via conventional and microwave irradiation route, to obtained excellent yields in microwave irradiation. The synthesized compounds were successfully characterized by FT-IR, 1 H NMR, 13 C NMR and mass spectrometry. Final compounds were screened for their in vitro antibacterial, antifungal and antimalarial activity against two gram-positive S. aureus, S. pyogenes;two gram-negative E. coli, P. aeruginosa bacteria, three fungal strains C. albicans, A. niger, A. clavatus and P. falciparum respectively. The tested compounds exhibited a good to moderate antimicrobial and antimalarial activity, when compared to reference ampicillin, chloramphenicol, ciprofloxacin, and norfloxacin for antibacterial; nystatin, and griseofulvin for

antifungal and quinine and chloroquine for antimalarial. Among them, compounds M5a, M5e and M1g showed the most active against P. falciparum strains with IC 50 values of 0.54, 0.45 and 0.58 ?g/mL, respectively. Moreover, in silico molecular docking and molecular dynamics studies were also carried out to all compounds. Compound M5e excellent binding affinities with the target proteins (7DI7), and the results were good correlation with the experimental findings.

OP-05 : One-Pot Three-Component Synthesis of Spirooxindoles Hybrids with Potential Antimicrobial Activity

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In this work, novel fourteen-compounds synthesized by assigner multicomponent reaction. The synthesized compounds were characterized by using FT-IR, H 1-NMR, C 13-NMR and Mass Spectrometry .The final compounds were evaluated for their potential antimicrobial activities using agar dilution method. The tested compounds show good to moderate activity with MIC value between 8 to 31 ug/ml, when compared to reference ampicilin and ciprofloxacine. Among them compounds l and m show most promoting activity against E.coli, B.cereus and B.substilis

OP-06 : Synthesis of Novel 1,2,3-triazole Bearing 1,3,4-oxadizole and Evaluation of their Antioxidant Properties

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Among the nitrogen-embedded heterocycles, 1,2,3-triazoles derivatives are widely explored and earned considerable attraction in pharmaceutical industry and academics. The copper (I)-catalyzed click chemistry has found application in bioconjugation, a growing field that is based on the use of biological probes that combine the activity of small molecules with the specificity of biomolecules. Oxadiazole is a versatile lead compound for designing potent bioactive agents. In view of these findings we have synthesised a new class of 1,2,3-triazole bearing 1,3,4-oxadizole via Cu(I) mediated 1,3-dipolar cycloaddition of azide with terminal dipolarophile (acetylene). Structures of the newly synthesized compounds were characterized by ^{1} H NMR, ^{13} C NMR,

IR, LC MS and elemental analysis. Hence we here in report a series of novel triazolo-oxadiazole derivatives 3-phenyl-1-(4-(4-(((5-phenyl-1,3,4-oxadiazol-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)phenyl)prop-2-en-1-one. The synthesised compounds were evallluated for their antioxidant property. These compounds showed moderate to good antioxidant activity.

OP-07 : Synthesis of Novel 1,2,3-Triazole based Schiff bases and Evaluation of their Antioxidant Properties

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Chalcones are of paramount interest of the synthetic and medicinal chemists because they are the key precursors for various synthetic and naturally available heterocycles. 1,2,3-Triazoles, a class of five-membered nitrogen heterocyclic compound present in a variety of biologically active molecules. The copper (I)-catalyzed 1,4-substituted-1,2,3-triazole forming reaction between azides and alkynes has become the gold standard of "click chemistry" due to its accuracy, specificity, and biocompatibility and gained remarkable utility in the development of novel lead molecules. A new class of Schiff base bearing 1,2,3-triazole has been synthesized via Cu(I) mediated 1,3-dipolar cycloaddition azide with various aromatic bearing terminal dipolarophile (acetylene). Structures of the newly synthesized compounds were characterized by ^{1} H NMR, ^{13} C NMR, IR, LC MS and elemental analysis. In view of these findings and as a part of our general search for biologically active Schiff base bearing 1,2,3-triazole, we here in report a series of novel triazole derivatives 4-((1-(4-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzaldehyde and novel Schiff base 1-phenyl-3-(4-(4-((4-(-(phenylimino)methyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)phenyl)prop-2-en-1-one derivatives. The synthesised compounds were studied for their antioxidant property which showed moderate to good antioxidant activity.

OP-08 : Reactive Dyes Having s-triazinyl Groups : Synthesis, Characterization and Application on Various Fibres

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A demand for novel reactive dyes with improved properties have led to synthesis of reactive dyes by coupling tetrazotised 3-sulpho 4,

4-Diamino diphenyl Sulphonamide with various cyanurated coupling components such as H-acid, K-acid, J-acid, N-methyl J-acid, N-phenyl J-acid, Peri acid, Tobias acid, Sulpho tobias acid, Laurent acid, Gamma acid, Bronner's acid, N-methyl Gamma acid and their dyeing performance as reactive dyes has been assessed on cotton, wool and silk fibres. The purity of dyes was checked by Thin Layer Chromatography. The IR spectra showed all characteristic bands and PMR spectra of representative dye showed all the expected signals. The percentage dye bath exhaustion on different fibres was good. The dyed fibres showed moderate to very good fastness to light, washing and rubbing.

OP-09 : Microwave-Assisted Multi-Component Synthesis of Betti Reaction and their Therapeutic Activity

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The Betti reaction, which 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.

OP-10 : Recent Advances of Carbon-Carbon Bond Activation by Transition Metal Catalyst in Organic Synyhesis

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Transition metals are well known for their catalytic behaviours for the activation of the Carbon-Carbon (C-C) bond. Many chemists have created various important development in this field of organic

synthesis during the last decades. only a few instances of catalytic activation of the C-C bond using the transition metal catalyst and their mechanism had been disclosed, which is useful information for creating new ways to break these bonds. This includes the recent advances in the activation of cyclic, saturated as well as unsaturated carbon-carbon bonds utilizing transition metals as a catalyst in number of different systems.

OP-12 : One Pot Synthesis of Substituted Coumarins using Nanoparticle under Solvent Free Conditions

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Green chemistry for chemical synthesis addresses our future challenges in working with chemical processes and products by inventing novel reactions that can maximize the desired products and minimize by-products, designing new synthetic schemes that are seeking greener solvents and environmentally free. The emerging area of Green chemistry is need in the design and attainment of sustainable development. Green chemistry is the utilization of a set of principles that will help reduce the use and generation of hazardous substances during the manufacture and application of chemical products. Substituted Salicylaldehyde, methyl amino acetate, magnetic NPs were mixed. The mixture was heated for 10-15 minutes under microwave. The mixture was allowed to cool to room temperature. The crude product was obtained and washed with water. The solid was recrystallized from methanol to give 80% of a solid product. NPs were separated at the time of recrystallization.

OP-13 : Synthesis of 2-Aminothiazole Derivatives from Thiourea and Alkyl /Aryl Ketones using Oxone and Iodobenzene Reaction System

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An innovative, rapid single step approach for the Synthesis of 2-aminothiazole derivatives from easily available Thiourea and alkyl / aryl Ketones with the help of Oxone and Iodobenzene reaction system has been developed in aqueous acetonitrile solution. The developed procedure is applicable to several types of substituted 2-aminothiazole derivatives to get the corresponding products. The developed methodology offers mild reaction condition, short reaction time, and

moderate to admirable yields. This is one of the most simple and environmentally benign protocols for synthesis of 2- aminothiazole derivatives. When reaction carried out in presence of oxone and Iodobenzene in aq. Acetonitrile solvent system there is formation of active Hypervalent iodine reagent in situ and that reagent is responsible for this conversion but, yield of reaction is less. We go in detailed in Hypervalent reagent study and got some literature in that researcher used catalytic KBr along with oxone and Iodobenzene and there is amplify in activity of Hypervalent iodine reagent because of catalytic amount of potassium bromide. So we decided to use catalytic amount of KBr along with oxone and Iodobenzene reagent and there is increase in yield of desirable product.

OP-13 : Ultra Sonicator Assisted Green synthesis of Coumarin using Citrus Maxima Juice as a Catalyst

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Coumarin derivatives have a myriad of applications in medical science, biomedical research, and many industrial branches. By considering their utility Coumarin derivatives are synthesized by green approach using the condensation between phenols and β-keto esters, in the presence of a Citrus maxima juice as a catalyst. The peel of Citrus maxima (C. maxima) is the primary byproducts during the process of fruit or juice in food industries, and it was always considered as biomass waste for further treatments. This approach is completely eco-friendly as it is synthesized in solvent free condition, green catalyst Citrus maxima juice and Microwave radiations.

OP-14 : New Phenanthrene Based Oxadiazole Derivatives: Synthesis, Molecular Docking Studies and Biological Activity

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Phenanthrene-based tylophorine alkaloids have been reported to exhibit anti-inflammatory, anti-immuno and antitumor activities. 1,3,4-Oxadiazole compounds are considered to be the distinct class of

heterocyclic compounds that have extensive biological activities including antiviral, antimicrobial, anti-neoplasticity, fungicidal, inhibition of tyrosinase and cathepsin K. In the light of fascinating biological activities that are displayed by naturally occurring phenanthrenes and oxadiazoles, synthesis of a series of novel phenanthrene linked oxadiazoles (7a-m) and their characterization by using ^{1}H NMR, ^{13}C NMR and mass spectral analysis are done. The synthesized analogues (7a-m) have been assessed for their in vitro antibacterial and antifungal activities towards the selected strains of Gram-positive, Gram-negative bacteria and fungus. It has been indicated from these preliminary bio-assays, that majority of the synthesized compounds showed up moderate to good antibacterial activities. Compounds 7e, 7b and 7j exhibited most potent antibacterial activities. Compounds 7c, 7i and 7l showed significant antifungal activities. Apart from the biological screening, the molecular docking studies assisted the biological activities by the correlated binding energy values. The synthesized compounds (7a-m) also followed the Lipinski's 'Rule of five' to observe drug-likeness.

OP-15 : Structure based Drug Discovery of 1, 2, 3-Triazolobenzoxepine Derivatives : Through Insilico Study

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1,2,3-triazole containing derivatives exhibit antibacterial and anticancer activities with excellent potency against various cell lines. In order to investigate the structural insights of synthesize compounds, we have used various computational methods for the identification of new compounds for triazolobenzoxepine derivatives. The 2-[1-(propan-2-yl)-1H-1,2,4-triazol-5-yl]-4,5-dihydrothieno[3,2-d][1]benzoxepine-8-carboxamide as a crystal ligand bound to the 3D structure of protein with PDB ID: 1HLE was employed for designing e-pharmacophore. Pharmacophore based virtual screening of large databases followed by molecular docking of identified potential compounds were studied. In order to identify the structural relationship and validate stability of triazolobenzoxepine derivative complexes, we performed molecular dynamics simulations for final selected hit compounds. Our studies revealed stable complex formation showed good H-bonding interactions, non-bonding interactions similar to crystal structure ligand. Further experimental validation would reveal that

these selected hit compounds acts as potential inhibitors for the development of novel antibacterial and anticancer therapeutics against proposed drug target.

OP-16 : Fatty Acids Composition and Elements Analysis of Cassia Siamea Lam Seed Oil

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Cassia siamea Lam is well known Ayurvedic medicinal tree. Cassia siamea Lam is a genus of family Fabaceae and sub-family Caesalpinioideae which is selected for investigation. In this study, we determined the fatty acid composition and elements analysis of Cassia siamea Lam seed oil. The oil was extracted from Cassia siamea Lam seed using a Soxhlet extractor with n-hexane as solvent. The fatty acid composition was analyzed by using the GC-FID technique and elements were analyzed by the ICP-MS instrument. Unsaturated fatty acids and saturated fatty acids are very important for pharmacological investigation. Linoleic and gamma linoleic acids are important unsaturated fatty acids that can be used in the synthesis of tissue hormones. Elements Pb, Cu, As, and Sn levels in this oil were measured. Although this oil contains lead and copper, it does not contain As or Sn. Cu is required in the body to prevent anemia, heart diseases and nervous disorders is found in this oil. A very small amount of Pb is present in this oil, which is not harmful to our bodies. Fatty acids and Elements of Cassia siamea Lam seed oil suggest that it may find application in both cosmetic and pharmaceutical natural product formulations.

OP-17 : Micellar Effect upon Dephosphorylation of 2-methyl Phenylphosphoramide Monoester by Peroxy Anions

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The micellar catalysed reaction between hydroxide or hydroperoxide anions and monester of 2-methyl phenyl phosphoramide (2-MPPA) has been examined in Buffered medium at pH 8-10 with borate ions. First order rate constant () for the reaction of hydroxide ion (OH -) with 2- MPPA through maximum with the concentration of cetyl trimethyl ammonium bromide (CTABr). The micelles of CTABr

are very effective catalysis to the reactions at phosphate monosters. The rate enhancement depends upon the hydrophobicity of the nucleophilic for the action of phosphate mono esters. Rate constants measured with hydroperoxy anion (HO - 2) ions are approximately twice and thrice than that of hydroxide ion (OH -) in presence of CTABr.

OP-18 : Pyrolysis of Kusum Seed Cake for the Production of Bio-Oil and Bio-Char

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The current research involves the preparation of bio-oil, bio-char and gas fuels, under a fixed-bed type reactor by thermal pyrolysis of Kusum press seed cake (KPSC) (Schleichera oleosa). The operating conditions are temperature 400°C - 550°C, N 2 flowrate 0.1 - 0.5 , and reaction time 30 - 60 min Response Surface Methodology (RSM) with Box-Behnken Design was used to obtain the optimum operational conditions for bio-oil production. RSM confirmed that the optimum outcome of 41.2% of bio-oil, 14.27% bio-char and 14.32% water in aqueous stage is obtained at temperature 550°C, N 2 flowrate 0.3 and reaction time 60 min. The experimental data is consistent with the model as indicated by the determination coefficient R 2 0.9985 for the bio-oil outcome. KPSC bio-oil and bio-char were analysed for their physicochemical characteristics. It was found that they had maximum amount of resources viz Octadecanenitrile, 1-heptacosanol, 8-Heptadecene, N-methyl-octadecenamide, N-methyl hexadecanamide, Octadecanamide, and Nonadecanenitrile. The Calorific Value of bio-char is 24.07MJkg -1 with a higher proportion and a higher carbon content of 71.15 wt.%. Bio-oil has a high heating value similar to diesel fuel 32.7 MJ kg -1.

OP-19 : An Ecofriendly HPTLC Method for the Quality Assessment of the Ayurvedic Drug "Bala (Sida Complex)"

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Sida complex denotes a collective term for similar species of Sida found in India and traded by the general name 'bala'.Sida species (Family: Malvaceae) is a potent and valuable medicinal herb used in the Indian system of medicine. For the globalization of herbal

drugs and international trade quality of the botanicals should be maintained. The present report focuses on HPTLC method development for QA/QC of Sida species.

Methodology: The HPTLC densitometric method was developed for the simultaneous quantification of cryptolepine and quindoline in Sida acuta, S. rhombifolia, S. cordifolia, S. coradta, and its possible adulterant abutilon indicum. The method is validated as per the current ICH guidelines applied to satisfy the validation criteria of linearity, Precision, LOD/LOQ, accuracy, and specificity.

Result: In the present investigation, the principal objective is to develop a high throughput and eco-friendly method for the simultaneous quantification of marker compounds in different sida species. This method involved the separation of two compounds with a mobile phase consisting of n-toluene: ethylacetate: methanol: triethylamine in a fixed ratio. The Rf values of cryptolepine and quindoline are 0.54 and 0.62. The range of linearity was defined from the calibration-response relationship curves showing an excellent correlation coefficient (r^2). Method sensitivities (LOD & LOQ) were in the range of sub-microgram/band. The method showed good precision and accuracy with overall acceptable intraday and inter-day variation. The greenness score of the method has suggested it be considered eco-friendly.

Conclusion: It is of paramount importance to develop a green method for cost-effective extraction and fast determination of marker compounds. In this study, ultrasonic-assisted extraction (UAE) using methanol proved to be the most efficient method for the extraction of marker compounds. The present HPTLC method was found to be precise, fast, cost-effective, and can be used for the quality control of sida species. The method can be directly implemented in QA/QC lab for quality evaluation of the sida complex.

OP-20 : Validated RP-HPLC-PDA Method for Simultaneous Determination of Four Bioactive Coumarins in Aegle Marmelos Root : Application for Genetic × Environment Interaction Studies

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Aegle marmelos Linn (Beal) is a highly reputed plant in Ayurveda, owing to its usage in many formulations including Dashmularista -a

popular Ayurvedic tonic for women's overall health. Almost all the parts of the plant i.e. root, leaf, trunk, and fruit are used in the traditional system of medicine. A. marmelos have a wide range of therapeutic actions including antidysentery, antipyretic, antidiarrheal, and hypertension activities. Therapeutic potential of the plant corresponds to the secondary metabolite flux. We have isolated the bioactive coumarins from the A. marmelos root for the quality assurance of the raw material and their derived products.

The aim of the present work is to develop and validate Reverse Phase-High Performance Liquid Chromatography (RP-HPLC) method for simultaneous determination of marmesin, marmin, imperatorin and auraptene in A. marmelos root extract.

Separation of A. marmelos phytochemicals was optimized for developing HPLC method respective plant part. A. marmelos showed good resolution with retention time within 60 min.

The method was found to separate the peaks for targeted compounds viz., marmesin, marmin, imperatorin and auraptene and appeared at 23.54, 27.67, 39.38 and 51.72 min, respectively. The chromatographic conditions have resulted in to optimum separation on a C_{18} column with acetonitrile– water as gradient mobile phase at a flow rate of 1.0 mL/min, UV was set at 254 nm for the quantitation while specificity was ensured with photo diode-array detector (PDA) spectral acquisition. The recovery was found to be satisfactory (99.11–100.19%) without interference from sample Metrix. The method seems to be reliable with intraday precision and intraday precision below 2.0%.

A simple, rapid, selective, and quantitative RP-HPLC-PDA method was validated for sensitivity, linearity, accuracy, precision, specificity and recovery as per the International Conference on Harmonization (ICH) guidelines, for the quantification of four (coumarins) characteristic analytical markers in the A. marmelos.

OP-21 : Ultrasound Assisted Ring Opening of Epoxides via $CuFe_2O_4$ as a Heterogeneous Magnetic Nano-Particles

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Development of highly efficient, reusable, economically viable, environment benign catalyst is highly desirable in the present scenario of exhaustive industrialisation globally to save mother earth. Heterogeneous catalyst like CuFe2O4 magnetic nanoparticles may be one of the option to mitigate mentioned global issue. Copper ferrite

nano catalyst, a highly efficient catalyst, has been used for the nucleophilic ring opening of epoxides with all aromatic, aliphatic and heteroaromatic primary as well as secondary amines under ultrasound assisted condition. Aminolysis is regioselective in nature for the synthesis of b-amino alcohols. MNPs were characterised SEM, X-rays and EDX moreover, all the products are characterised by NMR (^{1}H &^{13}C), FTIR, HRMS.

OP-22 : Synthesis, Characterization and Antimicrobial Studies of Some New Dihydrazones

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A facile synthesis of different thiodipropionic dihydrazones have been achieved by condensation of thiodipropionic dihydrazide with furfuryl(i), 2-acetyl furan (ii) and 4-acetyl pyridine (iii) resulted in the formation of different dihydrazones viz. furfuryl thiodipropionic dihydrazone (2a), 2-acetyl thiodipropionic dihydrazone (2b) and 4-acetyl pyridine thiopropionic dihydrazone (2c) respectively. All the synthesized compounds were characterized by their repeated M.P. determination, TLC for single spot, element analysis, IR and NMR spectral data. All compounds were screened for their antimicrobial activities against two bacteria Staphylococcus aureus and Escherichia coli and two fungi Aspergillus niger and Aspergillus flavus. All the synthesized compounds showed appreciable antimicrobial activities in comparison to the constituting fragments.

PHYSICAL CHEMISTRY SECTION

Sectional President's Address

Ionic Liquids as Green Solvents for Enhanced Stability of Proteins against Multiple Stresses

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Worldwide, there is growing awareness of the impact of hazardous chemical substances in the environment and economic view point. The judicious selection of chemicals and designing less toxic substances in chemical, purification processes and industries could offer safer and sustainable developments. Thus, control in generation of hazards and promotion of novel synthetic approaches must be followed. A wide area of research offering this incorporates the use of renewable feedstocks, catalysis and alternative solvents. Towards this, an environmentally benign solvent must be ascertained to ensure the biodegradability and enhanced applications in numerous fields like biotechnology and enzymology. Motivated by the demand for sustainable developments, researchers proposed ionic liquids (ILs) which fulfill the requirements of environmental sustainability. ILs render innumerable advantages over organic solvents in various fields like catalysis, electrochemistry, chemical synthesis and protein biochemistry. For a protein to be biologically active, the maintenance of its native structure becomes pre-requisite. Any deviation in native structure of protein results in misfolded or completely unfolded state of protein which in turn results in serious life threating ailments like type II diabetes, Alzheimer's disease and Huntington's disease. Most importantly, ILs as well as deep eutectic solvents (DESs) (a new generation of sustainable ILs) could be employed in enzyme biocatalysis as they enhance the solubility of products/ substrates without rendering them inactivation. The development of nontoxic ILs for biomolecules,

the ability of ILs in dissolution, suppression and cryopreservation has potentially aided the developments in cryobiology, pharmaceutical industry as well in biomedical treatments.

PIL-01 : A DFT Perspective on the Charge Transport Properties of Linear and Star-shaped Organic Materials

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Organic materials have developed as controlling supplies for their frequent applications in molecular electronics, which comprise organic photovoltaic cells, light-emitting diodes, super capacitors, and field-effect transistors. The effectiveness of the charge-transport processes is the key parameter for the performance of these devices; at microscopic level, the plenty of the electron transfer integrals by the hopping model from molecule to molecule between adjacent halves is one of the key constraints leading the transportation properties. Small organic materials based on thiophene-containing acenes and fused thiophenes are proven optoelectronic materials because of their improved air stability and high charge mobilities. These thiophene-based small organic molecules have versatile applications in OPV, OFET, DSSC, LED, OLED, NLOs, and LASERs. The structural impact of the linear and fused star-shaped organic thiophene-based molecules on the optical and charge transport characteristic features are investigated using density functional theory. The studied molecules have shown relatively smaller differences in the corresponding hole and electron reorganization energies, hence, these materials can be used as ambipolar charge transporting materials in optoelectronic devices.

PIL-02 : Environmentally Benign Methodologies for Waste Water Treatment and Processing of Hard to Degrade Polymers

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Inspired by surface active nature of many of the ILs called as surface active ILs (SAILs)[2]along with the utilization of ILs having metal ions incorporated in the anions (MILs) for the preparation of a variety of nanomaterials, our group conceived to synthesize surface active MILs for liquid phase exfoliation of graphene and in-situ

preparation of different nanomaterials in a sustainable manner for photocatalytic degradation of various effluents. The prepared nanocomposites have shown enhanced photocatalytic efficiency towards the degradation of toxic effluents in wastewater as compared to respective nanomaterials under sunlight or visible light. Further, we have prepared and utilized $ZnCl_2$ and lactic acid (LA) based DESs (LA:$ZnCl_2$) for the dissolution and degradation of Polythene under white light at 60 ^oC. The dissolved PE has been regenerated using water as an antisolvent and characterized, whereas DES was recovered and reused.

PIL-03 : Recently Developed Simple yet Highly Effective Approaches for Viscosity Prediction of Binary and Higher Order Liquid Mixtures

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Density and viscosity are two key thermophysical properties which can be used to optimize the process of mass and energy exchange. Determination of such properties helps in elucidating several excess properties such as excess molar volume, deviation in viscosity, excess free energy of activation of viscous flow etc. These properties are useful in understanding the nature and strength of molecular interactions between constituent components. Viscosity measurements of pure, binary and higher order liquid mixtures have been a principal factor leading to designing and optimizing various chemical processes. The deviations from the ideality of the thermophysical properties arise from the difference in molecular size, shape and structure and orientation and provide an important insight into the intermolecular interactions prevalent in the systems under investigation which provides the researchers and industry professionals with vital information for process and equipment design. The importance of computational calculations has enhanced significantly during the global shutdown of experimental research labs due to the COVID-19 pandemic.

There was and always remains a strong demand for strong and robust predictive approaches, especially for viscosity, the most important transport property. Unlike other thermophysical properties, viscosity does not exhibit a linear trend with the change in concentration. The problem is made more challenging as it is seen that viscosity is highly susceptible to temperature variations. Thus it is very challenging change to develop a model for predicting viscosity for binary and higher order liquid mixtures which works very effectively

at varying temperatures. Dey et al [1–5] have modified some of the well-established models and have also developed new models exhibiting an appreciable amount of success. Some of these recent approaches are also seen to work well for Ionic Liquid mixtures too as owing to their unique properties, ionic liquid (IL) mixtures deviate significantly from ideal behavior and exhibit a high degree of non-ideality as compared to organic liquid mixtures. The Dey Biswas model (2018) has now been tested on around 500 binary and good number of multicomponent mixtures and is showing great promise.

PIL-04 : Carbon Quantum Dots : Photoluminescence Properties and FRET Donor Efficiency for Sensing Applications

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Carbon quantum dots (CQDs) which are a new class of fluorescent carbon nanomaterials was discovery first time in 2004 during purification of single-walled carbon nanotubes (SWCNTs). A large number of investigations on CQDs has been made in last two decades due to their strong and tunable fluorescence (FL) properties, which enable their applications in sensing, catalysis, biomedicine, optoelectronic, and bioimaging. The intrinsic properties of nitrogen dopped CQDs upon doping of nitrogen atoms such as graphitic, pyridinic, pyrrolic and amine their roles in modulating the fluorescence QYs, energy levels and fluorescence decay life time of CQDs are concern of the recent reasearch. The FL quenching (Turn-off) and fluorescence recovery (Turn-on) properties of CQDs can be used to design fluorescence-based optical sensors for large class of analytes of environmental and biological importance. The Foster/fluorescence resonance energy transfer (FRET) based phenomena is most suitable technique for the development fluorescence-based sensors. We have investigated that the fluorescence tunability of CQDs make them suitable donors for fluorescence resonance energy transfer (FRET) with wide range of donor materials. Due to significant overlapping of FL spectra of CQDs with absorption spectra of gold nanoparticles (AuNPs), gold nanorods (AuNRs) and mangnese dioxide (MnO_2) nanostructures, we enabled to develop FRET-based sensors for detection of pesticides and biomolecules such as glutathione, cholesterol, acetylcholinesterase (AChE) enzyme and organophosphorus pesticides.

PIL-05 : Environmental Benign Solvents to Enhance the Extraction of Micropollutants and Heavy Metals

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Despite many waste management andwater treatment strategies, the removal of micropollutants from water bodies remains elusive. Micropollutants, which include pharmaceuticals, food additives, cosmetics, and dyes,present in trace amounts in the aquatic environment; but they have been associated with many adverse effects, including biomagnification and genotoxicity. The need to develop sustainable and cost-effective alternatives to eliminate these toxins has become a pressing issue. Apart from this, the rapid technological changes and the short life span of electronic devices create an abrupt accumulation of electrical and electronic waste in the environment. The heterogeneity of constituents in e-waste and the presence of hazardous materials raise complexity in e-waste treatment. Recently, ionic liquids (ILs) have emerged as a promising possibility for task-specific, efficient pollutant extraction because of the ease in structure tunability and other unique chemical properties. Deep eutectic solvents (DES), often referred to as a subclass of ILs, were also widely renowned for pollutant extraction capability. This talk will discussabout alkanolamine-based ILs as potential performance additives to eliminate pharmaceutical micropollutants in the aquatic environment, and choline chloride-carboxylic acid DES as an alternative to the conventional leaching acids for the recovery of valuable metals from e-waste. The proposed methodologies for extraction are rapid and facile without compromising environmental concerns.

PIL-06 : Experimental Spectroscopic, Quantum Chemical, Molecular Docking and Molecular Dynamic Simulation Studies of Medicinally Important Heterocyclic Compounds

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Compounds classified as heterocyclic probably constitute the largest and most varied family of organic compounds. Heterocyclic have been found a key structural in medical chemistry and also they are frequently found in large percent in biomolecules such as enzyme, vitamins, natural products and biological active compounds including antifungal, anti-inflammatory, antibacterial, antioxidant,

anticonvulsant, antiallergic, enzyme inhibitors, herbicidal activity, anti-HIV, antidiabetic, anticancer activity, insecticidal agents. Different N-based heterocyclic compounds have been studied spectroscopically as well as computationally such asAmpyra, Indole-3-carboxaldehyde, Amine-dimedone, 3-Pyridinepropionic acid, Pyridine-2,6-dicarboxalic acid, etc. examined with their Molecular Docking and Molecular Dynamic Simulations.

PIL-07 : Extreme Conditions in the Solar System – One Impact and one Thousand Reactions

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Amongst the icy objects of the Jovian and Saturnian planetary systems satellites such as Ganymede, Europa, Dione, Rhea, Callisto and Titan are embedded in their respective planetary magnetospheres and hence their surfaces are irradiated by a wide range of energetic ions as well as solar photons both of which release many secondary electrons. Such energetic processing of simple molecules within ices has been shown to synthesis complex molecules such as amino acids, sugar and even di-peptide links. However, another process by which molecules may be formed is physical impacts.

The observation of large scale craters on the surface of the icy satellites reminds us of the role of impact processes in planetary and lunar evolutions whilst many cometary bodies appear to the result of collision of constituent bodies. Such impacts release significant amounts of energy and therefore may provide pathways for large scale molecular synthesis. Indeed, it is important to recall that all planetary and lunar surfaces are constantly bombarded by micrometeorites. Such impacts and the impact associated shock processing of molecules in extreme conditions largely remains unexplored. In this meeting, we will discuss the need of a new experimental program to study molecules under astrochemical impact induced shock conditions.

PIL-08 : Polymer Electrolyte Membranes : Fabrication, Characterization and Potential Applications

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Polyelectrolyte membranes (PEMs) are a novel type of material that is in high demand in the health, energy, and environmental

sectors. If environmentally benign materials are created with biodegradable once, PEMs can evolve into practical technology. In this work we have fabricated environmentally safe and economic PEMs based on sulfonate grafted polysaccharide viz. pectin, sodium alginate. In the first step, 2-acrylamido-2-methyl-1-propanesulphonic acid (AMPS) and sodium 4-vinylbenzene sulfonate (SVBS) grafted on to polysaccharide by simple free radical polymerization technique. In the second step, sulfonated polysaccharide successfully blended with PVA to fabricate PEMs for in vitro controlled release of 5-fluorouracil (anti-cancer drug) at pH 1.2 & 7.4 and removal of copper(II) ions from aqueous media. Also, phosphomolybdic acid incorporated composite PEMs were developed to evaluate the fuel cell characteristics i.e., ion exchange capacity, proton conductivity and methanol permeability. The chemical structure of PEMs was verified by the FTIR. Crystallinity of PEMs was analyzed by the XRD studies. The surface morphology and elemental composition of the PEMs were recorded by scanning electron micro-graph and energy dispersive X-ray analysis, respectively. The results of present study demonstrate that, a simple and cost-effective approach to fabricate environment friendly PEMs from sulfonated polysaccharide and PVA that may be potentially employed as anticancer drug delivery systems for various cancer types, as adsorbent for removal of bivalent heavy metal ions and as polyelectrolyte membrane for transport of ions.

PO-CYSA-01 : Green Synthesis of Silver Nanoparticles and their Biocompatibility with Hemoglobin

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Nanoscience is garnering extensive attention due to their unique properties and potential application in biomedical sciences. Despite tremendous development in nanotechnology, limited knowledge is available regarding its possible effects on human health. In this study we present synthesis, characterisationof silver nanoparticles (AgNPs) synthesize using Drymaria cordata along with assessment of its antioxidant, antibacterial, and anti-diabetic activities. Additionally, herein we also evaluate the biocompatibility of the AgNPs using haemoglobin (Hb) as a model protein. A comprehensive analysis of Hb and AgNP interactions was carried out using various spectroscopic, imaging and size determination studies. Spectroscopic data revealed no alterations in the secondary structure of the Hb upon binding with AgNP. Furthermore, the thermal stability was also well maintained at different concentrations of nanoparticles. Overall, the synthesized AgNPs were found to be biocompatible with the protein Hb at the

physiological conditions. This study indicated an economical, simple and efficient eco-friendly technique using Drymaria cordatafor synthesis of AgNPs and confirmed that green AgNPs are also biocompatible. The spectroscopic techniques including UV-Visible spectroscopy, Steady State Fluorescence spectroscopy, UV-CD spectroscopy, Raman spectrometry, Fourier Transformed Infrared Spectroscopy(FTIR), Atomic Force Microscopy(AFM) were performed to study the interaction between Hemoglobin and AgNPs. Dynamic Light Scattering was performed to determine hydrodynamic size and zeta potential.

PO-CYSA-02 : Controlled Release of Iodine Entrapped in Hydrogels of Aloe Vera, Gelatin or their Blends in Aqueous Media and the Kinetics of the Release Process

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The Aloe vera gels have been reported to be good source of medicinal properties with health benefits. Hydrogels of Aloe vera, gelatinor blend of Aloe vera and Gelatinhave been prepared and employed as template for the entrapment of iodine. The release behavior of the entrapped iodine in the hydrogel was studied by dispersing the iodine entrapped hydrogel in aqueous media and monitoring the amount of iodine released spectrophotometrically against time until the saturation point.The results showed that almost the total amount of iodine entrapped in Aloe vera gel is released within a very short time, about 2-3 hours.On the other hand, iodine entrapped inGelatinhydrogel is released relatively much slower in about 13-15 hours which is much slower as compared to that of Aloe vera gel. With a view to controlling the rate of release of the entrapped iodine from the hydrogels to an optimum level, the release of iodine entrapped in the hydrogels of aloe vera blended with 20%, 50% and 80% (w/w) gelatin have also been studied. Blending of gelatin in the aloe vera gels resulted an increase in the iodine release time from 2-3 h to 5-6 h with 20% to about 11 h in 80% gelatin blended hydrogels.The results showed that the release of iodine from the aloe vera gels can be controlled by blending with gelatin. The kinetics of the iodine released from the hydrogel was found to follow first order kinetics.The variation of sol-gel transition temperature of Iodine entrappedhydrogelsas a function of Iodine concentration was studied using a Vibro-Viscometer. It was also observed that the swelling ratio of aloe vera gels decreased with the blending of the gel with gelatin. Most of the hydrogels or blended

hydrogels have been characterized using physical methods like FTIR, XRD,SEM, EDX, etc.

PO-CYSA-03 : Surface and Bulk Characteristics of Single and Mixed System Containing Surface Active Ionic Liquid

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The measurements of surface tension under controlled conditions, mixed surfactants sodium lauryl sulphate (SLS)/sodium lauryl ether sulphate (SLES) and double-tailed ionic liquid 1,3-didecyl 2-methyl imidazolium chloride were studied in aqueous solutions as a function of total concentration. Clint, Rubingh, Maeda and Rosen determined critical micelle concentration (CMC), surface excess concentration (T_{max}), minimum area per molecule (A_{min}), interaction parameter of mixed micelleand adoption monolayer (β^m, β^0) and thermodynamic and micellar properties. The synergism interaction between the ionic liquid and SLS is higher compared to the interaction of ionic liquid and SLES because SLS behaves as the anionic surfactant while SLES acts as the hybrid surfactant due to EO group present in it. The results are discussed in terms of the structural characteristics and chain of double tail cationic ionic liquid and the presence of ether group in the chain of the surfactant.

PO-CYSA-04 : Self-Assembly of pH-Responsive Diblock Copolymers Poly(N-Vinyl Pyridine)-b-Polyethylene Oxide in Water and Interaction with Anionic Surfactant

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The varied responses some polymers have to external stimuli has piqued much scientific curiosity. Poly vinyl pyridine is an example of this type of polymer that alters its behaviour in response to variations in pH. In this paper, we report on the aggregation behaviour in water of two PVP-PEO amphiphilic block copolymers with distinguishing molecular features, specifically PVP_{55}-PEO_{284} and PVP_{99}-PEO_{394}. The behaviour of these two copolymers during self-assembly was investigated in response to varying pH levels and temperatures. In addition, the micellization behaviour of these compounds is examined

at a range of anionic surfactant SDS and salt NaCl concentrations. PVP's pyridine ring has tertiary nitrogen, which can be quaternized or protonated at pH- 2 or acidic pH range, where the polymer demicellizes, becoming double hydrophilic and forming a unimolecular solution. Electrostatic interaction between protonated PVP-PEO and the anionic surfactant SDS is a primary factor in the production of micelles at low pH. In the presence of sodium dodecyl sulphate at an acidic pH, spherical micelles with low dispersions are shown to go through a transition into a variety of different shapes, as revealed by DLS, SANS data, and Cryo-TEM images.

PO-CYSA-05 : A Comparative Study of Hydrogen Production through Steam Methane Reforming Method and Photovoltaic Electrolysis Membrane Cell Method and their Environmental Emissions

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Hydrogen is one of the most important choices to be the future fuel with its high specific energy and low emissions.There are many countries that focus on it and they have worked closely together to obtain the best result to solve related problems. Hydrogen production plays an important role in deciding the future of hydrogen. Hydrogen is called green hydrogen, depending upon the method of its production.Today, majority of hydrogen productions are by steam methane reforming method which produces greenhouse gases as byproducts. These emissions restrict hydrogen from being a clean fuel. There are a number of methods which can be used to produce hydrogen and these methods can be divided on the basis of energy resources as like renewable or non-renewable. In this study, the focus is on two specific methods that are steam methane reforming and photovoltaic electrolysis membrane cell methods. These two methods have a strong hold over each other. Steam methane reforming method has high hydrogen producing efficiency and photovoltaic electrolysis membrane cell method has very low emissions in production. Specifically, photovoltaic electrolysis membrane cell method is studied. This method uses solar energy to produce electricity for the process. The discussion is based on required material in respective processes, the cost associated with it, and the production method in detail. The steam methane reforming method has better efficiency for hydrogen production.The emission comparisons are done on the parameters of carbon dioxide and acidification.

PO-CYSA-06 : Green and Efficient Recovery of Metals from used Lithium-ion Battery Cathode Materials using Deep Eutectic Solvents

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Due to the abrupt accumulation of electrical and electronic wastes (WEEE) produced by quick technological advancements and the short lifespan of electronic gadgets. In the modern technological world, the usage of lithium-ion batteries is inevitable due to their high energy density, which leads to over-demand and production. The overproduction expedites the formation of lithium-ion battery wastes, which are the prior source of $LiCoO_2$. Inorganic acids are employed in the hydrometallurgical leaching process to recover metals from discarded $LiCoO_2$ cathode materials, which has a detrimental effect on the environment. Deep Eutectic Solvents (DES) are a type of biocompatible solvents that emerged as a potential lixiviant for leaching applications. Here we have designed a choline chloride-carboxylic acid-based DES as an effective alternative to the conventionally used inorganic acids for the leaching of $LiCoO_2$. Differential Scanning Calorimetry (DSC) curves provide information on the eutectic composition and melting point of the prepared systems, and the reducing ability of HBD was studied using cyclic voltammetry. The high chloride content from the choline-based DES stabilizes the reduced Co^{2+} by forming a blue color cobalt-chlorocomplex, which was proved by the UV-Visible spectroscopy. As an extension of this, the molecular-level understanding of prepared DES and its leaching ability for different metal oxides are the future perspective.

PO-CYSA-07 : Development of a Hybrid Magnetic Nanocomposite Adsorbent based on Gum Ghatti for Removal of Cationic Dyes from Aqueous Solution

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The development of a novel hybrid adsorbent material Gum ghatti-graft-poly(2-acrylamido-2-methylpropane sulfonic acid)containing magnetite nanoparticles is presented. The nanocomposite(Ggh-g-PAMPS/Fe_3O_4) is characterized usingFTIR, XRD, TGA, SEM, VSM and BET techniques. The presence of magnetite nanoparticles imparted super-paramagnetic nature to the adsorbent material which helps in separation of the material after use with an external magnet. The

porousnature and large surface area of the nanocomposite is highly favorable for removal of dye molecules by adsorption.The Ggh-g-PAMPS/Fe_3O_4 exhibited maximum adsorption capacity of 403.2 and 427.8 mgg^{-1} for Rhodamine 6G and Methylene Blue respectivelyfrom a solution of concentration 500 mgL^{-1}. The adsorption of these dyes was evaluated by four different isotherm and kinetic models. The adsorption data were found to best fit Freundlich isotherm model and pseudo second order kinetic model.Negative $\Delta G°$ and positive $\Delta H°$ values confirmed the spontaneous and endothermic nature of adsorption. Further,desorption experiments affirmed the excellentregenerative efficacy of the nanocomposite, making it an ideal material for absorptive removal of cationic dyes from water bodiescontaminated with dye containing industrial effluents.

PO-CYSA-08 : Self-aggregation of Methylene Blue in Mixed Aqueous Organic Amine Media Leading to Formation of Red Methylene Blue Aggregates: Possible Application of using Methylene Blue for Detection of the Presence of Organic Amines

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The aggregational behaviour of Methylene Blue (MB) a thiazine dye in presence of homologues of ethylamine and ethanolamines has been investigated spectrophotometrically. The dimerization constant (K_D) of the dye in aqueous and aqueous organic amine media was computed using non-linear least square method. Geometry of the aggregates was analyzed in the light of exciton theory by evaluating the twist angles (θ_1) and tilt angle (θ_2) of the MB molecules in the dimeric species. A gradual change in colour from blue to red form of MB in presence of the amine with time was observed. The Rate constants (k) were evaluated to study the kinetics of the change. Glutaraldehyde or formaldehyde crossed linked chitosan gel can be succesfully used to check the change in colour from blue form to red form of MB. Flow behavior, triple test points, swelling behavior and swelling ratio of the crossed linked were also studied. IR spectra of the gel suggest that the dye molecules do not show any covalent interaction with the gel network and confirms that MB molecules may be incorporated in the pores of the gel network. Development and preparation of sensor for organic amines were done using gelatin gel evenly coated in glass slides.

PO-CYSA-09 : Near Unity Photoluminescence Quantum Yield of Green-emitting Graded Alloy Core/ Shell 'Giant' Quantum Dots by Z-type Ligand Passivation

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Due to outstanding optical properties, green-emitting graded-alloy core/shell 'giant' quantum can be utilized for different optoelectronic applications. But often, defects arise upon nonuniform growth of the shell. These surface defects limits the photoluminescence quantum yield (PLQY), lifetime, and stability of the green-emitting graded alloy core/shell 'giant' quantum dots. Therefore, to overcome these surface traps, the graded alloy core/shell g-QDs were passivated with z-type ligands ($ZnCl_2$, $CdCl_2$, and $MgCl_2$). The change in the PLQY, lifetime, and photoluminescence emission confirmed that the z-type ligands are passivating the trap states of g-QDs by bonding with an unsaturated chalcogenide atom on the surface, and this was confirmed by X-ray photoelectron spectroscopy. All three cases (treated with $ZnCl_2$, $CdCl_2$, and $MgCl_2$) were shown outstanding enhancement in the photoluminescence quantum yield. Fascinatingly, the $ZnCl_2$-treated g-QDs observed maximum enhancement in the PLQY from 62% to unity. Furthermore, the photostability test was performed under continuous UV light irradiation for 24 hours, which clearly shows superior photostability. Moreover, the temperature-dependent stability of untreated and treated was conducted from 10 to 90 °C. Furthermore, the green-emitting down conversion LED was fabricated by utilizing $ZnCl_2$-treated g-QDs, which shows great potential for display application.

PO-CYSA-10 : Preliminary Study on the Possible use of Aloe Vera Gel as an Adsorbent for Cu(ll)and Fe(ll) Ion from Aqueous Solutions

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Hydrogels of Aloe Vera gel have been extracted and prepared from the leaves of aloe vera plant and characterized by FTIR, XRD, SEM, AFM, etc. Preliminary studies were conducted to examine if the Aloe vera gels thus prepared can be effectively used to adsorb some metal ions like iron, copper, etc. from aqueous solution. The adsorption study was carried out using spectroscopic methods like AAS, UV-Visible, etc.The extent of adsorption of the metal ions was found to

be dependent on the adsorbent dose, sorbate concentration, contact time, etc. With an adsorbent dose of 2g (1.6 cm x 1.6 cm x 0.7cm) and metal ion concentration of $2.2x10^{-5}$ M for Cu (II) or $3.4x10^{-5}$ M for Fe (II) at 25°C, a maximum adsorption of about 76% of Cu(II) was observed in about 120 h time while it is only about 12% for Fe(II) in about 72 h. The adsorption amount may however be increased by increasing in the adsorbent dose. The release of the adsorbed metal ions was studied by dispersing the metal ion adsorbed aloe vera gels in aqueous media after which the gel may again be used for adsorption studies. The present study showed that there was no significant change in the adsorption behaviour of the gel at least during the five adsorption-desorption cycles. It was observed that the adsorption process under study was best described by the Langmuir model.The preliminary investigations showed that the properly prepared aloe vera gels may be effectively used for removal of metal ions like Cu(II) or Fe(II) from solution.

PO-CYSA-11 : W@$LaFeO_3$/MWCNT Thin Films for Solar Hydrogen Generation

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There is an urgent need for an environmentally friendly method for hydrogen production such as solar water splitting to produce green hydrogen. Thus, an intensive search for a novel semiconductor material is been carried out all over the world.

Perovskite like metal oxides have high activity, excellent compositional and structural flexibility, superior sunlight absorption capability and precise control of band gaps and band edges. Among them, Lanthanum Iron Oxide ($LaFeO_3$) is an attractive candidate for the desired application because of its stability, environmental friendliness and the relatively high earth abundance of the constituent elements. The strategy adopted is partial change in concentration of La ions through a similar oxidation state and ionic radius which can disturb the valence of the perovskite matrix, generate oxygen vacancies, and enhance the mobility of surface-adsorbed lattice oxygen.

Thus, we have synthesized $LaFeO_3$ loaded with analogous Tungsten (W) ion through a citric sol-gel route. We then incorporated MWCNTs to improve the overall conductivity of the system. Systematic investigation of the physicochemical properties, crystal structure, band gap, and texture properties of the as synthesized perovskites were

performed. The resultant system displayed an improved redox behaviour under environmental conditions because of an increase in majority carrier concentration.

PO-01 : Synthesis and Characterization of Chitosan-g-PAMPS Graft Copolymer and its Applications in Drug Delivery of Sodium Diclofenac

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Chitosan-g-AMPS was synthesized using free radical initiators and characterized by FTIR, PXRD, SEM and TGA analysis. The 2-acrylamido-2-methyl-1-propane sulphonic acid (AMPS) concentration has been optimized from 3.5 x 10^{-2} to 19.5 x 10^{-2} mol $dm^{-3}$to get maximum grafting of AMPS monomer onto chitosan. The FTIR spectral analysis proves the successful grafting and the PXRD spectra reveals the increase in crystallinity due to grafting of AMPS. SEM images exposed that smooth form of chitosan was changed into porous and fluffy structure after grafting. The cumulative drug diclofenac sodium release was studied in colonic medium. Delivery of drug was 13% and 55% during 4 h of assay in gastro-enteric and colonic system respectively and chitosan was dissolved about 53% and 65% in gastro-enteric and colonic system, respectively. The drug release behavior depends on the pH of medium as well as on the nature of beads, and AMPS grafted chitosan shows slow release of diclofenac sodium.

PO-02 : Synthesis of ABO_3 Type Perovskite Crystal Structure

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Energy is required in every aspect of our everyday life. The needs of humans are growing with every passing and with are increasing our need of energy. Unfortunately, the energy resources available to humans are mostly finite energy sources, that is, they provide energy for a limited amount of time and they cannot be reused. One solution of this problem is to produce renewable energy. After successful

production of renewable energy, the next step is to find ways to harness and store this energy. This research aims to study the energy storage capacity of a perovskite crystal. The structural, transport, energy storing magnetic properties of $LaCoO_3$ with Sr and Nb substitution are highlighted. The structural properties of the crystal were analysed using X-ray diffraction and the data received from the spectroscopy was analysed to obtain the values of dielectric constant, conductivity etc. The energy storage capacity of the perovskite crystal was determined. This research is aligned with one of the most crucial thrust areas identified in the sigma six qualities, values and attributes, and the UN sustainable goals which is Renewable Energy.

PO-03 : Quantum Chemical And Molecular Dynamic Studies on 5-Hydroxy Methyl Uracil

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The quantum chemical properties of 5-hydroxymethyluracil were explored by Density Functional Theory technique using B3LYP method with 6-311++G(d,p) basis set. The optimal structure was obtained that serves as foundation for other calculations. Orca programmer used to calculate thermodynamic parameters such as free energy, entropy and enthalpy at various temperatures. In the excited state, maps of hole and electron density distribution were generated using various solvents. The bio-active probability of the chemical was theoretically proven by computing the electrophilicity index. Molecular docking is used to calculate and confirm protein-ligand interactions. The title molecule was also used in medicinal fields and for drug development.

PO-04 : Harnessing the Novelty of Ionic Liquids: Ionic Liquid-controlled Dye Aggregation

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Ionic liquids (ILs) are salts that remain liquid over a wide range of temperature including room temperature. One can fine tune physical, chemical, and biological properties of these salts simply by changing the nature of cation, anion as well as side chains attached to them.ILs consists of ions only and hence these offer ionic environment to probe molecules. Many chemical processes demonstrate effects and outcomes that are very different within a milieu constituted of only ions as opposed to molecular solvents.ILs are known to show

anomalous behaviour as far as aggregation within them is concerned. In this talk we report unusual aggregation behaviour of dyes which interestingly depends on the identity of the ILs. Specifically, we found that dyes are triggered to form fluorescent H-aggregates by addition of 2 wt% 1 M aqueous NaOH to ILs 1-alkyl-3-methylimidazolium tetrafluoroborate ($[C_n mim][BF_4]$), whereas addition of 2 wt% 1 M aqueous NaOH to the same dye solutions in ILs with other anions results in J-aggregation. H-aggregation is unambiguously demonstrated to be specific to the $[BF_4]$ -based ILs. We propose the different hydrolytic properties of BF_4as compared to other anions in ILs to be the reason for this dramatic difference in IL-dependent dye aggregation.

PO-05 : Electrochemical Reduction of Mixed Complexes of Cu(II) With Some Substituted Malonamic Acid and Carboxylic Acid at D.M.E

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The mixed ligand complexes of Cu^{2+} with Succinate and 1-Naphthyl Malonamate, 2-(ethoxy) Phenyl Malonamate and 4-(methyl) Phenyl Malonamate ligands have been investigated polarographically at 25°C, μ= 2.0(KNO_3) and pH = 6.0. The reduction of all the systems involve a two electron reversible diffusion controlled wave. Schaap and McMasters method has been used to determine the composition and stability constant of mixed systems. Which were found to be more stable than simple systems.

PO-06 : String Operations on SMILES Notations : A Potent Data Encoding Resource

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Unique similarities are existing between chemistry and computer science. In chemical science, the representation of a molecule can be obtained through the repetition of symbols of elements. In computer science, sequences of instructions or programs were made through the repetition of specific commands and syntaxes. SMILES Notations provides an interface through which experts from both chemical science and computer science can interact with each other. The algorithm of SMILES Notations converts any molecular structure into a string made up of a set of alphabet, numbers, and parentheses. The advantage it provides is a reduction of space. While conventional image files and ChemDraw cdx files occupy space in megabytes to tens of kilobytes,

the smiles file occupies just a single kilobyte. Therefore, experts from machine learning are preferring to use SMILES Notation in the generation of databases and performing data mining. However, in this regard, a concern about the specificity of SMILES Notation to the respective chemical structure has been raised. Further, would SMILES strings be flexible enough to generate multiple molecule structures through applications of string operations?The present study explores these aspects. The result will improve the understanding of SMILES Notation-based data encoding.

PO-07 : Study of Structural qnd Optical Properties of Graphene Oxide Synthesized by Modified Hummer's Method

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Graphene oxide (GO) has been synthesized using Modified Hummer's method in such a way that crystalline phase GO has been obtained in powder form with average interlayer spacing of 0.82nm corresponding to (001) plane at $2\theta = 11.2°$. Structural properties have been analyzed by X-Ray Diffraction, Fourier Transform Infrared (FTIR) and Ramananalysis. FTIR analysis showed the presence of different oxygen containing functional groups which demonstrates the dispersive nature of GO in most of the organic as well as inorganic solvents. Raman analysis has been done to investigate the quality of the GO. The presence of graphitic (G) band and disorder (D) band at 1353 cm^{-1} and 1599 cm^{-1} respectively confirms the formation of GO. Further, optical properties have been investigated with UV-Vis and Photoluminescence (PL) spectroscopy. GO exhibited absorption in near visible region at 300 nm and broad PL with distinct five peaks at 360 nm, 443 nm, 480 nm, 690nm and 715 nm. Band-gap of the prepared GO and peaks of PL have been discussed rigorously. Also, Carbon hybridization states have been discussed from the data of Raman spectroscopy.

PO-08 : A Study of Substituent effects in Oxidation Kinetics between Anilines and Iridium Hexachloride (IV) : An Experimental and Computational Analysis

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Substituents effects in the oxidation kinetics of ortho and para substituted anilines with hexachloroiridate (IV) in aqueous perchloric

acid have been studied. The reaction is indicated first order dependence with respect to both reactants. Reaction rates accelerated with the introduction of electron-releasing groups and retarded with electron-withdrawing groups which are elucidated by Hammett's theory of linear free energy relationship. Hammett's reaction constant (ρ) has negative ($\rho < 0$) value. Furtherance, an increase in temperature increased the reaction constant (ρ). Various thermodynamic parameters have been reported and discussed the validity of isokinetic relationship. Isokinetic temperatures (β) observed from Vonthoff's plot, Compensation plot and Arrhenius plotare comparable. Observed β value from Exner's plot is above the experimental temperature range (303-323 K), indicating that the enthalpy factors are probably more important in controlling the reaction. Based on the kinetic results, a suitable mechanism has been proposed. To further support our proposed mechanism, density functional theory (DFT) computations at M06/6-311*G are also performingto predict the same reactivity trend as shown by the kinetics experiments.

PO-09 : How Kosmotropic and Chaotropic Osmolytes Perturb the Properties of an Aqueous Solution of a Pluronic Block Copolymer?

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Poloxamer 407 (P-407) has two distinct microenvironments: the interior core formed by the PPG unit, and the exterior shell formed by the PEG unit. Two fluorescent molecules Coumarin-153 (C-153) and 8-anilino-l-naphthalene sulfonic acid (ANS) of contrasting nature were used to characterize and probe the water dynamics in the core and corona region of the copolymer by means of spectroscopic techniques. Kosmotropic (betaine, sarcosine) and chaotropic (urea) known to perturb the water structure were added to aqueous solutions of P-407.[1] Our studies reveal that addition of kosmotropes decrease the critical micelle temperature (CMT) of the copolymer whereas, the chaotropic osmolyte increase the CMT.[2] Steady state studies reveal that addition of the osmolytes to the copolymer increases the polarity of the micelle formed, and hence the red shift in the ANS absorbance maxima. FTIR spectroscopy reveals that kosmotropes interacts with the PEG moiety of the copolymer whereas, the chaotrope interacts with both the PEG and PPG moiety of the copolymer. Solvent and rotational relaxation studies produced less changes upon addition of the kosmotropes whereas, a considerable change was observed in the presence of the chaotrope.

PO-10 : Density Functional Theory and Molecular Dynamic Studies on Pyridine-pyrozole-pyridine

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DFT calculation of Pyridine-pyrozole-pyridinecomputationally were determined using B3LYP method with 6-311++G(d,p) basis set. The optimal structure was obtained for other calculations like bond length, bond angle etc. Orca programme used to calculate thermodynamic parameters such as free energy, entropy and enthalpy at various temperatures. The bio-active probability of the chemical was theoretically proven by computing the electrophilicity index. Molecular docking is used to calculate and confirm protein-ligand interactions. The PPP molecule was also used in medicinal fields and for drug development.

PO-11 : Kinetic Study of Aquation of Cobalt(II) Terpyridine in the Waterpools of AOT/Heptane Reverse Micelles

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The surfactant aggregates formed spontaneously in organic solvents are called reverse or inverted micelles and water is solubilised in the core of reverse micelles. The water solubilised in the reverse micelles exhibits different properties compared to conventional aqueous medium. For eg.,the dielectric constant of the solubilized water is much less than bulk water and the solubilisedwater is highly nucleophilic compared to bulk water. These properties are dependent on a W parameter, { W =$[H_2O]/[AOT]$}. As the value of Wincreases, the properties approach that of ordinary water. In the case of AOT reverse micelles whenWis greater than 12the special properties of solubilised water reach that of bulk water.Since the solubilised water exhibits different properties, the rate of reactions are expected to change in this medium. In the present work a kinetic study of aquation of cobalt(II) Terpyridine complex has been carried out in AOT/Heptane reverse micelles. The reaction is markedly accelerated in the presence of AOT/Heptane reverse micelles compared to aqueous medium [The first order rate constant, k_1, 31.5 X 10^{-3} sec^{-1} at W = 3.33, [AOT] =0.3 mol dm^{-3}while the reaction is infinitely slow and incomplete in aqueous medium].Favourable partitioning of terpyridine ligand into the organic

phase is the reason for the high acceleration of rate along with the special properties mentioned above.The study of the reaction has been carried out at different W values and at different surfactant concentrations. The rate of the reaction decreases with increasing W at constant [AOT] and increases linearly with increase in [AOT] at constant W. The effect of surfactant concentration has been explained on the basis of Berezin pseudo phase model.

PO-12 : Nature Inspired Extreme Wettability Surfaces for Autonomous Drop Motion and Sensing

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Motion of water drops on surfaces such as window and car windshield can be observed daily but such phenomena have industrial applications such as in coatings, paintings, printing and for microfluidic systems. The drop motions are responsible for self-cleaning ability of insect's wings, bird feathers, and plant leaves. The surface wettability plays an inherent role in maintaining the self-cleaning behaviour of these natural materials. Nature developed these surfaces by creating a unique combination of surface chemistry and surface topology. Mimicking such materials has only been possible by studying the surfaces in detail and thus various man-made materials have been fabricated. Recently, the surface which show least adhesion to droplets due to negligible friction (very low contact angle hysteresis) have been fabricated and evaluated for drop motion. The aqueous and non-aqueous binary drops demonstrated autonomous drop motion and such motility provides an opportunity for sensing a nearby drop. The surface modification and wetting characterization was performed to understand the mechanism responsible for autonomous drop motion and sensing.

PO-13 : A Detailed Investigation of the Physicochemical Properties of Imidazolium and Phosphonium Ionic Liquids

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Ionic liquids (ILs) are gaining immense popularity currently as designer solvents owing to fact that their physicochemical properties can be conveniently tuned due the large number of combinations that are possible with its two components viz, the bulky organic cation and organic/inorganic anion. The selection of an IL for specific application demands an indepth understanding of the intermolecular interaction present therein. This can be achieved by studying their physicochemical

properties including density, viscosity, speed of sound, surface tension, ionic conductivity, refractive index, heat capacity, osmotic coefficient, activity coefficient, etc. The importance of the study of these physicochemical properties has been demonstrated by explaining the experimental observations perfomed on the aqueous systems of [EMIM][$EtSO_4$], [EMIM][$MeSO_4$], [EMIM][Tos] and [(iBu)3MP][Tos], [MMIM][$MeSO_4$] and [TBMP][$MeSO_4$]. The application of McMillan-Mayer theory and Pitzer model have shown water structure breaking nature of [EMIM][$EtSO_4$] and [EMIM][$MeSO_4$] whereas [EMIM][Tos] and [(iBu)3MP][Tos] show hydrophobic nature.

PO-14 : Electrochemical Impedance Aptasensor for PDGF-BB based on Succinic Acid Capped Selenomolybdate Nanodots/Antimonene Nanohybrid

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The motivation of present work was to design a unique bioelectrode for quantitative analysis of potential cancer biomarker, platelet derived growth factor-BB (PDGF-BB), which can be used for early detection of cancer. We report succinic acid capped selenomolybdate polyoxometalate nanodots, POM (SA), decorated antimonene hybrid film on glassy carbon as a suitable bioelectrode. Antimonene nanosheets, synthesized by chemical exfoliation of antimony provided large surface area for the symmetric dispersal of POM(SA) nanodots resulting in site-speciûc covalent immobilization of aptamer, PDGF-BB. A comprehensive electrochemical immunosensing investigation was performed on the electrode for sensing of target antigen, Ag-PDGF-BB. The sensitivity, selectivity, and reproducibility of bioelectrode were investigated using best-fit equivalent circuit model that fits the impedance response. The bioelectrode showed a linear impedimetric response in broad range of Ag-PDGF-BB (10 pM to 100 nM in pH 7.4 PBS) with limit of detection of 3.5 pM and sensitivity of 80 Ù cm^2 per decade. The response sensitivity of POM(SA)/ antimonene hybrid based bioelectrode towards PDGF-BB is approximated to be ~ 1.8 fold increased than that of only POM(SA) modified bioelectrode. The dissociation constant of immunoreaction between aptamer functionalized bioelectrode and target Ag-PDGF-BB is 76 nM, indicating high binding affinity between aptamer PDGF-BB and target Ag-PDGF-BB on the electrode surface.

PO-15 : Electrochemical Effect and Parametric Studies of Lead Carbonates and Cobalt Carbonate Composite Membranes

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This work is for comparative studies of Lead Carbonate and Cobalt Carbonate composite membrane on parchment paper this was prepared by co-precipitation method. The membrane was found to be crystalline in nature with consistent arrangement of particles and no indication of visible cracks. The prepared membranes were characterized by SEM, Membrane potential, Bi-ionic potential will be measured by using various combinations of 1:1 electrolyte at equal concentration on two sides of membrane or at a fixed concentration of one of the electrolyte and changing the concentration of the other electrolytes by setting up an electrochemical cell. The electrical potentials measured across the composite membrane in contact with univalent electrolytes (KCl, NaCl and LiCl), have been found to increase with decrease in concentrations. Thus the membrane was found to be cation-selective. Transport properties of developed membranes may be utilized for the efficient desalination of saline water and more importantly demineralization process. The antibacterial study of this composite membrane shows good results for killing the disease causing bacteria along with waste water treatment.

PO-16 : Physico-Chemical Studies on Stearate of Some Metals in Mixed Organic Solvents

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The CMC (critical micelle concentration) of Terbium and Dysprosium (Stearate) in a mixture of benzene and methanol (50:50 v/v) was determined from viscosity and conductivity measurements. The result shows that the CMC decreases with increasing atomic number of metal ion. The degree of dissociation and dissociation constant data show that the Terbium and Dysprosium Stearate behave as a simple electrolyte in the solution. The results of viscosity measurements have been explained on the basis of the equation proposed by Einstein, Moulik, Vand and Jones-Dole. The values of the molar volume are in close agreement with Vand's and Einstein's equation.

PO-17 : Self-Assembly of Bile Salts – Surfactant Mixed Aggregates in Aqueous Medium

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The bile salts are anionic bioamphiphiles that play an important role in fat solubilization in digestion. The self-assembly of bile salts emphasizing their mixed smart aggregates with a variety of ionic and nonionic amphiphiles has been examined. They self-assemble to form micelles in water similar to conventional surfactants but with a significant difference. Sodium deoxycholate (NaDC) and sodium cholate (NaC) are among the most investigated bile salts. We have examined the effect of bile salts on nonionic surfactants (TX-100, Block copolymers), cationic gemini surfactants and amphiphilic ionic liquids. The dramatic opposite behaviour of bile salts with these surfactants can be explained from their ionic nature; smaller mixed aggregates are formed with nonionic surfactants due to introduction of charge in the system while larger aggregates are formed with ionic surfactants due to the oppositely charged system. The mixed aggregates possess Ph-sensitivity as bile salts have carboxylate ($-COO^-$) group in theiroleculear structure. The extent of protonation of bile salts strongly depends upon the pH of solution so the size of mixed aggregates can easily be tuned simply by changing the Ph of solution. Different morphological transitions are observed which are confirmed by dynamic light scattering small-angle neutron scattering experiments.

PO-18 : Thermal Stability Studies on Some Metal Carboxylates of Rubber Seed Oil

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Alkaline earth metal carboxylates of Rubber Seed Oil (RSO) have been prepared by metathesis in aqueous alcohol solution have been carried out. Thermal stability of metal carboxylates were studied in the temperature range 60-600! under Nitrogen atmosphere using thermogravimetric analyzer (TGA). The thermal stability of alkaline earth metal carboxylates were evaluated in terms of temperature at which various weight of decomposition have been attained and data of weight loss at the initial stage of decomposition. The results show that metal carboxylates of Rubber Seed Oil (RSO) could be beneficial in various industries.

PO-19 : Photovoltaic Performance of Sio Thin Film and Its Applications

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Photovoltaic thin film is outstanding equipment supplementary to existing silicon mono oxide films. For the earlier few decades, the photovoltaic (PV) market was dominated by silicon-based photovoltaic cell. However, it will conversion to PV expertise based on flexible PV cell recently because of growing require for devices with high flexibility, lightweight, conformability, and bend ability. We highlighted the assorted photovoltaic cell SiO based films developed using the promising technology are introduced. We focused on SiO material for photovoltaic cell processing techniques, which is well-known for its extremely desirable coating material and excellent environmental stability. Its Dielectric properties can be achieved by proper selection of SiO film thickness and we have discussed about the temperature coefficient of SiO photovoltaic panel fabricated by various researchers. At the end of the review we have provide the applications of silicon mono oxide in photovoltaic cell.

PP-CYSA-01 : Monitoring the Conformational Behavior of PNIPAM-b-PACMO Polymer in a Medium Assisted by Ionic Liquid-Modified Gold Nanoparticles

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The subject of nanomaterials has created immense interest in the field of science and technology. Among various nanoparticles, metal nanoparticleshave remarkable physiochemical properties thereby widened the area of intensiveresearch. Particularly gold nanoparticles (AuNPs) offer various fascinating applications in many fields such as biosensing, catalysis, nanomaterial science etc. Moreover, ionicliquid-modifiedgold nanoparticles(IL-AuNPs) using different ILs, which are having common cation 1-ethyl-3-methyl-imidazolium (EMIM) and variable anions (CH_3OSO_3), ($CH_3CH_2OSO_3^-$) provide an attractive platform to tailor the properties of macromolecules such as proteins and thermoresponsive polymers. The unique structural and molecular attributes of thermoresponsive blockcopolymerare dominated in the field of advanced research. Herein, in the present study we have synthesized the blockcopolymer poly(N-isopropylacrylamide)-b-poly(acryloyl morpholine) (PNIPAM-b-PACMO) by RAFT

polymerization. No study reports the conformational changes of PNIPAM-b-PACMO in a medium provided by ionic liquid-modified gold nanoparticles (IL-AuNPs). Various biophysical techniques such as UV-visible spectroscopy, fluorescence spectroscopy and dynamic light scattering (DLS) are utilized to examine the interaction of ILs-AuNPs with PNIPAM-b-PACMO. Introducing IL-AuNPs with the polymeric solution promotes the coil-conformation of the polymer to higher temperature than the lower critical solution temperature (LCST) of the aqueous PNIPAM-b-PACMO. The current study can pave attention in the field of biomedical science specifically drug-delivery.

PP-CYSA-02 : Organometallic Astrochemistry : A New Frontier in Chemical Science

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The discovery of the simplest metallocene molecule, ferrocene, back in 1951 started a new branch of chemical science known as organometallic chemistry. Since then, verities of organometallic molecules have been discovered. Because of their unique structure, these organometallics play a vital role in different chemical reactions that start from catalytic reactions, charge transfer processes, and polymer reactions. The recent discovery of cyclopentadiene in the Interstellar Medium (ISM) has drawn attention to the astrochemistinvestigating organometallics' role in ISM chemistry. To understand the fate of organometallics in the extreme interstellar conditions, we subjected ferrocene to ~5.6 Mach (M) shock commensurate with conditions encountered in the ISM, leading to a temperature rise to 7300 K within 2 ms. Analysis of the post-shock residue showed the presence of a α-Fe and Fe_3C composite that responded to an external magnetic field. These results indicate that non-magnetic dust composed of molecules containing transition metals undergoing shock processing in the ISM can dissociate and synthesize dust that is then magnetic. In this meeting, we will discuss the importance of such results in interstellar polarization and its implications for cometary chemistry.

PP-CYSA-03 : Partitioning of DNA using Ionic Liquid-based Aqueous Biphasic System

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The separation and purification of nucleic acid is a widely studied

field as it has paramount importance. The disadvantages of conventional extraction methods include toxicity, complexity and time consumption[1]. The search for an alternative method for DNA extraction studies has led to ionic liquid (IL) based aqueous biphasic systemswhich is a benign method for biomolecule extraction[2]. The present work is focused on developing an ABS constituting ammonium-based ionic liquids (ILs) and phosphate buffer (K_2HPO_4-KH_2PO_4) for the partitioning of DNA. The optimization of cationic structure of the IL was done thoroughly by studying the influence of the functional groups in ABS formation as well as DNA partitioning. Further, the optimization of the partitioning was carried out with the ABS showing maximum extraction. The driving force behind the partitioningwasinvestigated through techniques such as FT-IR and circular dichroism spectra[3].Additionally, we have started the optimization of the anionic structure with the efficient cations and the extraction of DNA from the real sample using the optimized IL will be conducted in the future.

PP-CYSA-04 : Investigations on Self-Assembly and Super-Activity of Cytochrome-c in the Mixed Micelle System Comprising of Imidazolium-based Surface-Active Ionic Liquid and 14-2-14 Gemini Surfactant in the Aqueous Medium

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Ionic Liquids (ILs) are the substances comprised of ions only having a melting temperature below 100 °C. ILs having alkyl chain length more than 6 show surface activity like conventional surfactant and are called as Surface Active Ionic Liquids (SAILs). Herein, the self- assembly of imidazolium based ester functionalised SAIL $[C_{16}Emim]$ [Cl] in the presence of Gemini surfactant 14-2-14 has been investigated over the whole mole fraction range of Gemini surfactant. Theoretical models such as clint equation, motomura theory and Rubingh theory have been used to calculate the ideal critical micelle concentration (*cmc*) values, micellar mole fraction (x_m) and type of interactions i.e., synergistic or repulsive in the mixed micelle systems, respectively. Conductometric titration, Fluorescence and Surface tension measurements have been employed to investigate the cmc values in the bulk and at air-water interface, respectively. Isothermal Titrations Calorimetry (ITC) has been employer to quantify the thermodynamic aspects of micellization. Dynamic Light Scattering (DLS) and Zeta-

potential measurements have been used to have insights about the size and charge at the stern layer of the self- assembled structures. To investigate the morphology of the self-assembled systems, Small Angle Neutron Scattering (SANS) has been used. Further, self- assembled structures have been used as micro reactor to host and imparting super-activity to cytochrome-c (cyt-c). The kinetic study of the enzymatic reaction shows its dependence upon the nature of micelles formed. It is believed that the present work would provide basic understanding about the enzymatic activity in mixed micellar systems.

PP-CYSA-05 : Micellar Interaction of Sodium Cholate/Sodium Deoxycholate with Cationic Dihexadecyl Dimethyl Ammonium Bromide Surfactant in Anionic-Cationic Mixed Surfactant Systems

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Surface tension measurements of aqueous solution as a function of total concentration under standard conditions were used to study mixed anionic Sodium Cholate (NaC)/Sodium deoxycholate (NaDC) and cationic Dihexadecyl dimethyl Ammonium Bromide surfactant systems at different molar ratios. Clint, Rubingh, Maeda, and Rosen determined critical micelle concentration (CMC), surface excess concentration (τ_{max}), minimum area per molecule (A_{min}), interaction parameter of mixed micelle and adsorption monolayer (β^m, β^o), and thermodynamic and micellar properties. The results are discussed in terms of the structural characteristics and chain of double tail cationic surfactant and the presence of -OH in NaC/NaDC. In the current study, we have discovered that binary systems composed of the cationic Dihexadecyl dimethyl ammonium bromide and the anionic NaC/NaDC exhibit strong synergism and deviation from ideal behaviour. In pure water, cationic and anionic mixtures can spontaneously form vesicles, and synergism results in rich phase behaviour.

PP-CYSA-06 : Micellization Studies of Biocompatible Thermo-Responsive Graft Copolymers Containing ε-Caprolactam : A DLS and SANS Study

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Polymeric materials respond to external stimuli or changes in their surroundings. The biocompatibility, complexation ability, and

low toxicity of Poly(N-vinyl caprolactam) PNVCL, a thermosensitive polymer with an LCST at 37°C, makes it a promising candidate for use in medicine. Whereas, PCL polymer segments provide many benefits due to their biocompatibility, biodegradability, and the fact that they break down into 6-hydroxyhexanoic acid, a metabolite found in humans. However, PCL's high crystallinity limits its biodegradability and makes it incompatible with soft tissues. By blending PCL with different polymers or developing copolymers based on PCL, these issues can be addressed. Herein, we provide a micellization research of PCL-g-PNVCL polymers with diverse chain lengths in the presence of the anionic surfactant sodium dodecyl sulphate (SDS), as well as a study of PCL-g-P(NVCL-co-NVP) polymers at different temperatures. As revealed by the data obtained using SANS technique it is observed that due to the formation of micelles with thicker shells by graft copolymers with longer side chains,the micellar diameters of PCL-g-PNVCL graft copolymers increase with the length of the PNVCL grafts. While NVP monomer addition has little influence on micellar size, it greatly enhances graft copolymer LCST.

PP-CYSA-07 : Physico-Chemical Investigation of Ethylene Glycol at Low Temperatures and its Astrophysical Implications

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Ethylene glycol (EG, $CH_2OH)_2$, is one of the molecules detected in comets[1] and in interstellar medium[2]. In terrestrial conditions, EG prevents liquid H_2O from turning into ice i.e., it acts as an anti-freeze. To understand its behavior at astrochemical conditions, in the present work, wedeposited EG and H_2O mixtures at UHV and cryogenic temperatures (10 K) using the Simulator for Astro-molecules at Low Temperature (SALT) setup housed at PRL, and investigated this ice in-situ using IR spectroscopy. Since the OH peaks of H_2O and EG overlap, we used D_2O instead of H_2O. Mixtures and layers of EG and D_2O were deposited at 10 K and warmed gradually to higher temperatures up to 300 K.

We observed that interaction between EG and D_2O molecules exists even at such extreme conditions which affect the morphology (phase change) and the sublimation temperature of D_2O. The EG and D_2O mixture were present even up to 235 K while the sublimation temperature of pure D_2O is only 182 K. That is, EG doesn't allow D_2O

to either crystallize (hence anti-crystallizer) or sublimate at its usual temperatures. This implies that water can be present on comets containing EG at temperatures higher than previously known.

PP-CYSA-08 : Nanomaterials for Wound Healing

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Wound care management relies mainly on advancement of new and effective wound dressing material. The major complications associated with wounds are:- (i) The lack of an appropriate environment to enables the cell migration, proliferation and angiogenesis; (ii) The microbial infection; (iii) Unstable and protracted inflammation. But most of the available dressings methods have not solved these problems completely. To hasten the healing of acute and chronic wounds nanotechnology offers a superlative approach by stimulating proper movement through the different healing phrases. In nanotechnology the small size network nanomaterials nanoscaffolds,nanofibres, and biomaterials are used for topical drug delivery for wound healing. The details of these types of materials will be discuss in my presentation

PP-CYSA-09 : Environmental Importance of Pervoskite Nanomaterials

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Perovskite nanocrystals are the class of semiconductor nanocrystals. They have anABX_3 composition where A = cesium , methylammonium, formamidinium B = leador tin and X = chloride, bromide and iodide.These crystals possess numerousunique attributes like defect tolerance, high quantum yield, fast rates of radioactivedecay and narrow emission line width in weak confinementwhich make them idealcandidates for a various optoelectronic applications. A type of compound with thedefined structure of perovskite (ABX_3) was observed to play important roles inphotocatalysisandphotovoltaics. Thesematerials whichcanbeusedasphotocatalystsfor water splitting reaction for hydrogen production and photo-degradation oforganic dyes in wastewater as well as for photoanodes in dye-sensitized solar cell sand light absorbers in perovskite-based solar cells for electricity generation will be discussed in detail.

PP-CYSA-10 : Deep Eutectic Solvents as Sustainable Media for Thermoresponsible Polymer Poly(N Vinyl Caprolactam)

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When compared to typical ionic liquids and organic solvents, deep eutectic solvents (DESs) are known as a "green" option due to their unique characteristics, solvents. This research looked at the impact of DESs that contained choline chloride (ChCl), Urea, betaine, proline as a hydrogen bond acceptor and lactic acid operate as hydrogen bond donors (HBD) on thethermoresponsive behavior of poly(N-vinylcaprolactam) (PVCL) is investigated using various techniques such as UV"visible spectroscopy, steady-state fluorescence and Fourier-transform infrared (FTIR) spectroscopy. Furthermore, the lower critical solution temperature (LCST) was investigated using temperature-dependent dynamic light scattering, demonstrating a decrease in the LCST of PVCL in the presence of DESs. To elucidate the aggregation behavior of PVCL in the microenvironment of DES, dynamic light scattering (DLS) is also performed. This Results shows that the involvement of eutectic solvents in altering hydrogen bonding between the polymers and surrounding water molecules.Disruption of the hydrogen bond interactions resulted in early hydrophobic collapse of the polymers. Moreover, this change depended on the nature of the HBA groups in the DESs. The essential spectroscopic insights of thermoresponsive polymers in environmentally friendly deep eutectic solvents are highlighted in this study for usage as pulsatile medication carriers is a possibility.

PP-CYSA-11 : Self-Assembly Modulation in Star Block Copolymers by Amphiphilic Diol : A Scattering Insight

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The present study offers a better insight into the alteration in the aggregation characteristics of block copolymers Tetronics® T1304 and T1307 induced by Surfynolâ 104 using scattering and with complementary physical property measurement viz. solution viscosity and cloud point. The hydrophobic interaction that drives C_{14} diol

molecules to penetrate inside copolymer micelles resulting in dehydration that lowered the CP and markedly increase in solution viscosity. Quite interestingly, initial lowering in CP is followed by sudden increase at higher level of solubilization. A significant increase in the apparent hydrodynamic diameter (D_h) divulges the growth of micelles which is equally supported by SANS measurements. The preferential partitioning of C_{14} diol into the copolymer micelles is the driving force for morphological changes from spherical to unilamellar vesicles. Also, the effect of temperature and NaCl was examined with the aim to observe various micellar transitions. The observed changes are clarified in terms of the hydrophobic interaction of C_{14} diol with Tetronic® micelles and HLB value of copolymers. This investigation sheds light on C_{14} diol induced dehydration causing the micelle growth for both Tetronics® with varied hydrophobicity. Such hydrophobic diol-induced spherical to vesicular transition is observed for the first time in Tetronicâ-diol mixed system.

PP-CYSA-12 : Influence of Amphiphilic Diol on Aggregation behaviour of TX-100 Micelles

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Aqueous solution behaviour of non-ionic surfactant namely, p-tert-octylphenoxy polyethylene (9.5) ether, Triton X-100 (abbreviated as TX-100) was examined in the presence of an amphiphilic hydrophobic diol (Surfynol® 104) using viscosity, cloud point (CP), dynamic light scattering (DLS) and small-angle neutron scattering (SANS) measurements. Surfynol® 104 is a hydrophobic diol with limited aqueous solubility. It decreases the CP, elevates the solution viscosity of TX-100 solutions and leads to morphological changes of TX-100 micelles. The micellar transition was further confirmed from scattering techniques (DLS and SANS). With the aim to achieve different micellar transitions, the salt and the temperature effects were additional parameters used. It was revealed that the ellipsoidal to rod-like micellar transition observed at higher level of solubilization of Surfynol® 104 can be drag down to room temperature by incorporation of NaCl. Temperature and NaCl-aided micellar transitions were equally supported from SANS analysis. The observed structural transitions are explained in terms of the hydrophobic interaction between TX-100 and Surfynol® 104.

PP-CYSA-13 : Self-Assembly of Polyoxyethylene Alkyl Ether-based Multi-Responsive Nonionic Amphiphile

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The self-assembly of a polyoxyethylene alkyl ether carboxylic acids based nonionic amphiphile known as Akypo® RO90 VG (hereafter written as Akypo) in aqueous medium using cloud point, solution viscosity and scattering measurements. The surfactant micellizes in aqueous media analogous to conventional surfactants but with some dissimilarity. The influence of external stimuli viz. temperature, pH and electrolyte has been examined to assess the response on the microstructural changes in micelles. SANS experiments provided the exact size and shape of micelles; the micellar growth proposed by high solution viscosity and hydrodynamic diameter (D_h) of micelles from DLS and further reinforced by SANS data. This further divulges that increase of temperature and addition of electrolyte persuade the ellipsoidal to worm-like micellar transition. Change of pH towards an alkaline medium favors the transformation of ellipsoidal micelles into spherical ones which can be correlated with deprotonation of carboxylic acid groups that results in increased solubility of Akypo. The current study authorizes how the size of Akypo micelles can effortlessly be amended in the presence of external stimuli to the desired extent.S

PP-CYSA-14 : Sythesis of 2D ZIF-67 and g-C3N4 composed Electrode for High Performance Pseudocapacitive Supercapacitors

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The finite stock of fossil fuels has drawn significant attention towards alternative energy generation (wind energy, solar energy) and storage technologies (batteries and supercapacitors). Supercapacitors are excellent energy storage devices owing to fast charging- discharging, great power density and long cycling life. Typical supercapacitive materials include carbon (graphene, carbon nanotubes etc.), MOFs and its derived metal oxides, metal sulphides, metal phosphides etc. But each class of materials have some flaws, so in order to mitigate the limitations, we synthesized a nanocomposite composed of 2D zeolitic imidazolate framework-67 (ZIF-67) and graphitic carbon nitride (g-C3N4) nanocomposite for high performance aqueous supercapacitors. This nanocomposite avails the advantage of both g-

C3N4 and 2D ZIF-67, resulting in wider potential range and more pseudocapacitance due to large surface area and porosity of 2D ZIF-67, electronically rich conjugated layered g-C3N4 and redox active cobalt metal centre. Structural properties of the nanocomposite were analysed through powder XRD, FTIR and Raman spectroscopy whereas nanolayered type morphological features were studied through FESEM, EDAX. Electrochemical investigations (CV, GCD, EIS) were performed in 1M KOH electrolyte, where maximum specific capacitance of 550 F g^{-1} was obtained at a current density of 3 A g^{-1}. The fabricated electrode also displays an excellent cycling stability of 81 % after 5000 GCD cycles @ 10 A g^{-1}. This study is useful for enhancing the charge storage properties of traditional MOFs and bare graphitic carbon nitride based materials for practical applications.

PP-01 : Sythesis of 2D ZIF-67 and g-C_3N_4 Composed Electrode for High Performance Pseudocapacitive Supercapacitors

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The finite stock of fossil fuels has drawn significant attention towards alternative energy generation(wind energy, solar energy) and storage technologies (batteries and supercapacitors). Supercapacitors are excellent energy storage devices owing to fast charging-discharging, great power density and long cycling life. Typical supercapacitive materials include carbon (graphene, carbon nanotubes etc.), MOFs and its derived metal oxides, metal sulphides, metal phosphides etc. But each class of materials have some flaws,so in order to mitigate the limitations, we synthesized a nanocomposite composed of 2D zeolitic imidazolate framework-67 (ZIF-67) and graphitic carbon nitride (g-C_3N_4) nanocomposite for high performance aqueous supercapacitors. This nanocompositeavails the advantage of both g-C_3N_4 and 2D ZIF-67, resulting in wider potential range and more pseudocapacitance due to large surface area and porosity of 2D ZIF-67, electronically rich conjugated layered g-$C_3N_4$and redox active cobalt metal centre. Structural properties of the nanocomposite were analysed through powder XRD,FTIR and Raman spectroscopy whereas nanolayered type morphological features were studied through FESEM, EDAX. Electrochemical investigations (CV, GCD, EIS) were performed in 1M KOH electrolyte, where maximum specific capacitance of 550 F $g^{-1}$was obtained at a current density of 3 A g^{-1}. The fabricated electrode also displays an excellent cycling stability of 81 % after 5000 GCD cycles @ 10 A g^{-1}. This study is useful for enhancing the charge storage

properties of traditional MOFs and bare graphitic carbonnitridebasedmaterials for practical applications.

PP-02 : Spectral, Thermal and Structural Studies of Chromium Soaps

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The physico-chemical characteristics of Chromium soaps, (Stearate and Myristate) in solid state were investigated by IR, X-ray diffraction and TGA measurements. The IR result revealed that the fatty acids exist in dimeric state through hydrogen bonding and soaps possess partial ionic character. The X-ray diffraction measurements were used to calculate the long spacing's. The result confirmed the double layer structure of chromium stearate and myristatesoaps. The TGA results revealed that decomposition reaction of these metal soaps is kinetically of zero order.

PP-03 : Preparation and Characterization of Water-Pluronic-Ionic Liquid based Microemulsions and their Application in Superactivity of Cytochrome-C

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Microemulsions (μEs)[1], comprising water as polar component, pluronic[2] (normal, L35 and reverse, 10R5) as surfactant and a hydrophobic ionic liquid (HIL)[3] as non-polar component have been prepared and characterized. Owing to higher surface activity, pluronics have promoted the formation of μEs without the use of co-surfactant. Thus, prepared μEs have been utilized as nano-reactors for the oxidation of guaiacol in the presence of Cytochrome-c (Cyt-c) at 15, 20, and 25 ^{o}C. A 3.2- and 1.3-fold increase in the rate of formation of product of enzymatic catalysis in direct μE (HIL-in-water) with reverse pluronic (10R5) is observed at 15 and 20 ^{o}C as compared to that in buffer. However, negligible enzymatic activity is observed in the direct μE formed by normal pluronic (L35). The catalytic activity of Cyt-c decreases in reverse μEs (water-in-HIL) as compared to direct μEs irrespective of the nature of pluronic used. The contrasting nature of nano-interfaces formed by pluronics in μEs and the extent of hydration of these nano-interfaces controlled by temperature exerts varying influence on the catalytic activity of Cyt-c.

PP-04 : Optoelectronic and Charge Transport Properties of Heteroacene Molecules using DFT/ TD-DFT Studies

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In this work, density functional theory (DFT) and time-dependent density function theory (TD-DFT) calculations have been performed to explore the optoelectronic properties of the different Heteroacene molecules. New challenges in specific properties of organic-ð-conjugated molecules as Thiophene and Furan molecules are of great significance since they have become the most promising materials for the organic electronic devices such as solar cells and organic electronic devices. We have studied the effect of different heteroatoms and different aromatic rings present on the peripheri of the Thiophene and Furan ringsalongwithitsfused structures. The Hole Extraction Potentials(HEP), Electron Extraction Potentials(EEP), Ionization Potentials (IP), Electron Affinities(EA), Frontier molecular orbitals (FMOs), Reorganization energy (hole and electron) and HOMO-LUMO Gap are calculated by Density functional theory(DFT) and the absorption and emissionpropertiesarealsocalculated by the Time Dependent-DFT methods. The computationalfindings indicate that these designed heteroacene molecules can show better organic electronic parameters and are suggested for high-performance charge-transport materials.

PP-05 : Fabrication of Bimetallic MOF Nanosheets for High Performance Asymmetric Supercapacitor

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Energy storage devices are serving as the backbone in today's electronic world. Among various energy storage devices, supercapacitors are unique owing to their high power density and long cycling life. Metal-organic frameworks, as emerging supercapacitive electrode material, have drawn extensive attention due to their high specific surface areas, tunable pore structure and diverse structures. However, monometallic MOFs have few drawbacks such as low electrical conductivity and chemical stability. To address this issue, bimetallic layered-structure MOF is designed. Herein, we have synthesized 2D MnCo-MOF nanosheets by ultrasonication method at room temperature. 2D MnCo-MOF nanosheets were formed by varying atomic ratio of Mn to Co ions. So formed nanosheets were analysed through various

structural (XRD, FTIR, BET) and morphological (FESEM, HRTEM) techniques. Electrochemical investigations were performed by CV, GCD and EIS techniques. MnCo-MOF nanosheets in 3M KOH electrolyte solution exhibited a maximum specific capacitance of 1320 F g^{-1} at 1 A g^{-1} with an atomic ratio of 1:2 of Mn to Co inMnCo-MOF. It also shows specific capacitance retention of 52.6% at 5 A g^{-1} current density. Such performance is attributed to the presence of short channels for electron transport and electrolyte ion diffusion provided by nanosheets and synergistic effect between Co and Mn ions.

PP-06 : Effect of Surfactant-Solvent Interactions on Catalytic Function and Structure of Cytochrome-c in Aqueous Mixtures of Deep Eutectic Solvents

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The search for a suitable and versatile environmentally benign solubilizing media is an area of active research in modern science and technology. Deep eutectic solvents (DESs)satisfy key criteria for a green solvent technology, including non-toxicity, biodegradability, sustainability, and low price. Because DESs have H-bonded nanostructure,it has recently been found that they display a sufficient thermodynamic driving force for the formation of micelles,although this appears to depend strongly upon the specific DES and surfactant used. Herein, we have expanded on this recent research to investigate the self-assembly of an anionic bio-based surfactant,sodium lauroylsarcosinate (SLS),in choline chloride:glycerol based DES and their water mixtures(10wt%, 30wt% and 50wt% of water). Different techniques such as fluorescence, isothermal titration calorimetry (ITC), dynamic light scattering (DLS) and ^{1}H-NMR have been used to gain insight into the self-aggregation behavior of SLS in aqueous mixtures of DESs to study the micellar properties. Such micellar organizations in DESs and their water mixtures can be of potential use in enzyme technology.Cytochrome-cdissolved in DES/water colloidal solutions has shown extremely high peroxidase activity.

PP-07 : Isentropic Compressibility Studies of Trimethylamine with Non-Polar Solvents

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Ultrasonic velocity and density trimethylamine + benzene/ toluene/ o- xylene binary mixture was measured at 308.15 K as function of

concentrations. The measured Ultrasonic velocity and density have been utilized to calculate excess Isentropic compressibility, excess molar volume, intermolecular free length and available volume. These values are reported as a function of mole fraction X_1 of trimethylamine βs^E vs X_1 and V^E vs X_1 plots are explained in terms of specific/non-specific interactions between solute and solvent molecules. Ultrasonic parameters are useful for the studies of physicochemical properties and molecular interactions of binary liquid mixtures. The intermolecular interactions and related structural changes affect the compressibility of the system which in turn produces corresponding variations in the ultrasonic velocity and its derived parameters.

PP-08 : Morphology Controlled Synthesis of Layered Double Hydroxides for Aqueous Supercapacitor

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Layered double hydroxide (LDHs) are 2D Lamellar materials having general formula$M_{1-x}^{2+}M_x^{3+}(OH)_2]A_{x/n}^{n-}.mH_2O$. Theseare widely used because of tunability of cations in host layers and exchangeability of anions without altering structure. Herein, zinc-cobalt layered double hydroxide nanosheets (ZnCo-LDH NS) have been facilely synthesized using 2-methylimidazole as bifunctional alkali source (OH^-) and morphology controlling reagent. Themechanisticstudy shows that weak organic base of 2-methylimidazole induced slow release of OH^-in water/ethanol is the controlling factor for the formation of the LDH nanosheets. ZnCo-LDH with different Zn/Co molar ratios were synthesized which have influence on the morphology and electrochemical performance. An interconnected nanosheets structure and the highest specific capacitance were achieved when the Zn/Co molar ratio is 1: 2 (Zn_1Co_2-LDH). Resulting Zn_1Co_2-LDH was characterized through XRD, FTIR,FESEM and electrochemical investigations (CV, GCD, EIS) were performed in 2 M KOH electrolyte which delivers a specific capacitance (457 Fg^{-1}), Low solution resistance (1.6 Ω) and High Phase angle(56.6°) which holds huge potential for practical application in energy conversion and storage fields.

PP-09 : V_2CT_x MXene/reduced Graphene Oxide Nanoribbon Composite Electrode for High Performance Aqueous Supercapacitors

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In the current electronic era, it is imperative to create affordable, environmentally safe, and dependable renewable energy storage

technologies. Supercapacitors are a viable energy source due to their rapid power delivery, long cycling stability, and quick charge/discharge process. MXenes, a family of 2D layered early transition metal carbides and/or carbonitrides, have been explored as a potential pseudocapacitive electrode material for supercapacitors and rechargeable batteries due to their exceptional physical, chemical, and electrochemical properties. However, inevitable self-restacking of MXene nanosheets limits the electrolyte ion accessibility, resulting in its limited charge storage performance. Herein, we report a V_2CT_x MXene/reduced Graphene Oxide Nanoribbon based nanohybrid (MXene/rGONR) as an electrode material for supercapacitors. Insertion of rGONR prevents the self-restacking of MXene nanosheets, resulting into a porous structure. The resulting MXene/rGONR composite delivers a specific capacitance value of 738 F g^{-1} at a current density of 2 A g^{-1}, which is ~ 1.5 times higher than that of V_2CT_x MXene. The MXene/rGONR||MXene/rGONR symmetric cell operates upto 1.0 V, delivering high energy/power density (55 W h kg^{-1} and 452 W kg^{-1}).

PP-10 : Metal-based Ionic Liquids : Effective Catalysts in Aqueous Media for the Selective Production of Vanillin from Alkali Lignin at Room Temperature

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Catalytic depolymerization of lignin to value-added compounds is receiving increasing interest as part of the circular bioeconomy. This work describes the selective depolymerization of alkali lignin to vanillin at room temperature using metal-based ionic liquids (MBILs) as catalysts in an aqueous medium. Using a reaction mixture of 20 wt% lignin, and 5 wt% [BMIM][$FeCl_4$] catalyst in water, 12.5 wt% of volatile aromatic products were obtained of which 105 mg g^{-1} of vanillin could be extracted with 85% selectively. For this first, we optimized various solvents (ionic liquids; ILs, deep eutectic solvents; DESs, conventional organic solvents, and water) as reaction media and found water to be the best for lignin depolymerization. Following this, we optimized the effect of time, temperature, and catalyst loading on lignin conversion, product yield, and selectivity. We found that high solubility of alkali lignin in the water results in alkali lignin hydrolysis and subsequent conversion by [BMIM][$FeCl_4$] via heterolytic cleavage of Cα–Cβ bond along with β-O-4 to facilitate higher vanillin production. The purity

and structure of extracted vanillin have been confirmed by GC-MS, 1H, and 13C NMR analysis, whereas lignin depolymerization has been confirmed from 1H NMR, 13C NMR, SEM, FT-IR, 2D-HSQC, TGA, and PXRD.

PP-11 : Thermodynamics and Conductometric Studies of Nickel Myristate and Palmitate in Mixed Organic Solvent

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Conductometric mearusements of the solutions of nickel myristate and palmitate in mixed organic solvent (benzene –methanol 50-50% v/v) have been employed at different temperature to determine the C.M.C (critical micelle concentration), limiting molar conductance, degree of dissociation and dissociation constant. The results show that these soaps behave as weak electrolyte in dilute solutions and the value of CMC increases with increase in temperature.

The dissociation and association can satisfactorily be explained in the light of phase separation model and the micellization process is predominate over dissociation process.

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NOTE

NOTE

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