Poster Presentations

Poster Presentation-01

Study of Metals Characterization of *Andrographis Paniculata* Plant of Khordha Region, Odisha, India

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Abstract: Today plant materials represent a substantial proportion of the global drug market today. More often plant based medicines are derived from many kinds of plant leaves, stems and roots are taken by rural and urban people without knowing its toxicity effects despite of having therapeutic significance. According to a recent estimate of WHO, 80% of the world population relies on traditional or herbal medicines for their primary health. One such herbal plant is *Andrographis Paniculata*(Bhuin Nimb in Odia).This study represents characterization of different metals present in *A. Paniculata*. The plant samples were collected from urban and rural areas of Khordha region. The solid powdered sample from different parts of the plant were taken for XRF to know the presence of different metals qualitatively. Then these samples were taken for ashing and followed by acid digestion using (Aqua regia). Then the solutions were analyzed using ICP-OES (Pb, Cr, Mn, Co, Zn, Cu, Cr, V, Na, Ca and Mg), FES (Na & K) respectively. Details data are given project thesis. All the data provides a clear description about the metal and mineral contents in the plant parts qualitatively and quantitatively as well.It has been found that leaves of the plants of both the region are rich in Fe, Mg, Ca, K, Mn etc. But Pb, Cr, Co, Pd, V exist but in low concentration which have negligible impact on the medicinal characters of the plant. Further study on structural characterization (FESEM) is under process.

Keywords:*Andrographis Paniculata*, Acid digestion, heavy metals, AAS, ICP-OES

Poster Presentation-02

Effect of Nanosilver decorated functionalised Single-Walled Carbon Nanotube Hybrid Nanofiller based Polyaniline Nanocomposite on the Thermal and Dielectric Properties

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Abstract: The present study reveals the synthesis of silver nanoparticles (AgNPs) decorated functionalised single walled carbon nanotubes (*f*-SWNTs) based polyaniline (PANI) matrix, carried out through *in situ* polymerization process to study the thermal and dielectric properties. The nanostructured morphology and chemical interaction of the synthesized nanocomposites are investigated by using ultraviolet-visible (UV-Vis), X-ray diffraction (XRD), and Fourier-transform infrared (FTIR) spectroscopic techniques. The hydrodynamic diameter and particle size distribution of the nanocomposites in the solution medium is studied through dynamic light scattering (DLS) method. The morphological characterization of the nanocomposites are carried out by scanning electron microscopy (SEM) and Transmission electron microscopy. The thermal and dielectric properties of the nanocomposites are investigated by employing thermogravimetry-differential scanning calorimetry (TG-DSC) and dielectric relaxation spectroscopy (DRS). The main objective of the research work is to decorate the AgNPs on the surface of the *f*-SWNTs to fabricate hybrid nanofiller and the synthesized Ag@*f*-SWNT hybrid nanofillers are dispersed within the PANI matrix to enhance the overall materials properties of the nanocomposites.

Keywords: Silver Nanoparticles; Single-walled Carbon Nanotube;Polyaniline; Nanocomposites; Thermal and Dielectric Properties

Poster Presentation-03

Synthesis, Characterization, Thermal Study, Antimicrobial and Antioxidant Study of Some Pyrazole Derivatives with and without Inclusion Complex Formation with Β-Cyclodextrin

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Abstract: Pyrazole and their derivatives are regarded as versatile pharmacophore moieties. But poor solubility in polar medium may be a limiting factor reducing their pharmacological activity. In order to increase solubility and bio-accessibility, the inclusion complexes of the compounds have been synthesized with β-cyclodextrin by co-precipitation method. The formation of inclusion complexes have been ascertained by changes in melting point and spectral data (UV, IR, NMR, XRD etc). The determination of thermodynamic parameters like ΔH, ΔG and ΔS suggest that the inclusion complexes have appreciable stability and their formation is thermodynamically allowed. The study of the antibacterial and antioxidant activities of the compounds and their inclusion complexes concludes that inclusion formation increases antibacterial and antioxidant activities significantly.

Poster Presentation-04

Water Pollution: A Great Concern in Chilika Lake, Odisha, India

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Abstract: Chilika lake is that the largest coastal lake in India and also the second largest salt water lake within the world.The lake has rocks and stratum drainage area, a transitory atmosphere and water character. Chilika water is contaminated due to discharge of effluents from industrial units, fishponds, constant discharge of untreated water into the lake from drains, significant metals pollution in coastal lagoons, significant inflow of waste matter, domestic and agricultural waste that consists of variable risky chemical and inflicting hurtful effects on fish and different aquatic-organism. The physico-chemical parameters like pH, chloride, nitrate, phosphate,silicate,DO,BOD and COD from water samples were studied.The water is alkaline and pH starting from 7.1 – 9.6.Higher pH was due to the decomposition of submerged weeds.Highest pH scale and TDS at some places was thanks to evaporation,complex mix of fresh discharge,wind condition and periodic event influx of ocean water.The DO values were between 3.3–18.9mg/l.The vary of phosphate: 0 – 0.4 ppm, nitrate: 10–60 ppm and silicate:1–8 ppm were high within the north and northwest a part of the lake wherever most of the rivers discharge into the lake with giant amounts of mud or clay and nutrients.COD was terribly less thanks to absence of organic pollution.Chloride content of lake water ranged from 19.86g/l in ocean mouth space in summer to minimum 2.87g/l.To revive the lake, Chilika Development Authority (CDA) is established in 1991 by the Odisha government. Gap of natural new mouth helped to rise to salinity throughout the lake, disintegrate the weeds, and flush out the sediment load from lake increase the multifariousness and ecology.Detailed study is required to safeguard the lake scheme, migratory and home ground improvement of birds,preparation of atmosphere standing report,establishment of education centre for the lake,control of silt load of streams and rivers, property development of fisheries and aquacultures and desiltation.

Keywords: Fishponds, Physico-chemical parameters,DO,BOD,COD, CDA

Poster Presentation-06

Impact of Inclusion Complex of Ibuprofen with β-CD:A Brief Study

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Abstract: Ibuprofen is an anti-inflamatory drug used in many medical complications. However, poor solubility in polar medium may be a limiting factor reducing their pharmacological activity. In order to increase solubility and bio-accessibility, the inclusion complexes of the compounds have been synthesized with β-cyclodextrin by co-precipitation method. The formation of inclusion complexes have been ascertained by changes in melting point and spectral data (UV, IR, NMR, XRD etc.). The formation of inclusion complex reduces the side effects of the drug. The determination of thermodynamic parameters like ΔH, ΔG and ΔS suggest that the inclusion complexes have appreciable stability and their formation is thermodynamically allowed.

Poster Presentation-06

Synthesis and Characterization of highly Active and Selective, Mononuclear Cobalt(II)-salen Complex as Efficient Catalyst for the Formation of Cyclic Carbonates by Fixation of Carbon Dioxide

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Abstract: In this novel, A new efficient mononuclear cobalt(II)-salen complex has been developed successfully by the reaction of [-ONNO-] tetra dentate Schiff base ligand, i.e., N,N′-bis(2-hydroxy-1-naphthaldehyde)-1,3-diaminopropane with anhydrous cobalt(II)chloride salt in ethanol solvent under N_2 atmosphere with optimum reaction condition. The ligand and its complex have been characterized by NMR, FTIR, UV-Visible, elemental analysis, Vibrating sample magnetometer (VSM) and melting point (incorrect). The complex has a square planar coordination geometry, as determined by X-ray diffraction studies. The synthesized Co(II) complex as a catalyst with DMAP as a co-catalyst were found to play an important role in enhancing the catalytic activity for the formation of cyclic organic carbonate from carbon dioxide and liquid epoxides which served as both reactant and solvent. Cyclic carbonates are used as a polar aprotic solvent, electrolyte in lithium secondary batteries, precursors for the formation of polycarbonates, and intermediates in the production of pharmaceuticals and fine chemicals.

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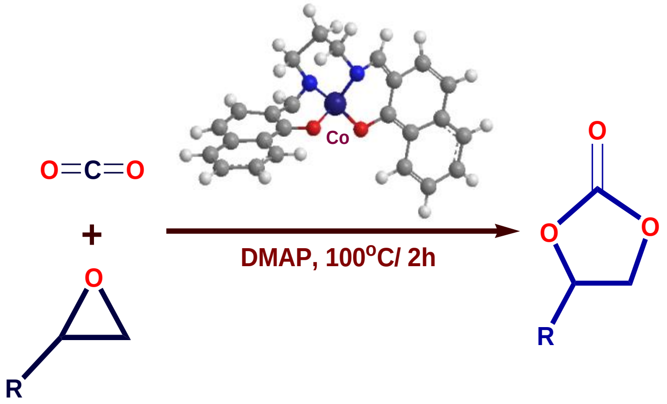
Graphical Abstract



Poster Presentation-07

Water in Cuttack Statistical Evaluation with Study of WQI of Different Parameters of Taladanda Canal and Paradeep City, Odisha, India

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Abstract: The precious natural resource is water. Canal is an artificial constructed channel; carry water from source (River/Reservoir) to fields.*"Life is the matrix of water. Within water life is originated, thriving and also it's medium and solvent."*The longest canal in Odisha is Taladanda canal. The canal was designed to provide irrigation, recreation and navigation and finally mixed with Bay of Bengal at Paradeep town. The total length of the canal is 82.3 km.The canal is contaminated by different polluting sources at its off taking locations. The water has become unfit for human consumption. Realising the importance of this problem the aims of our study is to determine the present pollution load of the canal with different physico-chemical parameters and based on the finding suitable models for prediction of the pollution behaviour at different locations of canal and its remedial measures.

Keywords: Canal water, WHO, Drinking water, Water quality.

Figure 1: *Talanda Canal Water.*

Figure 2: *At Laboratory.*

Poster Presentation-08

A Simple Synthesis of Ketone from Carboxylic Acid using Tosyl Chloride as an Activator

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Abstract: An effective process for the conversion of carboxylic acid to ketone has been discovered. In this process, carboxylic acid has been activated using p-toluene sulphonyl group. Under the optimized condition, aromatic, aliphatic heteroaromatic carboxylic acids have been proved to be good substrates for this methodology. The byproduct of this reaction can be removed very easily during work up process. In addition, one equivalent of organometallic reagent is sufficient to complete this transformation. The key advantage of this process is the ketone has been accessed from acid using one equivalent of organometallic reagent.

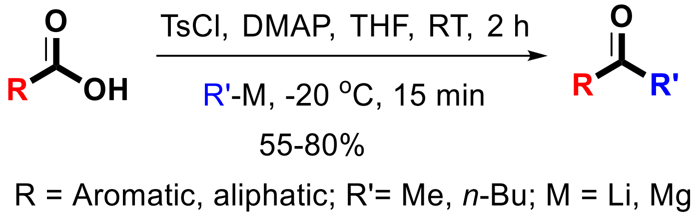

Figure 1: *Scheme for Synthesis of Ketone.*

Reference

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Poster Presentation-09

Single Walled Carbon Nanotubes

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Abstract: The different variations used for the production of SWNTs with the laser ablation process are briefly presented in this article. An attempt is made to point out the major differences and similarities of methods used by several researchers. Possible growth mechanisms for pulsed and CW laser excitations are presented. Several questions still remain about the role of small and large carbon clusters, the mechanism and growth of catalyst clusters, the dynamics of carbon–metal interactions including diffusion and surface adsorption, and finally how, when, and where the SWNT growth stops. It is hoped that additional work in the near future will provide answers to these questions and will help the community develop methods to improve SWNT production. This may enable choosing

parameters for large-scale production and controlling growth of SWNTs of a particular chirality and diameter.

Poster Presentation-10

What the Mutation Actually Does on Proteins:Loss or Gain of Function?

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Abstract: Regardless of advances in *in-vivo ,in-vitro and in-silico* studies, impact of the mutations on the protein structure remains an immense challenge.Recently, the computational programming particularly molecular dynamics based on Newton's equation and docking process are used to predict the structural and dynamical properties of small molecules has become an important component in the drug discovery process[1-13]. Molecular docking study has been carried out to study the molecular interaction between mutant and wild type models of the Podocin protein with biological active compounds of *Boerhaavia diffusa* plant extracts. Both boeravinone B and F are having higher binding energy as compared to others in mutant protein. Furthermore, molecular dynamics simulation study was carried out for both the wild type and mutant model and revealed that, flexibility nature decreases in the mutant protein[14].From the molecular docking study, it was found that, due to mutation the binding energy was decreased for aegeline, berberine diterpenoid and roseoside with mutant of PLCE1protein at S1484L compared to wild type. These dynamical behavior results of wild type protein show similar behavior with mutant protein [15].Several strategies are being needed to address this issue in future.

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Poster Presentation-11

Photo Catalytic Applications of doped g-C_3N_4towards Energy and Environment

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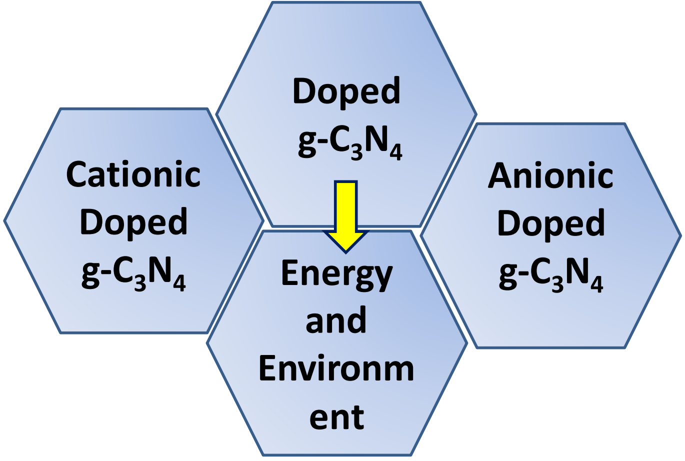
Abstract: In the last few years, tremendous theoretical as well as experimental efforts have been made to understand the characteristic properties of graphitic-C_3N_4, an organo-polymeric semiconducting material. However, owing to its low-dimensionality and quantum confinement effect various modifications including doping, defecting and forming heterojunction/composites etc. are proposed to extend its potential applications. Among all, band gap engineering through elemental doping is reported as an effective strategy to tune its optical as well as electronic properties. "Structural doping" has been attracted researcher's attention since long and supposed to be the best method to enhance the photocatalytic ability. Doping significantly introduces impurity levels in the band gap, broadens the light absorption and increases the electron-hole separation efficiency. In case of anionic doping, the dopants either through substitutional or interstitial doping, modulate the textural as well as electronic structure. Whereas, in case of cationic dopants, orbital hybridization may also occur among the dopant's orbital and molecular orbital of g-C_3N_4, leading to tunable VB and CB potentials. Incorporation of non-metallic/metallic dopants play an exceptional role to enhance light absorption and change the band edge potentials to carry out targeted photo catalytic redox reactions to carry out pollutant remediation and hydrogen energy generation. Doped g-C_3N_4 photo catalytic systems can pave a novel avenue towards visible-light driven photocatalysis.



Poster Presentation-12

Synthesis of $CuSbS_2$ Nanoplates and $CuSbS_2$-Cu_3SbS_4 Nanocomposite: Effect of Sulfur Source on Different Phase Formation

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Abstract: In the recent decades, Cu-Sb-S ternary nanomaterials have been attractive for their wide potential and technological applications in solar cell as well as in supercapacitors. In particular, Cu-Sb-S nanomaterials exhibit exclusive optical properties such as unique band gap, p-type conduction and high absorption co-efficient. Moreover, the components Cu, Sb and S are earth abundant, low/nontoxic and economic. In the present work, we developed a facile approach for synthesis of $CuSbS_2$ nanoplates and $CuSbS_2$-Cu_3SbS_4 nanocomposite using hot injection method with varying sulfur precursors. The role of solvent, sulfur precursor and reaction temperature has been investigated. As prepared nanomaterials were characterized by PXRD, UV-Vis, XPS, TEM, FESEM, etc. Further, the Electro chemical measurements were thoroughly studied for supercapacitor applications.

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Poster Presentation-13

Preparation and Study of Antimicrobial Properties of Chitosan/Cu-Al LDH/Ag Bio-nanocomposites

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Abstract: Biopolymer based nanocomposites (bio-nanocomposites) are an emerging class composites, which are formed by the combination of a polymer and an inorganic or organic nanoparticle. Chitosan is among one of the most important and most studied natural polymers. The present work deals with the application of a relatively new class of hybrid filler such as Cu-Al LDH/Ag, for synthesizing polymer based bio-nanocomposites. The CS/Cu-Al LDH/Ag bio-nanocomposite materials were synthesized by a simple and environmentally friendly *in situ* polymerization technique. The CS/Cu-Al LDH/Ag bio-nanocomposites were characterized using Field emission scanning electron microscopy (FESEM), High-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). The antibacterial activity the bio-nanocomposites film against pathogenic bacteria viz. *Escherichia coli*, *Staphylococcus aureus* and *Bacillus subtilis* was measured by agar diffusion method. The XRD pattern indicated the presence of Cu-Al LDH, silver and chitosan in the bio-nanocomposites. The spherical morphology of silver nanoparticles was confirmed from the FESEM and the HRTEM images. FTIR spectroscopy was used for the structural elucidation. It is observed that CS/Cu-Al LDH/Ag bio-nanocomposites film exhibits good antimicrobial and antitumor properties.

Keywords: Chitosan, nano silver, bio-nanocomposites, morphology, antimicrobial activity

Poster Presentation-14

Probing the Conformations of Intrinsically Disordered Protein Utilizing Fluorescence Spectroscopy

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Abstract: The intrinsically disordered proteins (IDPs) belong to an important class of proteins due to their higher structural flexibility and diverse functions. IDPs lack stable three-dimensional structure and exist as structural ensemble in solution. Furthermore, IDPs have been found to be associated with various neurodegenerative diseases like Alzheimer's, Parkinson's, diabetes and spinocerebellar ataxia. Several spectroscopic techniques are being employed to predict the structure of IDPs as the X-ray crystallography is immensely challenging due to their structural dynamism. κ-Casein, an important milk protein containing net negative charge, belongs to the class of IDPs. κ-Casein has been found to assume different structural conformations at various pH and surfactant concentrations. In this work, we have utilized quenching efficiency of ionic liquid (1-butyl-3-methylimidazolium bromide) and energy transfer efficiency between tryptophan and 1,6-Diphenyl-1,3,5-hexatriene (DPH) to evaluate the conformation of κ-casein at various pH and cetyltrimethylammonium bromide (CTAB) concentrations. Our results validated the applicability of above-mentioned methods to determine the polarity of tryptophan environment in κ-casein at different conditions, where κ-casein assumes diverse structural conformations. The present work opens up the possibility to employ quenching properties of ionic liquid in conjunction with energy transfer efficiency between tryptophan and DPH for the elucidation of protein conformation.

Poster Presentation-15

Interaction of Eugenol with α- and β- cyclodextrins: Implication in Drug Delivery

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Abstract: Eugenol, a natural compound available in clove, serves as an analgesic, anti-inflammatory, antiviral, antifungal, antiseptic and a local anesthetic that is widely used in the pharmaceutical world. The major challenge with eugenol is its lower cellular partitioning and that has been improved significantly by utilizing macromolecular carriers. In this work, we have evaluated the partitioning efficiencies of eugenol with α- and β- cyclodextrins using steady state and time resolved fluorescence methodologies in tandem with molecular docking to find out a better carrier for eugenol to overcome its lower partition coefficient in biological systems. Our experimental results suggest that eugenol has relatively higher affinity toward β-CD compared to α-CD. The relatively higher partition coefficient leads to preferential binding of eugenol in β-CD, which was evident from fluorescence lifetime measurements in a competitive experiment. However, the molecular docking results indicate that the α-CD-eugenol inclusion complex is more stable compared to the β-CD counterpart. This could be due to the molecular docking experiment in vacuum, which ignores the interaction of eugenol and/or cyclodextrins with water. Taken together, our results demonstrate that eugenol is having adequate affinity toward α- and β-CD and CD-Eugenol inclusion complexes could be used for delivering eugenol in biological system.

Poster Presentation-16

Construction of Fluorophoric Thiazolo-[2,3-b]quinazolinone Derivatives: A Multicomponent Domino Synthetic Approach

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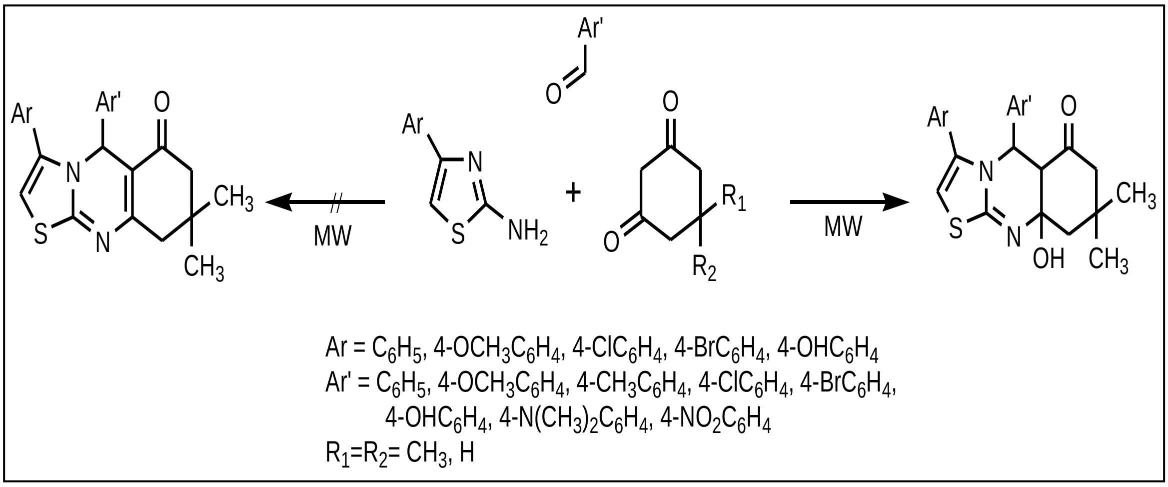
Abstract: Fusion of biodynamic heterosystems for designing new molecular framework has pivotal importance in the process of drug discovery. Thiazole serves as a privileged scaffold in many natural and synthetic medicinal compounds. Conversely, quinazolinones have interesting structural architecture, which contribute to develop the medicinally relevant products along with the fluorescence properties. Assembling such vital nuclei make them intriguing scaffold not only in pharmacology, but also in photochemistry. Benzothiazolo[2,3-b]quinazolinone scaffolds exhibit assorted biological and pharmaceutical properties such as cytotoxicity against HL-60, inhibitory activities towards EGFR, anti-bacterial, antiviral, antitumor activities, electrochemical sensors for glutathione, amoxicillin or L-cysteine and

photo-antiproliferative activity.As, the syntheses of diverse heterocycles are important in all facets of chemistry, we herein, developed a one-pot domino reaction of substituted 2-amino thiazole, benzaldehyde and cyclic diketone for the synthesis of novel thiazolo[2,3-b]quinazolinone possessing angular –OH group (Scheme 1). The unique structural arrangement is found to be potential fluorophore which gave us an inducement to synthesize a library of such type of fluorescence molecules with various substituents. All the newly synthesized compounds were elucidated on the basis of elemental and spectral (NMR and Mass) analysis and their fluorophoric properties were explored with respect to various substituents.



Ar = C_6H_5, 4-$OCH_3C_6H_4$, 4-ClC_6H_4, 4-BrC_6H_4, 4-OHC_6H_4
Ar' = C_6H_5, 4-$OCH_3C_6H_4$, 4-$CH_3C_6H_4$, 4-ClC_6H_4, 4-BrC_6H_4, 4-OHC_6H_4, 4-$N(CH_3)_2C_6H_4$, 4-$NO_2C_6H_4$
R_1=R_2= CH_3, H

Scheme 1

Poster Presentation-17

Science of Materials Components, Composition, and Configuration

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Abstract: Materials are made up of chemical elements. Smartness of materials depends on its components, composition and configuration, which can be explained with the help of masterpiece of arrangement of chemical elements the Mendeleev's Periodic table. In the 150th birth anniversary of table precursors, co-cursors and rein forcers of the table will be dealt in the present talk. Story of two and a half millennium starting from Democritus (500BC) to the present day Pekka Pykko(2019) will be narrated in a lively style so as to attract experts and curious laymen alike. The notable amongst those starts from Dobereiner, Gladstone, Cooke, Odling, Lenssen, Boyle, Priestley, Davy, Faraday, Gmelin, de Chancourtois, Lother

Meyer,Newland, Ramsay, Rayleigh, Thomson, Rutherford, Moseley, Bohr, Summerfield, Segre, Frankland, Lockeyer, Travers, Owen, Nilson, Del Rio, Vauquelin, Brandt, Stromeyer, Gadolin, Ekeberg, Wollaston, Mosander, de Broglie, Schrodinger, Planck, Heisenberg, Seaborg, Ghiorso, Oganessian, Flerov, Penzias, Wilson, Peebles, Goodenogh, Poliakoff and Eric Scerri.The most smart material of the present millennium is Graphene, a 2D material whose use as a superconductor by adjusting quantum band gap and magic twist angle in bilayer Graphene is occupying the frontline in material science research.

Poster Presentation-18

Cholesterol Alters the Inhibitory Efficiency of Peptide-based Membrane Fusion Inhibitor

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Abstract: Membrane fusion is one of the most important events in the entry of enveloped viruses in the host cell. The membrane composition modulates membrane fusion by altering membrane physical properties as well as the structure, organization and dynamics of fusion proteins and peptides. The journey of developing peptide-based inhibitors for viral fusion is often stalled by the change in lipid composition of the viral and target membranes. This makes it important to study the role of membrane composition on the organization, dynamics and fusion inhibiting abilities of the peptide-based fusion inhibitors. Cholesterol, an important constituent of mammalian cell membrane, modulates bilayer properties in multiple ways and impart its effect on the membrane fusion. We have previously shown that TG-23 peptide derived from coronin 1, a phagosomal coat protein, show significant inhibition of fusion between membranes without cholesterol. In this work, we have studied the effect of the TG-23 peptide on the polyethylene glycol-mediated membrane fusion in presence of different concentrations of membrane cholesterol. Our results show that the inhibitory effect of peptides is being completely reversed in the membrane containing cholesterol. We have measured the effect of these peptides on the depth-dependent membrane properties, organization and dynamics of the peptides to elucidate the composition-dependent fusion efficacy of the peptides. Our results demonstrate that cholesterol alters the membrane organization and dynamics of TG-23 peptide and thereby manifest differential efficacies on membrane fusion. Therefore, we envisage that the study of peptide organization and dynamics is extremely important to determine the effect of peptide on the membrane fusion.

Poster Presentation-19

Fluorescence Spectroscopic Study on Interaction of Anticancer Drug Molecule Doxorubicin and Pluronics

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Abstract: The study on drug release in a precisely controlled and active way is highly demanding and challenging for tumor precision therapy. Techniques to improve the accumulation of therapeutic agents in tumors, which subsequently enhance the therapeutic efficacy of anticancer drugs against malignant tumors and reduce their side effects remains a great challenge. Doxorubicin is one of the most powerful anticancer drug molecule known for its sustained and target delivery to tumor cell, although its clinical use is impaired by severe undesired side effects.[1]Use of amphiphilic copolymers such as pluronics is being studied widely for the formulation of doxorubicin.[2,3] In this fundamental work, the interaction of doxorubicin with the pluronics F127 and P123 has been studied extensively using steady state and time dependent fluorescence measurements at different pluronics concentrations and temperatures.It has been observed that, doxorubicin is experiencing change in its microenvironment on increasing temperature and concentration of pluronics. From the quenching experiment, it was found to locate itself near the hydrophobic-hydrophilic interfacial region of the pluronics network. Quenching in the fluorescence intensity of doxorubicin could be due to collisional quenching and transient effects at the concentration of the drug used.The particle size study shows that the D_h of copolymer F127 is larger than that of P123. This may provide more information on encapsulation of the drug molecule.

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Poster Presentation-20

Impact of Size and Charge of the Flavin Mediators on Reductive Iron Mobilization from *Mycobacterial* Ferritin

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Abstract: Nature uses flavin, both in its free and protein-bound form as electron relay molecule (mediator) for various oxidation and oxygenation reactions. As reported earlier, the reductive iron mobilization from ferritin nanocage largely depends upon the reduction

potential of electron transfer mediators. However, the current work utilizes three flavin analogues (Riboflavin, FMN, and FAD), which differ in size and charge but have similar redox potentials, to mediate electron transfer from NADH to the ferritin mineral core. Of these, the smallest/neutral analogue, riboflavin, exhibited the fastest kinetics of NADH oxidation, dissolved O_2 consumption and released higher amount of iron than the larger and negatively charged FMN and FAD. The presence of O_2 under normoxic conditions marred the process of ferritin iron mobilization by oxidizing the reduced form of flavins, resulting in initial lag phase, which further, gets inhibited in the presence of superoxide dismutase ($O_2^{\cdot -}$ scavenger) indicating the generation of $O_2^{\cdot -}$ *in situ*. Overall, the flavin mediated reductive iron mobilization occurs via two competitive pathways (Fig.1). One, the formation of reduced form of mediator which participates in long range electron transfer to facilitate iron release and second, the generation of $O_2^{\cdot -}$, which acts as an intermediate to assist the reduction of iron mineral core and its release.

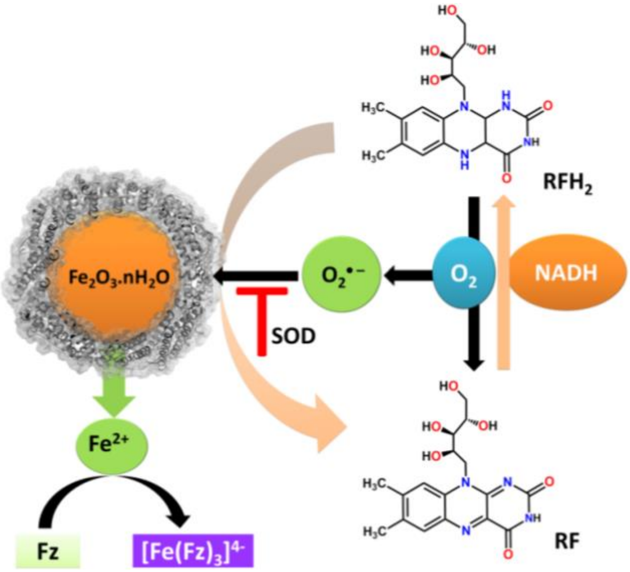

Fig.1. Competitive pathways of Flavin mediated reductive iron release from ferritin nanocage

Poster Presentation-21

Reusable Pd-Catalyzed Oxidative Coupling between Amides with Olefins towards Stereoselectve Synthesis of Z-enamides

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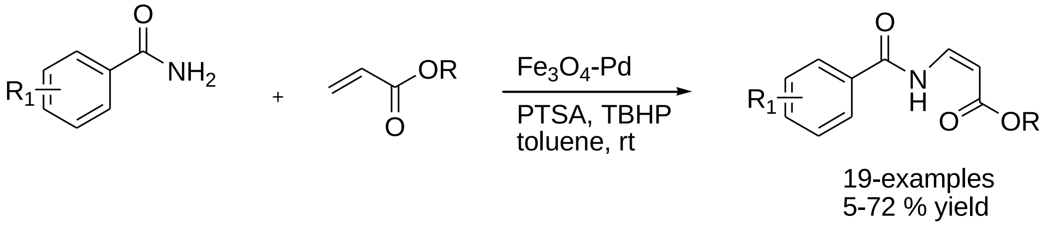
Abstract: Over the past few years, transition-metal-catalyzed oxidative coupling reactions have received much attention due to their being atom- and step-economic approaches for the preparation of complex molecules.[1] In oxidative coupling reactions, two C—H and heteroatom—H bonds are directly coupled to form C—C and C- heteroatom bonds in the

presence of oxidant and transition metal catalyst.[2] Here in we described a convenient method for the synthesis of palladium decorted ferrite nanoparticles (Fe_3O_4-Pd). The catalytic application of the Fe_3O_4- Pd nanoparticles was explored for the first time in oxidative coupling between amides and olefins. p-Toluenesulfonic acid plays a significant role in the oxidative amidation reaction. The reaction proceeds at room temperature, resulting in stereoselective synthesis of (Z)-enamides under ambient air in the absence of co-catalyst and ligand.[3] The superparamagnetic nature of Fe_3O_4-Pd facilitates easy, quantitative recovery of the catalyst from a reaction mixture, and it can be reused for up to three consecutive cycles with a slight decrease in catalytic activity.



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Poster Presentation-22

A Defect Study in TiO_2-rGO-ZnS Composite for Photocatalytic Applications

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Abstract: Developing an efficient photocatalyst for environmental remediation from solar energy is a challenge. Defect engineering although offers a strategical promise to enhance the photocatalytic performance. In the current work, a comprehensive study on defects in TiO_2-rGO-ZnS compositewas done. The composites were synthesized by one pot solvothermal method. The content of graphene was varied to study its effect on the defect sites in the

composites. Characterization techniques such as FTIR, SSA, XPS, ESR and PL were employed to characterize the composites. The photocatalytic performance was studied by conducting degradation of methylene blue (MB) under solar radiation. Graphene acted as an effective electron sink as understood from luminescence spectra. The superior activity of TiO_2-ZnS-rGO is attributed to low bandgap and rapid separation of photo-excited charge carriers. This work may assist to explore the fundamental role of defects in the photocatalytic processes and improve the selectivity in heterogeneous catalysis.

Poster Presentation-23

Synthesis, Characterization and Thermal Property of $Cu_3(PO_4)_2\cdot 2H_2O\cdot Na_3PO_4\cdot NaHSO_4\cdot H_2O$

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Abstract: The phosphate compounds of copper and sodium along with sodium hydrogen sulfate monohydrate mixture has been synthesized and characterized with different measurement techniques such as Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA) and Differential Thermal Analysis (DTA), Fourier Transform Infrared (FT-IR) Spectrometry, C-H-N-S elemental analyzer, Inductively Coupled Plasma -Atomic Emission Spectrometry (ICP-AES), Ultraviolet–Visible and near Infrared (UV–Vis-NIR) Absorption Spectrophotometry and X-ray Powder Diffraction (XRD). The thermal property of this mixture has been studied up to 573 K from 173 K in different thermal cycles with DSC. The specific heat capacity of this mixture has been measured in atmospheric O_2 at a rate of 10 K min^{-1} in all cycles. The net specific heat capacity of this mixture is found endothermic in all thermal cycles. So, it can be used as heat storage material as a combination of sensible and latent heat technique.

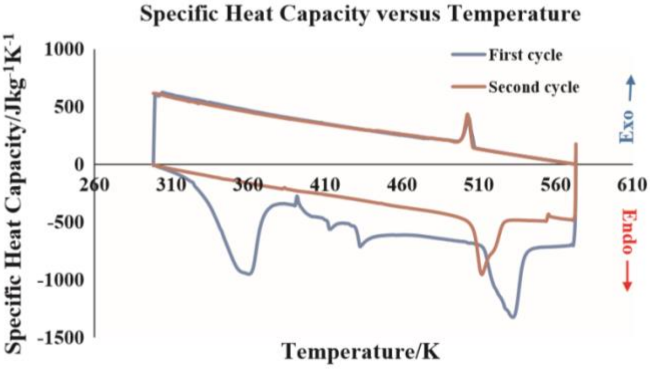

Figure 1:*DSC Graph of Specific Heat Capacity Versus Temperature in the Temperature Range 298 K to 573 K and Vice Versa in Two Thermal Cycles and Kept at 573 K for Two Minutes of the Mixture* $Cu_3(PO_4)_2\cdot 2H_2O\cdot Na_3PO_4\cdot NaHSO_4\cdot H_2O$.

Poster Presentation-24

Nano Silver embedded Chitosan incorporated Polymethyl Methaacrylate/Graphene Oxide Nanocomposite as Packaging Materials

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Abstract: A simple *in situ*polymerization technique is used to synthesize polymeric nanocomposite of PMMA/Chitosan-GO@Ag. The thickness of the PMMA/Chitosan/GO@Ag nanocomposite mainly depends on the polymerization of the methylmethaacrylate and concentrations of the GO. Phase analysis, microstructure, and chemical composition are examined by X-ray diffraction (XRD), Fourier transform Infrared Spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), X-ray photoelectron spectroscopy (XPS) and high resolution transmission electron microscopy (HRTEM). The surface and nano-tribological characteristics of the polymeric nanocomposite are investigated by atomic force microscopy (AFM). The thermal, antibacterial, and oxygen barrier properties of the polymeric nanocomposite are studied. The incorporation of the Ag NPs enhances the barrier, thermal, and antimicrobial properties of the PMMA/chitosan-GO matrix by which the material is suitable for good packaging applications.

Keyword: Nano silver; nanocomposite; AFM; FESEM; Packaging

Poster Presentation-25

Synthesis of Pd decorated Carbon Quantum Dots modified Fe_3O_4 Nanoparticles: Application in C–C bond Forming Reactions

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Abstract: Carbon nanodots (C-dots) constitute a fascinating new class of carbon structures showing size and excitation wavelength dependent photoluminescence (PL) behaviour.[1]With their high photostability and lack of known cytotoxicity, C-dots are considered to be a green alternative to fluorescent semiconductor nanoparticles and have shown potential use in optical detection, bioimaging, light emitting diodes, fluorescent ink and photocatalysts.[2] C-dots might also function as excellent supports for nucleation and growth of nanoparticles leading to the formation of new functional materials where C-dots play a critical role in prevention of agglomeration and effective catalysis by the metallic component. In this respect, carbon quantum dots coated Fe_3O_4 magnetic nanaoparticles were synthesized and used for the reduction of Pd(II). The synthesized catalysts Fe_3O_4@CQDs@Pd were characterized by PXRD, SEM, TEM, EDS and VSM. The synthesized catalysts were applied for the coupling

reactions between aryl halides with olefins. Interestingly, the reaction proceeds in aqueous medium using triethanol amine as the base. Subsequently, the scope and mechanism of the reactions were investigated. The easily synthesized and air-stable catalyst Fe_3O_4@CQDs@Pd NPs could be separated from the reaction mixture by using an external magnet and reused in eight consecutive runs with no significant loss of catalytic activity.

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Poster Presentation-26

Green Synthesis of Gold Nano-Particle and Its Applications

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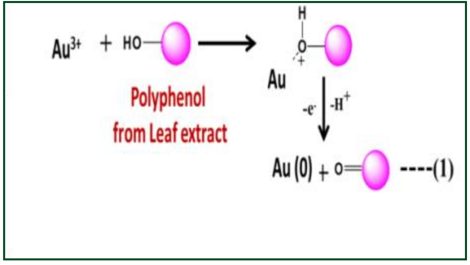
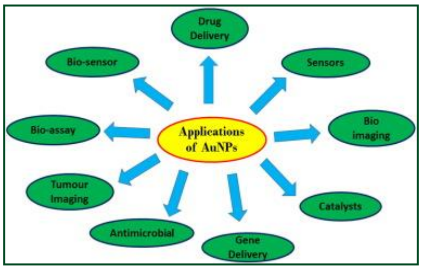
Abstract: Nanoparticles are particles that exist on a nanometre scale (i.e., below 100 nm in at least one dimension).These can possess properties such as uniformity, conductance or optical properties that make them desirable in materials science and biology. Green chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products. An *insitu* green synthesis of gold nanoparticles using Hirakud sand as source of gold solution and red tea infusion as a reducing and stabilizing agent and their applications have been presented. The size and shape of gold nanoparticles are modulated by varying the ratio of metal salt and tea leaf extract in the reaction medium. The nanoparticles obtained can be characterised by UV-vis, transmission electron microscopy (TEM) and X-ray diffraction (XRD) (continuing) A special attention to varying nano gold particle size, Tyndall effect and Target drug delivery have been presented in the form protocol.





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Poster Presentation-27

Effect of Metallic Ions, pH, Moisture Content of Host Plant Leaves on Silk Formation in Tasar Silkworm *Antheraea Mylitta*Drury: A Review

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Abstract: Sericulture is the term associated with silk industry, which involves rearing of silkworm using advanced scientific and technological knowledge to enhance silk productivity. Tasar silkworm *Antheraea mylitta* Drury is one of the important *Vanya* silkworms that produces commercially important silk. This silkworm is polyphagous in nature, inhabits in Sal forests and also reared on its primary host plants *viz*. *Terminalia tomentosa* (Asan) and *T. arjuna* (Arjun). Leaf nutrients have direct bearing on the quality as well as quantity of silk. Tasar silkworm converts concentrated fibroin and sericin solutions to insoluble silk fiber and adhesive gum respectively, through silk ducts instantly before the silk is drawn down into filament. Silk fibers possess dramatic mechanical properties and are partly dependent on the crystalline β-sheet silk conformation under shear or rapid elongation flow. The protein conformation to β-sheet is dependent on several factors such as concentration of metal ions in the soil and host plant leaves (Na^+, K^+, Mg^{2+}, Cu^{2+}, Zn^{2+}), pH of the soil besides the moisture content in the soil as well as leaves. In this paper, we present a detailed review on the impact of metallic ion, pH and moisture content of host plant leaves in relation to silk production and productivity of tasar silkworm.

Keywords:*Antheraea mylitta*, host plant, metallic ions, moisture content, tasar silkworm, soil

Poster Presentation-28

Nano Gold based Composites for the Reduction of Cu^{2+}Ion

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Abstract: Recently, researchers are running behind the developing of nanosensor for the detection of toxic metal ions from the environmental and biological samples. Among different metalions, Cu^{2+} ion is one of the important environmental pollutant. Generally, Cu^{2+} ions are third abundant metals in the human body. However, excessive amount of Cu^{2+}ion not only imbalance the cellular process that lead to Wilson's disease, Parkinson's disease.According to

World Health Organization (WHO) maximum permissible limit is 20.5 µM in drinking water. We have designed metal induced aggregation of gold nanocomposites; an efficient approach for the detection of Cu^{2+} ion. Sensing of Cu^{2+} ion using gold nanocomposites is based on aggregation of gold nanoparticles in nanocomposites. The as-synthesized gold nanocomposites in contact with Cu^{2+} ion forms co-ordinate bond which leads to aggregation of gold nanoparticles (AuNP). Therefore, the surface plasmon resonance peak of AuNP in nanocomposites is decreased with a red shift. Scanning electron microscope (SEM) micrograph reveal the aggregation of gold nanoparticles in the nanocomposites. The limit of detection and limit of quantification for Cu^{2+} ion are 40 nM and 133nM respectively.

Keywords: Nano Gold; L-alanine; Copper; Metal induced aggregation

Poster Presentation-29

Solvent Free Green Synthesis of Porphyrin and Metalloporphyrin

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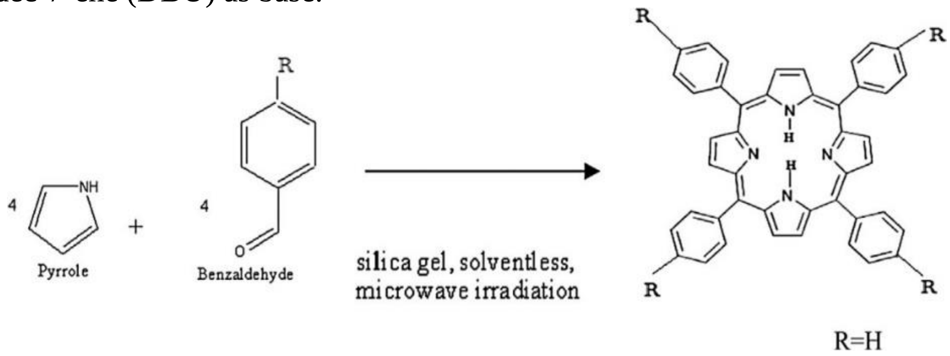
Abstract: Traditionalmethodofsynthesisofchemicalcompoundsinvolvesuseoftoxic,corrosive chemicals, which affect very badly our environment. Again, during these reactions the byproducts also create harmful effect on environment. To overcome this difficulty, researchers developednearlyadecadeanalternativemethodofecofriendlysynthesisofcompounds.

Environment friendly synthesis or green synthesis of small molecules is comparatively easy compare to synthesis of macrocyclic molecules. Porphyrin, a macrocyclic molecule consists of four pyrrole rings joined together through methine (=CH−) bridge are synthesized in various conventional methods by using high boiling propionic acidor large amount of halogenated solvents containing corrosive lewis acid catalysts. In many cases, toxic oxidizing compounds are used to convert porphyrinogen to porphyrin. A solvent free microwave assisted synthesis of porphyrin using benzaldehyde and pyrrole followed by the preparation of the nickel porphyrin by a solvent free microwave assisted reaction using 1,8-diazabicyclo [5.4.0] undec-7-ene (DBU) as base.



The use of mechanochemistry to bring about an acid-catalysed condensation between aldehydes and pyrrole followed by oxidation of the intermediates to produce porphyrin, which enables the elimination of both solvent and high temperatures from the synthesis of these important compounds. It represents a significant reduction in environmental impact.

Keywords: porphyrin, Microwave irradiation, Green synthesis, Solvent, Silica gel

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Poster Presentation-30

A Comprehensive Review on Biopolymers with Special Reference to Fire Retardant Property

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Abstract: The impact of pollution load in the world by the use of synthetic non-biodegradable plastics materials increases day by day, which forced us for searching of new materials from natural renewable sources, having the property of biodegradability and nontoxicity in nature. The important biomaterials that replace the synthetic polymeric materials are the biopolymers and its composites. The biopolymers can be synthesized from plant and animal products by using variety of microorganisms in controlled environmental condition. In this work, we discuss about the present development, synthesis, characterization and application of biopolymers and biopolymer composites with special reference to fire retardant materials, which becomes new construction materials and helps our society for dangerous fire hazards. The emphasis given in this chapter is different characterization specifically thermal stability and fire retardancy along with some specific application in the field of nanotechnology.

Keywords: Biopolymers, Fire retardancy, Nano composite. Biomolecule, biopolymer

Poster Presentation-31

Biodegradable, Superabsorbent with Potential Biomedical Application as Drug Delivery System of “Pectin-g-P (AN-co-AM)/Chicken Eggshell” Biocomposite

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Abstract: The outer cover of the Chicken egg having a mesh size of 100-350 μm serves as a good bio-filler and a versatile material for manufacturing of advanced composite materials. Pectin-g-P(AN-co-AM)/chicken eggshell which was synthesized by using water soluble cobalt complex as catalyst and its properties were studied by using FTIR and on-off switching swelling graph. Moreover, water absorbency and biodegradability along with a drug delivery property of the prepared material was studied by using the conventional method. It was observed that the synthesized material shows property of super absorbency (hydrogel) and demonstrate interesting results at pH= 2 and 8 being responsive to swelling-de-swelling behaviour. This material also shows potential application in drug delivery system. This bio-composite is environmentally friendly as it is synthesized in microwave assisted medium without emission of any gaseous toxic materials to the environment.

Keywords: Pectin, Hydrogel, Acrylonitrile, Acrylamide, Drug Delivery, Ibuprofen

Poster Presentation-32

Assessment of Pollution Load of Taladanda Canal in and arround Paradip City, Odisha, India in terms of Physico-Chemical and Bactriological Analysis

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Abstract: The quality of the water was usually analyzed in terms of its physical, biological and chemical characteristics. From the present analysis, it was found to be revealed that TC and FC of all the sampling points are much higher than the standard actable limit. The TC value ranges from 52.9 to 25.3 whereas FC value ranges from13.1 to 6.4 per 100 ml as per MPN test. The pH value of the water is less than 6.7and is acidic in most of the sampling point. The TDS values and SS values are much higher than the permissible limit. All other water parameters are also more than the permissible limit but less than the tolerance limit. Due to high bacterial contents, acidic properties and much higher value of TSS, TDS the water is almost not suitable for human use and it affects the socio-economic conditions of the dwellers living nearby the Taladanda Canal in and around Paradip area.

Keywords: Water quality, Pollution, Physicochemical assessment, bacteriological parameters. FC.

Poster Presentation-33

Sustainability and Eco-Utilization of Blast Furnace Slag Generated From Rourkela Steel Plant, Odisha, India

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Abstract: During the production of Iron, the major solid waste obtained is BF slag, which can be utilized as a resource material in the manufacturing of bricks and concrete slab with high value of tensile strength, load bearing capacity and durability. The Rourkela steel plant generated huge amount of BF slag at every day and creating increase in pollution load, if it is eco-utilized in the manufacturing of bricks and concrete slab, it will be more economical, energy saving and eco-friendly to our environment. The aim of our the present work is designing and manufacturing of bricks and concrete slabs of high stability and strength by using the BF slag produced from RSP with combination of lime, sand and marble dust. From different Characterization it was found that the bricks and slabs obtained is of high quality and more suitable for construction,

Keywords: BF slag, concrete slab, brick, pollution load, Eco-utilization

Poster Presentation-34

Corrosion Inhibition Studies of 4-Aminoantipyrine based Schiff Base

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Abstract: Acid solutions are widely used in industries for processes like acid descaling, cleaning and pickling. These acidic solutions cause corrosion in various metallic parts leading to loss of material. Inhibitors are needed to stop the corrosion process to maximize the lifetime of metals. Schiff bases have received enormous attention as an excellent class of corrosion inhibitor since they can be synthesized easily and are cost effective. A series of Schiff base based on 4- aminoantipyrine with different substituents on the aromatic aldehyde were synthesized, characterized and the effect of various substituents on the corrosion inhibition property was studied. The electrochemical study was carried out in 1 N HCl taking mild steel samples at different concentration (10_{-2} – 10_{-5} M) and temperature (303K-333K). Schiff base having $-N(CH_3)_2$ and (-OCH3) as substituents exhibited maximum inhibition tendency at 333K and 303K respectively. All the Schiff base ligands followed Langmuir adsorption isotherm confirming the formation of monolayer at the mild steel surface. The surface morphology was studied by SEM and EDX, which confirmed the formation of protective layer on the MS surface. DFT Study and experimental results were found to be in agreement with each other.

Keywords: Schiff base, 4–Aminoantipyrine, Corrosion inhibition, DFT

Poster Presentation-35

Polymer Bionanocomposite (PNC): An Ecofriendly and Novel Adsorptive Tool for Removal of Rare Earth Metals from e-Waste in the Environment

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Abstract: In recent years Polymer Nanocomposites (PNC) have attracted the focus and attention of young and dynamic researchers in water remediation and its purification due to its cost effectiveness, high processability, modified surface area, enhanced adosorptivity for heavy metal ions and also for its tunable properties as well as reusability. Chitosan, a deacetylated product of chitin is a most promising and prospective biopolymer for adsorption of heavy metal ions from the diluted waste water. But when it is functionalized with any of its co-polymers its effectiveness and usability capacity is enhanced thousand times in comparison to the virgin biopolymer as it Iess soluble in acidic aqueous solution. The functionlization is very efficient for binding the rare earth ions (lanthanide ions) from the waste water solution and it is done by grafting of biopolymer with variety of co-polymers. This grafting of biopolymer lanthanides (Nd^{3+}& Pr^{3+}) was investigated by various FTIR, XRD, FESEM, TEM, AFM technologies. The influence of several parameters such as P_H, adsorbance doses, contact time, metal ion concentration, kinetic parameters with proper isotherms, desorptibility, and reusability of the PNC was studied in batch adsorption mode. The adsorption efficiency by the PNC with increasing metal ion concentration was found to be 99% from the waste diluted water followed by Freundlich model along with Pseudo-second order kinetics. Desorption of the lanthanides were also done with 1M sulphuric acid and hydrochloric acid solution. The adsorption efficiency of the PNC did not alter much as with the original in reusability of maximum three times. Thus, in the conclusion The PNC can be effectively used as the novel adsorbent for treatment of waste water containing pollutants along with transition rare-earth metal ions.

Keywords: Polymer nanocomposite, Chitosan, Rare earths, Adsorption, Waste water, Desorption

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Poster Presentation-36

Sustainable Biodiesel Production from Microalgae *Chlorella Vulgaris*

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Abstract: Increasing energy demand, pollution and dwindling of non-renewable energy sources, has compelled us to look for ecofriendly sustainable energy sources. India, the tropical peninsular country, is suitable for large scale cultivation of microalgae and cyanobacteria coupled with its species richness mega biodiversity hotpots. This led to identification of the potent strains, which can be used to produce biodiesel and to meet the challenges of 4th generation biofuel research. *Chlorella vulgaris* isolated from Hirakud reservoir of Odisha, India, was screened for their lipid content for biodiesel production. Cost effective outdoor mass cultivation technology has been developed to microalga *Chlorella vulgaris* with Mahanadi water. Growth conditions were optimized toward maximum lipid and biomass production. Lipid with saturated FAME (fatty acid methyl esters) to biomass ratio has been optimized and optimized conditions have been applied in large scale production. Under the optimized conditions approximate 28.64% yield of lipid and 80% yield of FAME was obtained in *Chlorella vulgaris*. The formation of the biodiesel was ascertained by TLC, FTIR and GC-FID spectroscopy.

Poster Presentation-37

Fuel Gas Production using Solar Radiations

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Abstract: Of late to meet the high demand for energy from all possible sources, most of the researchers throughout globe are curious and fascinated towards the discovery of new materials capable of storing and providing green energy at our convenience. In this last decade, numerous advanced functional materials have been explored for their high-energy applications. Solid Oxide Fuel Cells (SOFCs), Solar cells, gas sensors and membrane technology have employed many of them as reliable electrode and electrolyte materials for energy conversion [1-2]. Oxide materials of specific structure are potential candidates for such applications [3-8].Certain catalytic nanomaterials (0-10 nm size) based on oxides of cerium, zirconium, titanium, tin, molybdenum etc., their metal doped oxides and mixed oxide systems have the potential of losing and reabsorbing oxygen at high and low temperatures respectively through their lattice oxygen framework [9-13]. This tendency of these tailored functional nanomaterials is exploited to split carbon dioxide and water in presence of solar radiations into mixture of carbon monoxide and hydrogen (commonly known as water/synthetic/syn gas) which is used as fuel gas for energy production [14-16]. It resembles artificial photosynthesis. A device/set-up can be envisaged using quartz window equipped with Fresnel lens in order to concentrate solar radiation into the chamber lined with the suitable nanocrystalline catalytic oxide materials where CO_2 and H_2O of air/supplied source can be converted to syn gas/alternative transport fuel [13-16]. A solar device big enough to fit on average house rooftop (or shiptop in sea) could be engineered capable of generating required fuel to fulfill the transport need fully/partially.

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Poster Presentation-38

Cyclic Voltammetry Study of a Novel Phase Transferring Oxidant Cetyltrimethyl Ammonium Ferricyanide (CTAFC) in Organic Medium

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Abstract: Phase transferring oxidants have gained much interest due to their solubility in organic solvents and mildness of the oxidants. We have synthesized a novel lipopathic oxidant cetyltrimethyl ammonium ferricyanide $(CTA)_3[Fe(CN)_6]$ (CTAFC), from cetyltrimethyl ammonium bromide (CTAB) and potassium ferricyanide and have characterized it from UV,

IR, NMR spectral data and elemental analysis. Its cyclic voltametry investigations have been performed in organic medium at different scan rates (Figure 1). The linear dependency of peak current with square root of scan rate indicates the reduction of Fe (III) to Fe(II) in CTAFC to be diffusion controlled. A comparison has been made between the cyclic voltammograms of CTAFC in acetonitrile and mixture of potassium ferricyanide and CTAB in aqueous medium. Though the medium are completely different, the higher diffusion of CTAFC may be attributed to the hydrophobic CTA group enveloping the Fe (II) ions.

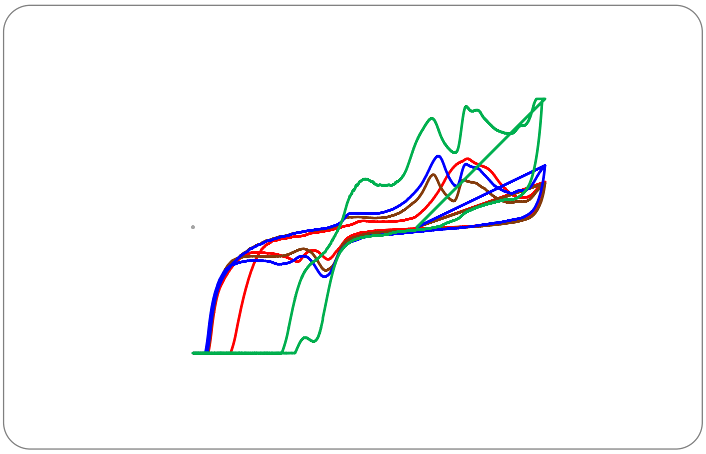

Figure 1:*Cyclic voltammograms of CTAFC inCH_3CN at different Scan Rates.*

Poster Presentation-39

Characteristic Studies of One Dimensional Nanocomposites

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Abstract: The project involves synthesis of one dimensional heterocyclic polymers – metal nanocomposite. Cobalt in nano form was prepared from cobalt chloride hexahydrate by reduction method. The one dimensional nanocomposite was prepared in situ by taking a solution of polypyrrole in acidic medium followed by ammonium persulphate /HCl with continuous stirring. Cobalt in nano form was added to it with different wt% with continuous stirring for 2 Hrs. The work highlights the determination of optical properties, band gap and Refractive index of nanopolymers and nanocomposites using UV-Vis spectra. Characteristic peak around 300 nm was observed in the nanopolymer and nanocomposites. Confirming the formation of nanopolymers and nanocomposites. The energy gap was determined using Tauc’s plots. The results revealed that the band gap of polymer changes on doping with nanoparticles. The band gap of pure nanopolypyrrole was found to be 1.6 eV. The nanocomposites of polypyrrole-Ni-nanocomposite has band gap 2.1eV and refractive index 2.651. The nanopoypyrrole and polypyrrole-Mn-nanocomposite has lowest band gap 1.6 eV and highest refractive index 2.893 among all nanocomposites.

Keywords: Polymers, Nanocomposite, Polypyrrole and Band gap

Poster Presentation-40

Solvent Polarity Sensing using Some Bischromophoric Styrylpyridinium Dyes

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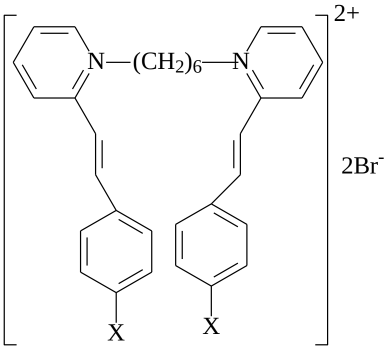
Abstract: Two bischoromophoric α-styrylpyridiniumdyes with hydroxy (OH: **1**) and N,N-dimethylamino (NMe_2: **2**) substituents with flexible spacer have been synthesized (Figure 1). Their solvatochromic behavior in 13 solvents of various polarities has been studied. Both the dyes clearly sense the polarities of the solvents. Based on the sensing, the solvents can be classified into three categories: non-polar, dipolar aprotic and polar protic. In each class of solvent, positive solvatochromism is observed (Figure 2).



X = OH (1), NMe_2 (2)

Figure 1

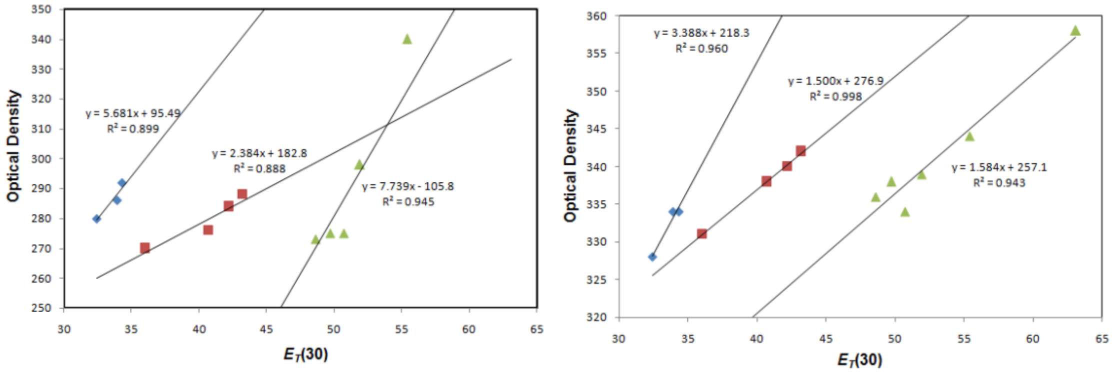


Figure 2

The dyes can further be used as molecular tweezers and can be utilized for the study of molecular recognition.

Poster Presentation-41

Unmodified and modified Silica Scaffolds for the Adsorption of a Methine Dye from Organic Solvent Medium

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Abstract: The work describes the adsorption of a methine dye on unmodified silica surface and sodium dodecylsulphae (SDS) modified and polyethylene glycol (PEG) modified silica surfaces from dichloromethane medium at 25$_{\text{o}}$C. The rate of adsorption in all cases obeys second order kinetics. A negative enthalpy change (ΔH = -41.8 kJ/mol) indicates the adsorption to be an exothermic process and low entropy change (ΔS = 0.13 kJ/mol/K) depicts the involvement of an ordered adsorption mechanism. Comparison of rate constants shows an increase in the order, Unmodified silica < SDS-silica < PEG-silica. The surface silanol groups propel adsorption on unmodified silica, whereas adsorption of SDS-silica may be due to the coulombic force of attraction between the anionic surface and the cationic dye. The hydrophobic tail of PEG may be responsible for the adsorption of the dye on PEG-silica. Temperature, adsorbent amount, concentration of the dye, solvent polarity as well as substituent on the dye molecules will be varied to obtain a clear significance of the work.

Poster Presentation-42

Cr(VI) Oxidation using Cetylpicolinium Dichromate (CPDC) – Kinetics of Oxidation of Aliphatic Alcohols

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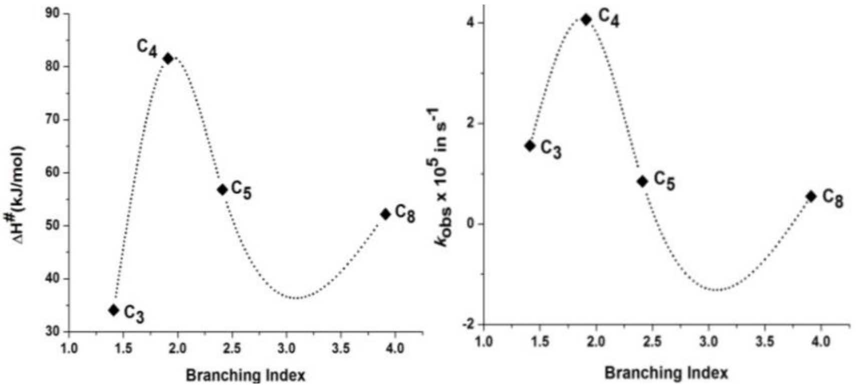
Abstract: Oxidation kinetics of various alcohols having varied hydrocarbons has been studied using cetylpicolinium dichromates (CPDC), a class of novel phase transfer oxidants, in DCM medium. The rate of reaction is first order with respect to oxidant and fractional order with respect to the substrates. Michaelis-Menten type oxidation was observed with respect to the substrates. Alcohols are found to be oxidized to their corresponding aldehydes. The mechanism of oxidation reaction has been suggested based on solvent isotope effect, and thermodynamic study. Solvent isotope effect ($k_{\text{CHCl3}}/k_{\text{CDCl3}}$= 1.42) indicates the involvement of hydrogen exchange with the medium during oxidation reactions. A strong influence of specific solute–solvent interactions on the rate of the reaction is observed. The graph of χ, Randic topological parameter,against $k$obs for normal chain alcohols is shown in Fig. 1b. A similar trend is also observed when the enthalpies of activation of the alcohols are plotted against χ

(Fig. 1a). Both the plots indicate a similar change at *n*-butanol, which is considered to be the most active substrate out of all the normal chain alcohols.



(a) **(b)**

Figure 1

Poster Presentation-43

Nano Silver decorated Propylene Oxide/Polyethylene Oxide-Cellulose Nanohybrid Composite Hydrogels for Drug Delivery Applications

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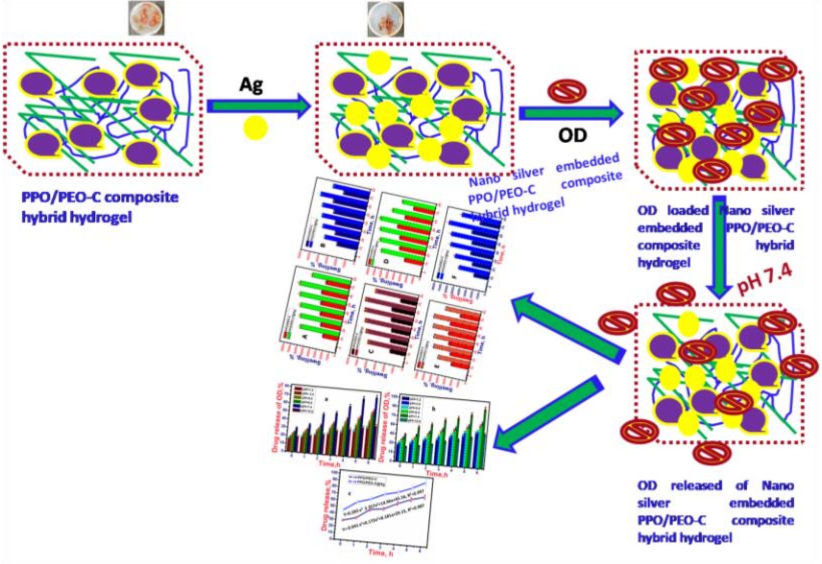
Abstract: In this work, nano silver embedded polypropylene oxide/poly ethylene oxide-cellulose (PPO/PEO-C@Ag) biodegradable nanohybrid composite hydrogel are synthesized by *in situ* polymerization technique for the *in vitro* release of ornidazole drugs.The change in structural, morphological and functional properties are noticed due to combine effect of PPO/PEO-C and nano silver by FTIR, XRD, XPS, SEM, EDX mapping and TGA. The distribution of particle in the nanohybrid composite hydrogel is determined from zeta potential measurement. The interaction between the Ag NPs and PO/PEO-C are elucidated using different spectroscopic techniques, which in turn are responsible for the uniform distribution of the Ag NPs in the PPO/PEO-C matrix. The resulting hydrogels structure, morphology, thermo responsive property, water retention and swelling behavior are investigated. The thermal stability of the as-synthesized nanohybrid composite hydrogel is studied by TGA. The rheological measurements confirmed the incorporation of equally distribution of nano silver to PPO/PEO-C system significantly enhanced the viscoelasticity and stiffness of hydrogels. The antibacterial activity of the biodegradable silver nanohybrid composite hydrogel is studied by inhibition zone method against *Shigella Flexneri* (SF), *Bacillus cereus* (BC), *Escherichia coli* (EC) and *Listeria Inuaba* (LI). The drugs are incorporated either during cross-linking by dissolving it in the reaction medium or after cross-linking by the soaking technique. The *in vitro* drug release showed a dependence on the extent of cross-linking, amount of drug loading, nature of drug molecule and method of drug loading. Even through the release of drugs is swelling controlled in the initial stages, in the later stage diffusion of the solute is dominating. The drug delivery applications of the nanohybrid composite hydrogel are evaluated using ornidazole as a model drug. Maximum drug release of 96.4% is recorded at7.4 pH after 5 hour. Cytotoxicity of the nanohybrid composite hydrogel is verified using mouse fibroblast cell line L-929 (ATCC CCL-1) cells for their possible use as controlled drug delivery vehicles. Nanohybrid composite hydrogel are found to be nontoxic in nature and more biocompatible as compared to neat PPO/PEO-C, as observed through cell viability. The results indicated that the PPO/PEO-C@Ag nanohybrid composite hydrogel exhibited pH-sensitivity and could be applied efficiently as biodegradable carriers for colon-specific ornidazole delivery.

Keywords: Nanohybrid composite hydrogel; Ag NPs; Rheology; Ornidazole; *In vitro*



Scheme 1: *Schematic Illustration of Ornidazole Drug loaded and released of PPO/PEO-C@Ag Nanohybrid Composite Hydrogel*

Poster Presentation-44

Nano ZnO imprinted poly (N-isopropylacrylamide)/Polyacrylamide Nanocomposite Hydrogels for *in vitro*Release of Olifloxacin

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Abstract: In recent times, hydrogels have made tremendous progress in the field of biomedical application as drug delivery system because of its unique biodegradable nature, along with its high sensitivity to several environmental factors. This work is focused on the novel thermally-sensitive nano ZnO imprinted poly

(*N*-isopropylacrylamide)/polyacrylamide)(PNIPAM/PAM@ZnO) nanocomposite hydrogels are synthesized by *in situ* polymerization technique for the *in vitro* release of olifloxacin drugs.The chemical interface in PNIPAM/PAM@ZnO nanocomposites hydrogels is confirmed through Fourier transform infrared (FTIR) spectroscopy. The formation of nanocomposite hydrogel is evidenced by XRD, FESEM, EDX mapping, XPS, and TGA. The distribution of particle in the nanocomposite hydrogels is determined from zeta potential measurement. Moreover, swelling behavior, water retention, thermo responsive and mechanical properties are systematically investigated. The gelling strength and gelation time of synthesized materials are noticed from the rheological study. The antibacterial activities of the nanocomposite hydrogel are studied against *Shigella Flexneri* (SF), *Bacillus cereus* (BC), *Escherichia coli* (EC) and *Listeria Inuaba* (LI). The drugs are incorporated either during cross-linking by dissolving it in the reaction medium or after cross-linking by the soaking technique. The *in vitro* drug release showed a dependence on the extent of cross-linking, amount of drug loading, nature of drug molecule and method of drug loading. Even through the release of drugs is swelling controlled in the initial stages, in the later stage diffusion of the solute is dominating. Cytotoxicity of the nanohybrid composite hydrogel is verified using mouse fibroblast cell line L-929 (ATCC CCL-1) cells for their possible use as controlled drug delivery vehicles. Nanohybrid composite hydrogel are found to be nontoxic in nature and more biocompatible as compared to neat PNIPAM/PEG, as observed through cell viability. The capability of the synthesized nanohybrid composite hydrogels to be employed as a colon-specific drug delivery vehicle is executed at various pH using olifloxacin as a model drug. The capability of the synthesized PNIPAM/PAM@ZnO nanocomposite hydrogels with improved thermal, mechanical, and rheological properties make suitable as a good carrier for release of drugs.

Keywords: Nanocomposites hybrid hydrogels; Nano ZnO; Rheology; Olifloxacin

Poster Presentation-45

Plastics and Bioplastics in Packaging: An Overview

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Abstract: The largely use of these traditional synthetic polymers/plastics has already resulted in a serious ecological problemsas plastic products have become a vital asset for humanity and have brought benefits to society in terms of economic activity. It concerns with the dumping of non-biodegradable plastics in landfills. In the present review, the major advantages and challenges of these bioplastics over conventional synthetic plastics were compared [1]. Several important biopolymers such as polylactic acid (PLA), starch and cellulose were discussed in details [2]. The chemical structures, mechanical properties, thermal properties, and recycling of these biopolymers were summarized. The bio plastic-based materials have garnered increasing attention to packaging market due to the concerns from both

environmental and economical perspectives of traditional petroleum based polymers in recent years.

Keywords: Bioplastics, Packaging, Environmental, Sustainability

About the Fact: Certain limitations of using bioplastic over conventional plastics:Plastics are a comparatively low thermal resistance and a strong interdependence among thermal mechanical and barrier properties. For this we can use polymers directly extracted from biomass such as the polysaccharides, chitosan, starch, cellulose, proteins, polycaprolactones, polyvinyl-alcohol, ethylene-vinyl alcohol copolymer and sustainable monomers of polylacticacid (PLA).

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Poster Presentation-46

Nano Silver based Composites for Catalytic Reduction of 4-nitrophenol

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Abstract: Recently, metal nanoparticles are gaining special attention in the field of nanocatalyst along with their other technological applications like optoelectronics, photography, surface-enhanced Raman scattering, biological labelling, formulation of magnetic ferrofluids and photonics. It is because of their size and shape dependent optical and electronically behaviours. Although, 4-nitrophenol (4-NP) is widely used in many pharmaceutical industries for formation of pesticides, fungicides and insecticides, but it is a toxic water pollutant present in waste water that discharges from industry and agriculture, since it is highly soluble and more stable in waterand it may cause problems in both plant and aquatic organisms. Therefore, it is a challenge to adopt an effective technique for elimination of 4-NP from waste water. Herein, a low cost and eco-friendly approach are adopted for the synthesis of L-cysteine assisted silver/reduced graphene oxide (L-cys-r-GO/Ag) nanocomposites for catalytic reduction of 4-NP. The excellent behaviour of L-cys-r-GO/Ag nanocomposites acting as a heterogeneous catalyst for the conversion of 4-nitrophenol to 4-aminophenol with $NaBH_4$ is achieved which is due to the high adsorption of reactant on the surface r-GO and more transfers of electron from r-GO to Ag NPs.

Keyword: L-cysteine; Nanocomposites; Heterogeneous catalyst; Catalytic efficiency

Poster Presentation-47

Rhodamine based Nano Silver decorated Graphene Oxide Nanocomposites for Sensing of Hg^{2+} Ion

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Abstract: Present day, monitoring of toxic pollutants such as heavy metal ions from water resources is important and challenging, since these, pollutant affects not only the human health but also the environment. Among different heavy metals, mercury (Hg^{2+}) is one of the most toxic pollutant due to its strong affinity to sulphur containing group so that it affects the enzyme and protein in the body. Exposure of mercury can cause many diseases such as Hunter-Russell syndrome, acrodynia, and Minamata disease. Therefore, development of low cost, selective and sensitive method is required for mercury detection. Herein, we have synthesized rhodamine B based Ag/r-GO nanocomposites which are non-fluorescent using Ag/r-GO nanocomposites as quencher. Transmission electron microscope (TEM) and scanning electron microscope (SEM) of nanocomposites are carried out to investigate the morphological analysis. When these Ag/r-GO@RhB nanocomposites interact with Hg^{2+}, rhodamine B is separated out from Ag/r-GO with producing a highly fluorescence emission. This is due to the soft-soft interaction, cationic- π interaction and interaction of Ag & Hg^{2+} ion in the nanocomposites. The present fluorescence approach shows very small limit of detection (LOD) of 2 nM at optimized pH and optimized contact time.

Keywords: Silver nanoparticle; Reduced Graphene Oxide; Rhodamine B; Hg^{2+} ion

Poster Presentation-48

Green Synthesis of Water Soluble Gold Nanoclusters for the Detection of Hg^{2+} Ions

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Abstract: Recently, environmental pollution is attributed due to presence of many heavy metal ions and human beings are affected due to this problem because many heavy metals are toxic and non-biodegradable. Among them, mercury (Hg^{2+}) is one of the important environmental pollutants that is widely spread in soil, water and food. Mercury can cause various diseases such as minamata, acrodynia and hydragyria and also affects kidney, brain and nervous system that constitute a serious threat to human being. Therefore, developing a sensor that detects ppb level of mercury is a significant step for environment safety and health monitoring for researchers. Herein, a simple, facile and biocompatible fluorescent sensor using L-cysteine assisted chitosan reduced gold nanocluster (L-cys/CS-AuNC) is prepared by "one pot" synthetic protocol for ultrasensitive detection of Hg^{2+}ion, which produces a strong orange fluorescence emission at 575 nm. The morphology of nanocomposites are studied by transmission electron microscopy. The detection limit (LOD) for mercury (II) is found to be 3 nM. Moreover, the L-cys/CS-AuNC can be applied to real water samples such as pond, river and tap water for detection of Hg^{2+} ion.

Keywords: Chitosan; Gold Nanocluster; Mercury; L-cysteine; turn off

Poster Presentation-49

Nano Silver incorporated Polyacrylic Acid/GO Hybrid Nanocomposites as Packaging Material

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Abstract: Herein, a low-cost and eco-friendly approach is adopted for the synthesis of poly acrylicacid/GO/Ag (PAA/GO/Ag) nanocomposites using sodium alginate as reducing agent in aqueous medium via*in situ* polymerization technique. The formation of AgNP in nanocomposites is confirmed by SEM and XRD study.The chemical interactions of PAA/GO with AgNPs are established by Fourier transferred infrared (FTIR) study. The average diameter of dispersed Ag NPs is 50 to 70 nm, which is evidenced by transmission electron microscope (TEM) and DLS study. Thermogravimetric analysis reveals more differences of weight loss (i.e. 11%) between PAA/GO and PAA/GO/Ag nanocomposite.The enhanced thermal stability of the PAA/GO/Ag nanocomposites is achieved by incorporation of AgNPs. The tensile properties and antibacterial behaviour of PAA/GO/Ag nanocomposites are also increased by incorporation of AgNPs. The oxygen barrier behaviour of PAA/GO/Ag nanocomposites is increased by eleven folds with reinforcement of $27x10^{-3}$ wt% of AgNPs as compared to PAA/GO Matrix. Therefore, the incorporation of AgNPsenhances the oxygen barrier, thermal, chemical resistance and antimicrobial properties of the PAA/GO matrix by which the synthesized material is suitable for packaging applications.

Keywords: AgNPs; Antibacterial; Oxygen barrier; Nanocomposites; Packaging

Poster Presentation-50

Thermal Degradation Behaviour and Kinetics of Pyrolysis of Electronic Plastic Waste

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Abstract: Advances in the electronic telecommunication and information technology have improved all aspect of lifestyle by providing high-end electronic gadgets with new functionalities. Due to its virtual nature, the IT sector appears environmental friendly but in actual practice, it contributes different pollutions. One of the major problems is generation of e-wastes that describes discarded electrical or electronic devices otherwise called waste from electrical and electronic equipment (WEEE). Plastic materials constitute a most important share in the electrical and electronics accessories due to their distinct properties. Therefore, the amount of waste plastics from such sector is increasing continuously and this situation causes serious environmental issues. As plastic wastes cannot be subjected to composting or land filling due to their non-biodegradable properties, the recycling of waste plastics by pyrolysis has attracted much interest as an alternative method for their disposal and management over the last few years. Thermal or catalytic pyrolysis of waste plastics yields gas and liquid products that can subsequently be utilized as fuels and valuable chemicals. The optimal design of the pyrolysis process and thus the reactor design require kinetics and thermodynamics data of the thermal degradation, and must be determined for better design and operation of the process. Thermogravimetric analysis technique is an excellent way for studying the kinetics of thermal degradation. This work focuses on the study of thermal degradation behaviour of discarded computer key board plastic waste; a type of electronic plastic (EP) waste using thermogravimetry analysis (TGA) at wide range of heating rates of 5, 10, 15, 20, 40, 60 and 100°C/min., leading to the study of kinetic using established equations. The average values of activation energy of the reaction are found to be 198.883, 193.612, and 197.765 $kJmol^{-1}$ calculated from model free methods such as Friedman, FWO, and Coats-Redfern method respectively. The kinetic data obtained in this work would be useful for accurate prediction of reactions behaviour, optimization of the process towards products and in the design of efficient commercial process for conversion of such electronic plastic wastes to energy.

Keywords: e-Wastes, Plastic wastes, Pyrolysis, TGA, Kinetic study

Poster Presentation-51

Photocatalytic Activity of mixed Oxides derived from ZnAlTi-Ternary Layered Double Hydroxides (LDHs)

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Abstract: Organic pollutants from the textile industry represent one of the major sources of water contamination. About 15% of commercially used dyes are discharged in to the environment, which requires suitable treatment before their discharge to reduce the environmental pollution. Although a host of processes has been tried and some of them are in use, search for a greener and energy efficient treatment process is desirable. In this regards, photodegradation process, especially under visible/solar light, has attracted much attention due to the advantages of low cost, no generation of secondary pollutant and wider applicability. Therefore, developing new visible-light-driven materials with improved photodegradation efficiency of dyes has acquired greater relevance.LDHs have been most extensively employed as a bifunctional acid-base heterogeneous catalyst. In recent years, there is a growing interest to develop LDH based photocatalysts as an alternative to

conventional semiconductor oxides for degradation of variety organic pollutants including dyes as well as for generation of H_2 from water. In particular, the mixed oxides derived from ZnAl/MgAl containing LDHs (with or without Fe, Sn, Ce and Ti as a component) have shown potential for degradation of some commonly occurring organic water contaminants like phenols/phenolic, dyes etc. In this work the photocatalytic behaviours of derived mixed oxides from corresponding LDHs towards a model dye Alizarin Yellow 2G (AYG), under visible light irradiation was reported. The mixed oxides containing Zn. Al and Ti, derived from corresponding ternary LDH precursors, were characterised by different physicochemical methods (PXRD, Uv-Vis-DRS, TEM, FT-IR). The mixed oxides showed relatively lower band gap energies compared to ZnO or TiO_2-P25 and showed better activity towards photo-degradation of aqueous AYG dye. Under identical conditions, the photodegradation activity increased with increase of Ti content in the catalyst. The results of photocatalytic activity under various experimental parameters were discussed and a suitable mechanism was also proposed for the degradation process.

Poster Presentation-52

Recogination of a Bromnide Ion by the protonated form of 2-(1-H-Imiddazole2-ylthio)-3-methylnapthalene-1,4-dione

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Abstract: Supramolecular chemistry of anions is an important field of research in biological and environmental science. Hosts for different anions are generally formed by protonation of a neutral molecule(s) to offer electrostatic interactions to bind an anion. Thus, understanding host–guest binding of a neutral host interacting with an acid in a selective manner has great potential for the design of a new host for anions as well as acid recognition. Furthermore, the anion-directed assemblies of coordination polymers are also used for molecular recognition, guest inclusion, and catalysis. Imidazole-containing compounds are of interest in anion binding; because they occur as amino acid residues of natural proteins. The interactions of various acids, such as hydrochloric, hydrobromic, nitric, perchloric, and tetrafluoroboric acids with (1Himidazole-2-ylthio)-3-methylnaphthalene-1,4-dione (L) enhance the intensity of the fluorescence emission of L. Exceptionally ,the interaction of hydrogen bromide with L not only enhances the emission intensity, but also leads to a sharp characteristic emission at l=480 nm (lex=350 nm), which is different from the other acids. Bromide-ion recognition by protonated L is explained based on a tautomeric equilibrium. The Stokes shifts were calculated for each case and they were dependent on the anions and, in general, were found at l>100 nm. Fluorescence lifetimes were measured and it was shown that two independent paths operated for the emission processes in solutions of the salts of L.

Keywords: Anions; Fluorescence; Imidazoles; Molecular recognition

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Poster Presentation-53

Unusual C–H Bond Activation at Ambient Condition of 2,2'-(1,4-dihydro-1,4-dioxo-naphthalen-2,3-diylthio)dipropanoic Acid

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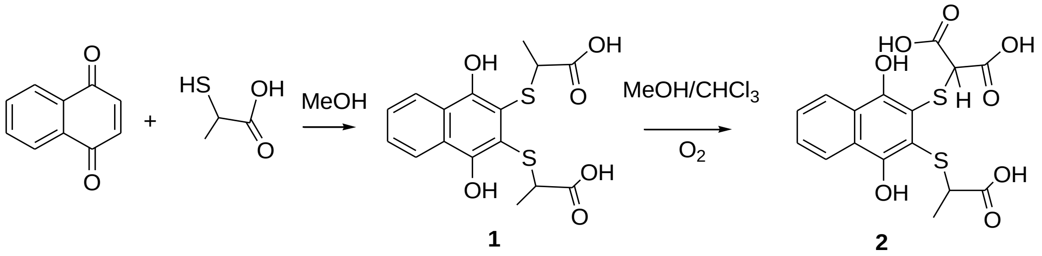
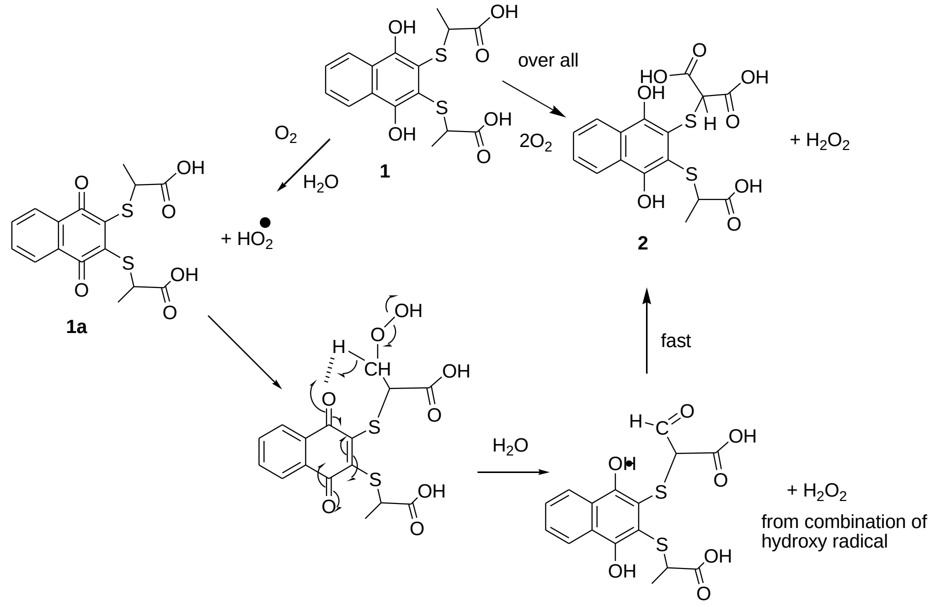
Abstract:2,2'-(1,4-dihydro-1,4-dioxo-naphthalen-2,3-diylthio)dipropanoic acid undergoes oxidation under ambient condition to form 2,2'-(1,4-dihydro-1,4-dioxo-naphthalen)-3yl-thiomalonicacid, 2-propanoic acid.

Keywords: Naphthoquinone; Thiolactic acid; Side chain oxidation; C–H activation.

General Reaction:



Mechanism:



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Poster Presentation-54

Phosphoric Acid (H_3PO_4) promoted [2+2] Cycloaddition of 2-methyl-1,4-naphothoquinone Derivatives *via* C–S bond Cleavage and Study of Their Protein Interactions

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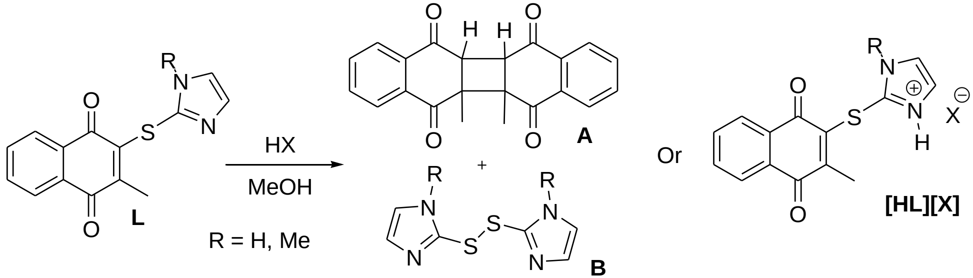
Abstract:Phosphoric acid (H_3PO_4) promoted [2+2] cycloaddition of 2-methyl-1,4-naphothoquinone derivatives *via* C-S bond cleavage was synthesized and characterized by physicochemical and spectroscopic tools. The effect of binding interaction of Bovine Serum Albumin (BSA) and Human Serum Albumin (HSA) proteins with cycloaddion compound were studied by fluorescence titration method. From the binding constant, it was shown that BSA has higher affinity towards cycloaddion compound over HSA. Finally, molecular docking study was also performed with BSA to support the experimental results. From the docking analysis it was found that the cycloaddition compound formed hydrogen bonding (N-H···O) interaction with different amino acid residues, namely, Val-342 (N-H···O, 1.8 Å) and Lys-291 (N-H···O, 1.9 Å), whereas Arg-194 exhibits cation-π interactions with cycloaddition compound. Trp-213 present near 7.7Å from the cycloaddition compound.



Scheme 1:*[2+2] Cycloaddition Product Formation through Phosphoric Acid (H_3PO_4) assisted C–S Bond Cleavage.*

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Poster Presentation-55

Extraction of Nano-silica from Wheat Straw Black Liquor: A Green Route

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Abstract: Pulp and paper production from agricultural residues is an attractive future option from the standpoint of environment friendliness. The black liquor obtained from wheat straw pulping with caustic soda and anthraquinone as cooking additive contains much silica content, which causes severe problems during evaporation, combustion and recovery of alkali, using the conventional recovery method. In this study, silica nano particles are precipitated by decreasing pH of agricultural residues (e.g. wheat straw) black liquor by using sulphuric acid and carbon dioxide gas under controlled conditions. The morphology and microstructure analysis of the precipitated nano-structured silica particles was characterized through TEM, EDAX, FT-IR, XRD, TGA, XRF and BET. The nano-structured silica particles' yield reached more than 94 percent and the particles' diameter ranged 150 to 200 nm. The quality of the filtrate after precipitate separation was also monitored in each step. The black liquor, which involves perecipitation of silica was found high calorific value than without separation of silica from black liquor.In summary, agricultural residues black liquor with high content of silica can become a potential resource of low cost precursors for the production of high value-added silica/silicon materials for practical applications.

Keywords: Pulping, Black liquor, Agricultural resides, Nano-silica, Calorific value.

Poster Presentation-56

Equilibrium and Kinetic Study of Lead (II) Sorption from Aqueous Medium by a Fibrous Ion Exchanger

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Abstract: The quality of water is deteriorating by the geogoenic & anthropogenic activities mostly rapid growth of industries in different city of the world. The present investigation aims to remove Lead ion from aqueous medium by using a Cerium Phosphate based fibrous ion exchanger as an adsorbent material. Batch studies were carried out to study the efficiency of the adsorbent. Further the effect of various parameters like effect of Adsorbent dose, Temperature, pH, Contact time, Competitive ion adsorption and kinetic, equilibrium and

thermodynamic studies were also carried out to find out the effectiveness of the adsorbent towards adsorption of Lead. From the study it was revealed that the preliminary sorption start within 5 minutes of contact time. The maximum adsorption capacity was found to be 97.3% after one hour rotation of contact time at pH 5 and at a temperature of 50°C. The synthesized material was found faster and effective. The test results were applicable to both Langmuir & Freundlich model.

Poster Presentation-57

Recycling of Waste Plastics to Nanocomposites

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Abstract: With the increase in population leading to enormous usage of plastic that’s causing a threat to environment it is highly necessary that the waste plastics are converted into valuable materials by upcycling processes. One such process is preparation of polymer nanocomposites by recycling the waste plastics and as polymer nanocomposites have attracted remarkable attention from the scientific community for their unique combinations of advantageous chemical and physical properties, such as excellent heat conductivity, chemical stability, advanced optical properties, and high mechanical strength and the remarkable changes on physical and mechanical properties of polymers due to the addition of nanoparticles. With this preview, different types of waste plastics (polypropylene, High density polyethylene, low density polyethylene, polystyrene) are blended with functionalised Carbon nanotubes (CNTs) in different proportion by melt mixing method and the nano composite obtained are characterized by means of Fourier transform infrared (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), thermo gravimetric analysis (TGA), differential thermogravimetric (DTG), and differential thermal analysis (DTA) to understand the improvement in the properties.

Keywords: waste plastics, polymer nanocomposites, CNT, Melt mixing

Poster Presentation-58

Computer Aided Drug Design on HIV-1 Protease Inhibitors

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Abstract: Human Immunodeficiency Virus type I (HIV-1) is a pathogen that causes a continuous and depressive disease of the human immune system known as human acquired immune deficiency syndrome (AIDS).[1] The human immunodeficiency virus type 1 aspartic protease (HIV-1 PR) has been found to be an important enzyme due to its vital role in viral maturation. The accurate prediction of enzyme-substrate interaction energies is one of the major challenges in computational biology. The enzyme therefore is an attractive target in anti-AIDS drug design, and the effect of binding various inhibitors on the protease, structure is currently the focus of intensive research. In this study, we illustrate the importance of molecular docking method by using AutoDock tools to predict the HIV-1 protease-inhibitor binding energies. The present study illustrates the irreversible HIV-1 PR containing small epoxide molecule and its substiuent based on Computer Aided Drug Design. The molecular docking study provides best solution based on highest binding energy and lowest RMSD values of receptor-ligand complexes. The clustering histogram for all the 10 different conformations of ligand -1, ligand-2 and ligand-3 bound to HIV-1 have been analyzed. The cluster RMSD value indicates for the conformation-7 of ligand-1 as lowest with highest binding energy 6.37 kcal/mol, conformation-3 of ligand-2 as lowest with highest binding energy 5.40 kcal/mol and conformation-5 of ligand-3 as lowest with highest binding energy 5.37 kcal/mol revealed as stable protein-ligand complexes as compared to EPNP having highest binding energy 5.33kcal/mol and lowest RMSD value.

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Poster Presentation-59

Theoretical Investigation on Spectral Signature of Astro Molecules: Glycine and Aminoacetonitrile

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Abstract: The prebiotic chemistry of the Earth has been explored with the discovery of glycine in space, which brings enormous research interest2 for last several years.The aminoacetonitrile is also an interesting organic molecule because it was detected in SgrB2, which could be a precursor of the smallest amino acid molecule, glycine, in astrophysical environments.The present investigation reports the conformational studies and spectral spectral signature of astro

molecules: Glycine and Aminoacetonitrile. Density functional methods with dispersion corrections have been used with Pople triple zeta basis sets for all possible conformers, based on the $-NH_2$, -COOH and -CN group orientation of the glycine and aminoacetonitrile molecules with respect to both conventional and non-conventional interaction with water molecule. We report the molecular structure and the characterization of the rotational and IR spectra, the most important issues for a correct theoretical description and a proper comparison with experiment.

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Poster Presentation-60

Studies of the Formation of Iron Oxide Nanocrystals Synthesized by Emulsion Method

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Abstract: Iron Oxide (Fe_2O_3) is an important material and widely used in many industries such as electronics, sensors, catalysts, dyes, biotechnology, medicines and thermite materials. In the present studies, iron oxide nanorods were synthesized by emulsion-precipitation method. The precursor material so obtained was calcined at different temperatures. The samples were characterized by XRD, TG-DTA, FTIR and SEM. Precursor material contained FeOOH phase may be due to γ-Fe2O3 along with crystalline water. Thermogram of the precursor showed two step weight losses with a broad exothermic DTA peak at $346_{o}C$. First step weight loss may be due to loss of crystalline water and combustion of remaining surfactant of the precursor samples and second step may be due to transformation of gamma to alpha Fe_2O_3. Crystallite size of the maghemite was 19.0nm and it remained unchanged up to $600_{o}C$. Conversion of gamma to alpha phase tends to form nanorods with a diameter of 80-200 nm and increase in crystal growth with a maximum crystal size of 176.5 nm. Iron oxide nano crystals are ideal materials for biomedical applications and also in magnetic separations for arsenic and uranium removal due to their well-established biocompatibility.

Key words: Iron oxide, Nanorods, XRD, SEM, Emulsion

Poster Presentation-61

Synthesis, Characterization and Study of Sensor Properties of Some Xylene based Molecular Tweezers

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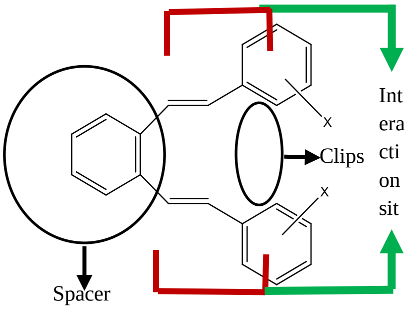
Abstract: The present work describes the synthesis, characterization and sensing properties of some xylene based polymethine molecules, which act as molecular tweezers towards foreign guests. The molecules were synthesized by the condensation of xylene and substituted benzaldehydes in 1:2 ratio in presence of a strong base. The compounds having a benzene spacer bridged between the two interaction sites with various substituents such as -OH and -NMe$_2$ create an electron-rich cavity, thus acting as molecular tweezers (Figure 1). The molecules were characterized from melting point, FTIR and ^{1}HNMR analyses. The clefts predominantly respond towards the cationic and neutral guests following the mechanism of host-guest model. The sensing property of the host molecules for Hg^{2+} ion was studied by measuring the fluorescence intensity in dichloromethane medium. A decrease in fluorescence intensity of the host molecule was observed, which can be attributed to the formation of host-guest complex between the polymethine molecuels and Hg^{2+} ion (Figure 2).



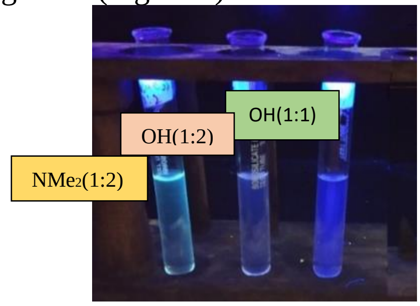


Figure 1:*Structural Representation of Xylene based Tweezer* **Figure 2:***Fluorescence Intensities of Clefts with Various Clips*

Poster Presentation-62

Defluoridation of Drinking Water using New Adsorbent Materials

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Abstract: Defluoridation using adsorption technique is accepted worldwide for its simplicity of operational procedure which serves as an effective method for design process as well as cost factor. Development of new materials and technology often involves critical evaluation of material performance characteristics as well as regeneration capability for sustainable use. Current attempt is focused on development of hybrid materials from combination of suitable organic functionality with a fluoride selective metal and the hybrid material was prepared using environment friendly sol-gel process. The cooperative effect of organic functionality and inorganic constituent were studied as a function of parameters. The synthesized adsorbents were characterized using FTIR, XRD, SEM-EDS and TGA-DTA. The pore

structure of the material was also evaluated using Hg-porosimeter. From the studies of adsorption kinetic and isotherms, the material – anion interaction parameters were evaluated for spiked samples as well as collected ground water samples under defined experimental protocols.

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Poster Presentation-63

One Pot Hydroxylation of Benzene to Phenol using Metal supported Red-Mud

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Abstract: Phenol is a key intermediate in chemical industry. Currently, phenol production is recorded as nearly about 10 million metric tons all over the world. Direct hydroxylation of benzene to produce phenol quite challenging goal to achieve. Phenol is synthesized commercially from benzene using three steps cumene process involves compression of both benzene and propylene at 30 bar pressure and at a temperature of 250°C. Such a process involves formation of intermediate such as cumene-hydroperoxide that requires careful monitoring of process parameters for industrial safety and production. Apart from this, requirement of high temperature and pressure including acidic condition of the process often resulted in low selectivity. In view of the above, the objective of the present work is development of a new catalytic material for hydroxylation of benzene to phenol using metal supported red-mud. Red-mud is easily available from alumina industry and the material can be useful as a support material due to some of its suitable properties. The catalytic material was prepared, characterized and tested for its efficiency for hydroxylation reactions. The protocol was established after several trial and error methods and successfully implemented in a lab-scale conversion process. It was observed that various factors such as reaction temperature, time, amount of oxidant plays an important role on the performance of the catalyst and the result significantly dependent upon the amount of H_2O_2 used in the reaction.

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Poster Presentation-64

Purification of Contaminated Water by using Novel Chelating Resins Containing Heterocyclic Moiety

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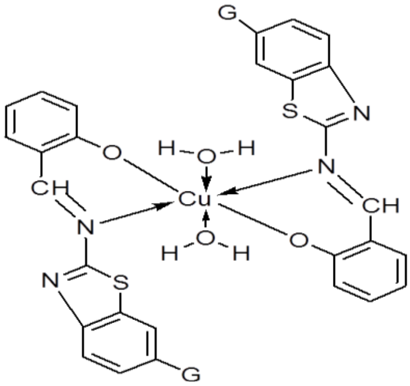
Abstract: The concentration of different toxic metals has increased beyond environmentally and ecologically permissible levels due to the increase in industrial activity. More than 1 billion people of the world are affected by drinking ground water contaminated with arsenic copper, cadmium and other toxic and heavy metals. Extraction of these metal ions is a difficult process as they are associated with a variety of complex species present in the natural aquatic systems. Again Copper, lead, nickel, cadmium, etc. are present as cations in ground and surface water while arsenic is present as anions like AsO_4^{-} and AsO_3^{-}. Therefore, different methods and mechanism are required to separate them from water. Chelating ion exchange resins having specific chelating groups attached to a polymer are excellent material for sorption and pre concentration of metal cations with specific selectivity at appropriate pH. Polymeric ligand exchanger, which is a metal complex of chelating resins, is one of the effective material for separation of arsenic. We have designed some novel chelating resins having heterocyclic ring systems and multiple functional groups. Their metal complexes with Cu^{2+}, Ni^{2+}, and Fe^{3+}were prepared. The adsorption behaviour of the synthesized resin towards Cu^{2+}, Ni^{2+}, and $Fe^{3+}$was studied by batch as well as column techniques with the variation of different parameters. The resin showed more effectiveness in the adsorption process towards Cu (II) ions in both competitive and non-competitive conditions. Simultaneously the copper and iron polychelates of the resin were used as polymeric ligand exchanger (PLE) to remove arsenate from drinking water. A comparative study was also done between the copper and iron PLE.



Poster Presentation-65

A Study of Physical, Mechanical and Thermal Aspects of Polyester Composites with Inorganic and Organic Fillers

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Abstract: This research throws light on the physical, mechanical and thermal properties of hexagonal boron-nitride filled polyester composites as well as hybrid composites with organic as well as inorganic filler. The inorganic ceramic filler like hexagonal boron nitride tends to enhance the thermal properties and provides hydrophobic character whereas an organic fiber such as Peanut husk tends to enhance strength of the composites. The effect of h-BN on the physical properties like density, water absorption and mechanical properties like tensile strength as well as compressive strength are studied. The density of the composites keeps on increasing with increase in filler content. With the rise in BN content in polyester resin from 0 to 35 wt%, a rise in density of the composites was registered in spite of an increase in void content. However, in case of hybrid composites, keeping the BN content constant and increasing the PH content there is a gradual fall in density, even when the void fraction still continues to increase. The increase in void content along with addition of low density PH fibers as well as due to air trapped inside voids together are responsible for decrease in the density of the composites which eventually decrease the weight of the composites. A gain in mechanical strength and hardness is also registered with the addition of peanut husk fibers. Similarly, an enhancement of thermal conductivity was there in case of single filler BN-polyester composites but PH fiber does not enhance thermal properties unlike mechanical and physical characteristics. Hence, a balance is maintained between BN and PH particulates to get the desired design specifications for different application areas according to our need. Therefore, with superior physical and mechanical properties, and enhanced thermal properties due to addition of h-BN ceramic filler and its hybrids, these polyester composites with appropriate amount of particulates can be utilized in various fields like heat engine laminates, engine casings, military equipments, fins and heat sinks, printed circuit board substrates etc. where faster heat transfer along with higher mechanical properties is an essential.

Keywords: Composites; Density, Tensile Strength, Thermal Conductivity; Boron Nitride; hybrids

Poster Presentation-66

Double Emulsion:An Ideal Candidate to Deliver the Drugs

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Abstract: Treatment of diseases using different drugs can cause various side effects due to uncontrolled release. Thus, researchers have put emphasis on controlled release of drugs. Drugs act by blocking enzymes, ion channels, transporters and receptors. Water-in-oil-in-water double emulsion technique is used to control the release of drugs. The choice of the emulsifying agent is usually done based on the HLB index. This work presents the application of Biovia software to identify the bio-surfactants. Different schemes have been proposed to control the release of a pair of drugs obtained from medicinal plants. Microencapsulation and bilayer micelization techniques have the potential to separate the drugs in the double layer emulsion. This work can help release of drug at target specific sites.

Poster Presentation-67

Spectroscopy and Molecular Docking based Biophysical Characterization of the Binding Interaction between Bone Morphogenetic Protein – 2 and Quercetin

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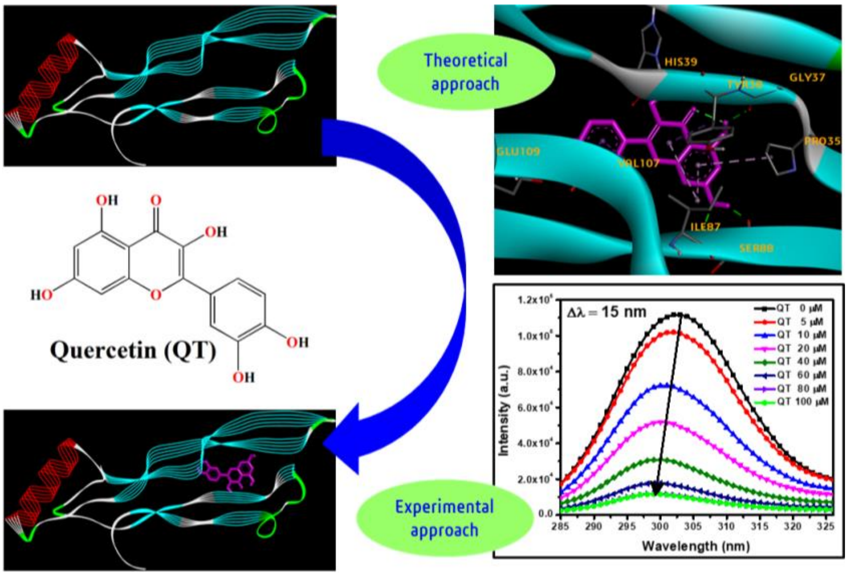
Abstract: Bone morphogenetic proteins (BMPs) are multi-functional growth factors that belong to the transforming growth factor beta (TGF-β) superfamily. We investigated the binding interaction between quercetin and BMP-2 by various spectroscopic, calorimetric and theoretical studies. Interaction profile represented a reduction in the absorbance of protein along with a prominent red shift under absorbance spectroscopy. The complexation was further confirmed from steady-state fluorescence quenching. It was accompanied by a significant blue shift. To narrow down the involvement of aromatic residues, synchronous fluorescence spectroscopy was utilized. Shifting was noticed only in case of Tyr residues; thus, confirming the alteration in confirmation is mediated upon reduction in polarity of tyrosine residues of the protein. The binding constant (10_{-2} M) of the protein increased with increase in temperature. Thermodynamic analysis revealed the involvement of van der Waals and hydrogen bonding which was further confirmed from molecular docking studies. These studies confirms a significant effect on the structure and confirmation of the protein in presence of quercetin and it may be used as a potential therapeutic for bone regeneration.



Poster Presentation-68

Physicochemical, Functional and Morphological Characterization of Starch isolated from Palm Tuber (*Phoenix Dactylifera)* for Prospective Applications

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Abstract: Starch is one of the digestible natural polymers found in vascular plants. This natural polymer is the primary source of polysaccharides to produce energy for humans. In this work, starch was extracted from underutilized date palm (*Phoenix dactylifera*) tuber using water treatment method and characterized it with respect to physico-chemical, functional and morphological characteristics. Starch yield was equal to 43.79 %, with low content of protein (14.34%) and fat (3.09%), 79.37 % of purity and with amylose content of 13.67 %, indicating low level of retrogradation after gelatinization process. Water and oil absorption capacities were 88.45 and 68.11 %, respectively. FTIR spectra reveals that the band at 3377 cm^{-1} might be attributed to -OH bond stretching and its width ascribed to the formation of inter and intra molecular hydrogen bonds. Spectral band range between 900 to 1100 cm^{-1} have been shown to be sensitive to changes in starch structure, in particular band at 1021 cm^{-1} and 1167 cm^{-1} may refer to anhydroglucose ring C-O stretch of C-OH stretch and crystallinity nature of native starch. The bands near 1653 cm^{-1} were attributed to deformation vibrations of hydroxyl groups. The peak near 2924 cm^{-1} was ascribed to asymmetric C-H stretching. XRD data was well correlated with FTIR study. The shape and size of starch granules differ according to the botanical source and the environmental condition under which a crop is grown. Palm tuber has oval and spherical shaped granules with different size ranging from 1µm to 10 µm (Figure 1). Starch granules play important role in size and shape of the amylose and amylopectin structure. Results indicated that, starch from palm tuber (*Phoenix dactylifera*) had potential in developing food and non-food applications.

Keywords:*Phoenix dactylifera*, Starch, Functional properties, FTIR study, Scanning Electron Microscopy.

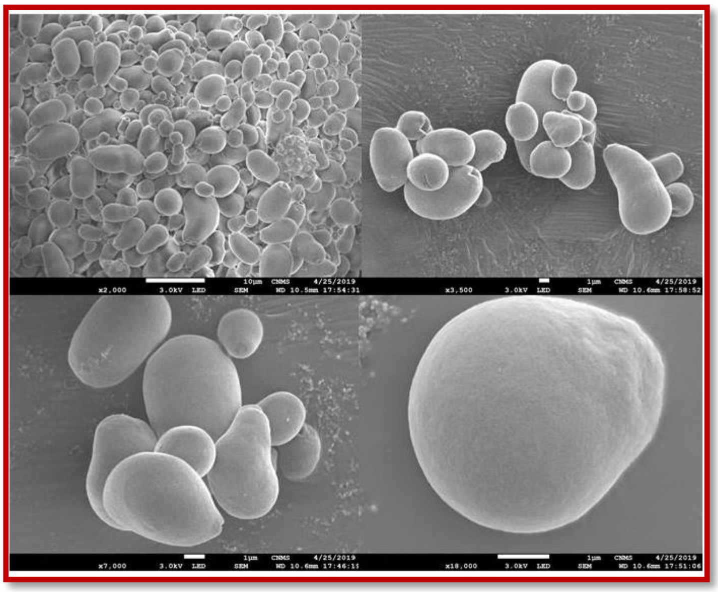

Figure 1: *Morphological Characterization of Plam Tuber (Phoenix Dactylifera) Starch Granules*

Poster Presentation-69

Designing a Method: The First Step in Bench-top Mimicking of Nature

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Abstract: Cycloisomerization reactions leading to the formation of functionalized bicyclic enol-ethers and spiroketals which constitute important functional moieties in many natural products, are characterized by their complete atom economy and provide attractive tool for delivering complex molecular diversity. A Pd-mediated cycloisomerization of 3-C-alkynyl-allo- and ribo-furanose derivatives was investigated in detail to understand the influence of electronic factors on the regioselectivity in ring closure reaction. A preference for *endo-dig* cyclization over *exo-dig* was noted, if the alkynyl substituent is not sufficiently electron

withdrawing. In continuation of our interest in the synthesis of bridged/spiro-bicyclic ketal skeletons,[1] we explored the Pd-mediated intramolecular ketalization of an alkynediol for the synthesis of Cyclodidemniserinol trisulfate (1),[3] a nonsteroidal integrase inhibitor of HIV-1 integrase, isolated from Palauan ascidian *Didemnum guttatum* (Figure 1).[4] Herein, the application of Pd-mediated intramolecular ketalization of alkynediols to construct the central [3.2.1]-bicyclic ketal core of cyclodidemniserinol trisulfate has been discussed.

Keywords: Palladium, C-Alkynyl furanose, Bridged bicyclic ketal, Alkynol cycloisomerization, Cyclodidemniserinol trisulfate

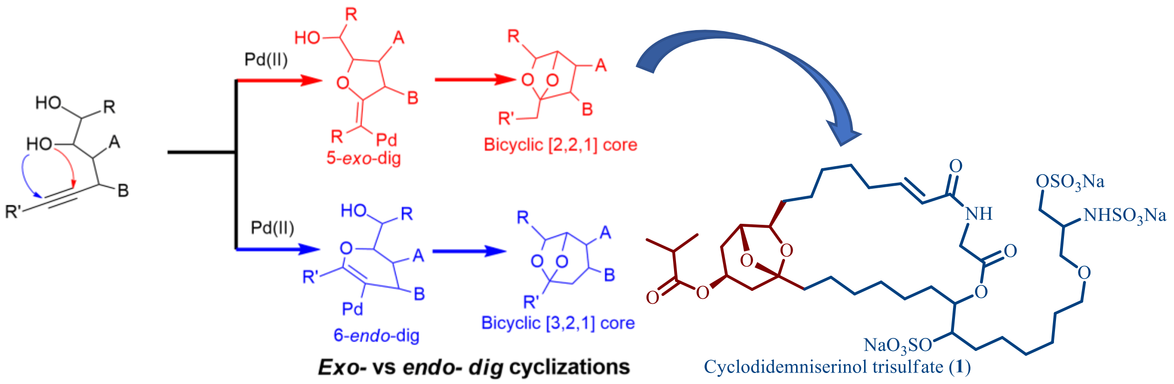

Figure 1:*Pd-mediated Cycloisomerization and Its Application in the Synthesis of Cyclodidemniserinol Trisulfate.*

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Poster Presentation-70

Cobalt Metal Organic Framework (Co-MOF) for Oxygen Electro Catalysis

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Abstract: The scarce availability of traditional energy resources (fossil fuels) motivates the energy researchers throughout the globe to develop alternatives. Therefore many of the energy conversion and storage systems (like fuel cell, batteries etc.) have developed and uses fuel like oxygen, hydrogen and small organic molecules like methanol, formic acid etc. Out of them, the hydrogen assumed to be the clean and green energy source for these purposes. One of the

efficient ways to generate hydrogen is the catalytic splitting of water, in which both the hydrogen (HER) and oxygen (OER) liberates efficiently. The effective generation of hydrogen depends on the conversion of water to oxygen. However, the OER associates with a multistep reaction mechanism, thereby faces sluggish reaction kinetics demanding more overpotential to execute the reaction. Additionally, in case of metal air batteries (i.e. Zn-air and Li-air batteries) the gaseous oxygen is widely used and both the oxygen reduction and evolution reactions are observed to be the heart of these metal air batteries. Here the molecular oxygen is reduced at cathode and combines with dissolved metals in electrolyte at the time of discharge and the reverse process occurs during the charging. Therefore, stable and efficient electro catalysts for the generation of these gaseous fuels and their efficient conversion to energy are highly imperative for smooth operation of these conversion/storage systems for future sustainability. Traditionally the noble metals (like Pt, Ru, Ir, etc.) and their oxides (RuO_2, IrO_2 etc.) were used as catalysts for this purpose. However, the high cost, low durability and detrimental environmental effect of these noble metal/metal oxide based nanostructures demand to develop new electroactive material. So we report the synthesis of Co-MOF $[Co_4(BTC)_3 (BIM)_6]$and explored it's electrocatalytic behaviour towards OER and ORR. The Co-MOF catalyses the ORR efficiently with a lower onset/reduction potential and higher reduction current density by a four electron reduction path. The MOF shows higher durability with >70% performance retention after 25 hour of reaction. The more active sites and accessible surface area of the Co-MOF enable to perform well towards OER with lower onset potential and small Tafel slope compared to the commercial RuO_2 nanoparticles. Additionally it needs only 280 mV overpotential to deliver the state of the art current density (10 mA/cm^2) and robust stability. It shows high value of TOF of 93.21 s^{-1} at as overpotential of 350 mV in comparison to the reported MOF/nanoparticle based electrocatalysts and the state of the art RuO_2; presume to use as both the cathode and anode electrocatalysts for the future energy storage and conversion systems.

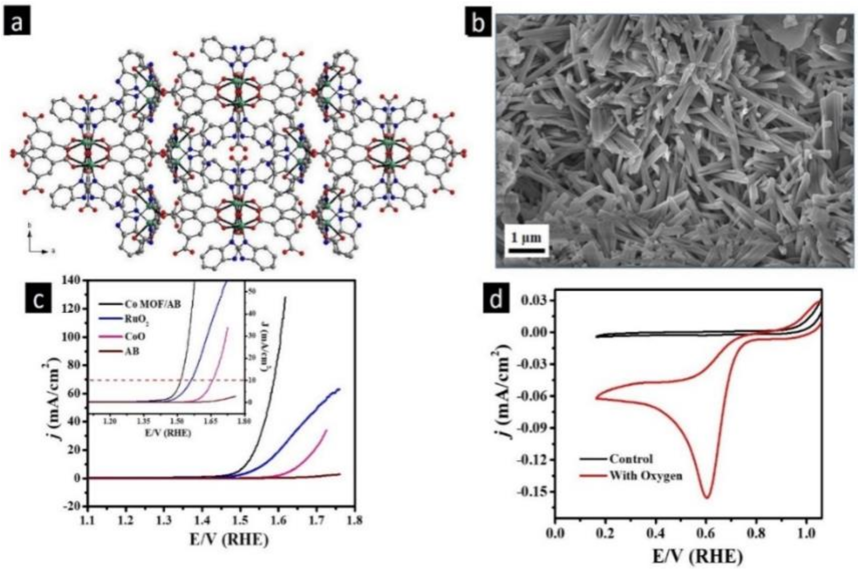

Figure 1:*(a) 3D View of [$Co_4(BTC)_3$ $(BIM)_6$] along c-axis, (b) FESEM Images for the Co-MOF, (c) LSVs for OER by Co-MOF/AB, Commercial RuO_2, CoO (after TGA) and AB in 1 M KOH Electrolyte at a Sweep Rate of 5 mV/s, (d)Cyclic Voltammogram for the ORR by the Co-MOF modified GCE in Oxygen saturated 0.1 M KOH Electrolyte at a Sweep Rate of 10 mV/s. The Control Experiment was carried out in Argon saturated Electrolyte.*

Poster Presentation-71

Synthesis of Polypyrrole Modified Layered Double Hydroxides for Efficient Removal of Cr(VI)

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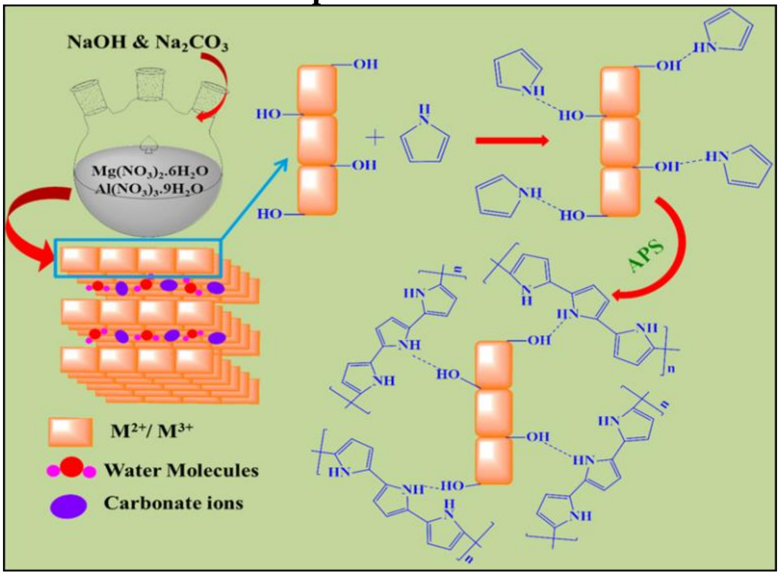
Abstract: Designing a stable, selective and efficient adsorbent for the removal of pollutants like chromium poses serious concern. Herein, an organic-inorganic hybrid material, polypyrrole modified Mg-Al layer double hydroxides has been reported as an adsorbent for Cr(VI) removal. The inorganic framework Mg-Al layer double hydroxides (LDHs) are synthesized via co-precipitation followed by hydrothermal treatment. The synthesized LDHs are enriched with polypyrrole coating via in-situ oxidative polymerization followed by microwave irradiation. The structure of the as-synthesized composite was delineated using various characterization techniques like FESEM, TEM, XRD, FTIR, RAMAN, BET, TGA-DTA and XPS which confirmed the successful formation of polypyrrole modified layer double hydroxides nanosheets (PPY-LDHs). The PPY-LDHs are applied towards the abatement for Cr(VI) from aqueous solutions at varying temperatures. The adsorption data fits well to Langmuir isotherm, and pseudo-second-order kinetics models suggesting monolayer

chemisorption in the superficial and interlayer regions. The adsorption mechanism is proposed which asserts that the removal of Cr(VI) onto the adsorbent was a combined effect of reduction of Cr(VI) to Cr(III) and chemical sorption which takes place through ion-exchange in the interlayer regions; on the surface through electrostatic attractions and hydrogen bonding. Hence, PPY-LDHs is an ideal adsorbent for the treatment of Cr(VI).

Graphical Abstract



Poster Presentation-72

Chitosan Hybrid Polyacrylic Acid Nanocomposite Hydrogels for Wound Healing Applications

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Abstract: When nanostructured materials are incorporated in the conventional gels, wound healing behaviour is enhanced due to high stability, good selectivity as well as improved antifungal and antibacterial properties. In the present work, chitosan (C) hybrid poly (acrylic acid) (PAA) nanocomposite hydrogels are synthesized using *in situ* technique by incorporation of nano $CaCO_3$ and reduced gold nanoparticles (Au Nps). As-synthesized PAA/C- $CaCO_3$/Au nanocomposite hydrogels are characterized by UV-visible spectroscopy, FTIR spectroscopy, X-ray diffraction (XRD) and scanning electron microscopy (SEM). The molecular interactions and the functionality of the polymeric chains are studied from the FTIR spectrum. From morphological analysis, it is found that the synthesized nanocomposite hydrogels contain micropores of non-uniform size. The particle size distribution of the incorporated nanomaterials is investigated by dynamic light scattering (DLS) technique. From the thermogravimetric analysis (TGA), it is noticed that the synthesized nanocomposite hydrogels have higher thermal stability due to the combined effect of nano $CaCO_3$ and Au Nps. The wound healing properties of the as-synthesized nanocomposite hydrogels are investigated by *in vitro* method. The antibacterial properties of the synthesized materials is studied ant it is found that nano gold and $CaCO_3$ are responsible for enhancing the antibacterial behaviour of the nanocomposite hydrogels. The combining effect of nano $CaCO_3$ and Au Nps on the PAA/C hybrid polymeric chains, the antifungal and antibacterial behaviour of the composite hydrogel are enhanced which enables the material used for wound healing.

Keywords: Au nanoparticles, *In situ*, Morphology, Wound healing, Nano $CaCO_3$.

Poster Presentation-73

Fabrication of Carboxymethyl Cellulose-Alginate based Nanocomposite Films with Antibacterial Applications

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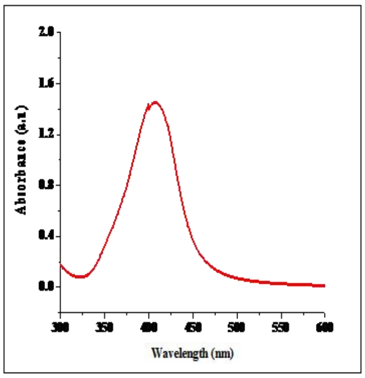
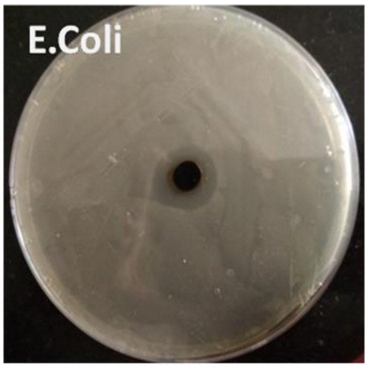
Abstract: Polymeric nanocomposites fabricated from polysaccharides have been extensively used in food industry, packaging, biomedical applications, protective films and coatings, etc due to their properties such as biocompatibility, nonantigenicity, nontoxicity and ability to improve wound healing. The embedding colloidal nanoparticles and graphene based nanofillers into the polymer matrices is an effective method for enhancing the functions of these functional materials.Carboxymethyl cellulose, Alginate, Graphene oxide and Ag nanoparticles based hybrid nanocomposite films have been prepared by solvent casting method. The polymeric nanocomposite is characterized by FTIR Spectroscopy, XRD, SEM, TEM and TGA-Analysis. The formation silver nanoparticles have been confirmed by UV-Vis spectroscopy. Further, the formation of silver nanoparticles is evident from the XRD patterns of polymer nanocomposites. The presence of graphene oxide has been confirmed from the corresponding peaks observed in the FTIR-spectra analysis of the polymer nanocomposites as well as thermogravimetric analysis.The films showed very good antibacterial activity on Escherichia coli.





Poster Presentation-74

Synthesis of Surface functionalized Gold Nanoparticulates for Cancer Therapy

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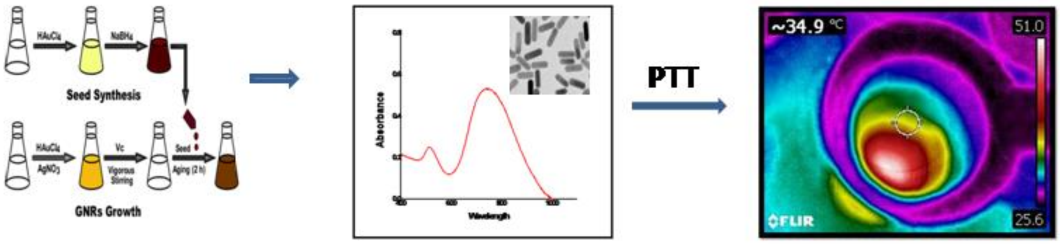
Abstract: Currently a popular area in nanomedicine is the implementation of nanoparticles for cancer diagnosis and therapy. Nanotechnology has revolutionized cancer therapies. Among various cancer therapy modalities, photothermal therapy (PTT) has gained popularity and very quickly developed in recent years due to minimally invasive treatments for patients.Among the available NIR light-responsive nanomaterials, gold nanorod has become attractive options owing to its excellent optical properties, ease of synthesis and outstanding photothermal conversion efficiency. Peptide conjugated gold nanorods have been synthesized for photothermal therapy of breast cancer cells MDA-MB 231. The nanoparticles have been characterized by FTIR and UV-Visible spectroscopy. The size of the nanoparticles have been determined using Zeta sizer and TEM. The photothermal response of nanoparticles has been tested using laser studies. The cytotoxicity of the nanoparticles has been evaluated using MTT assay. The high perfoming functionalized gold nanorods exhibit great potential in tumor targeting and photothermal therapy.



Poster Presentation-75

Intriguing Aspects of Chemical Reactivities of Aminothiazole Derivatives Possessing Amine-Imine Tautomerism

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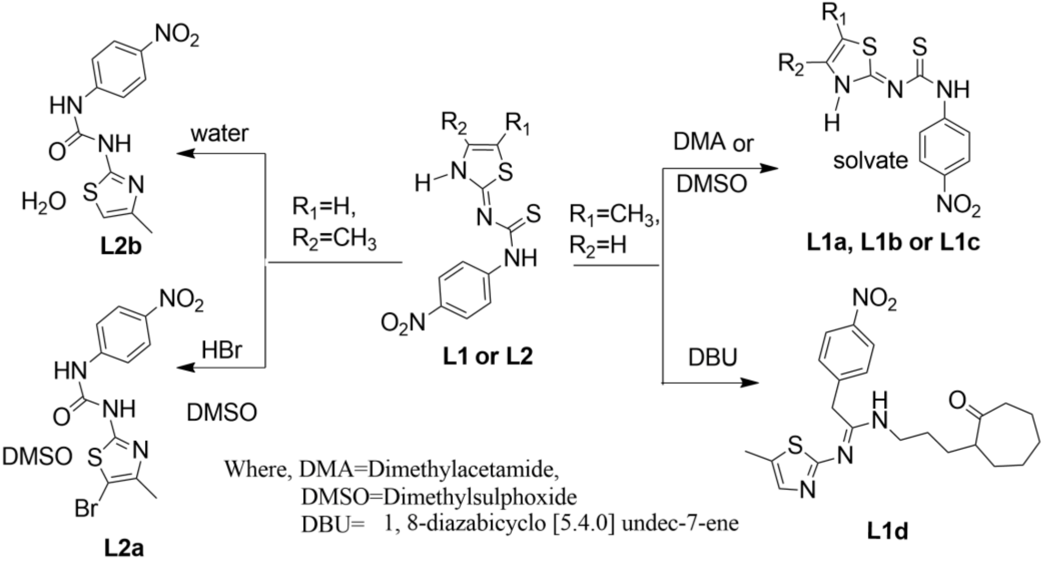
Abstract: Intriguing reactivities of positional isomers 1-(5-methylthiazol-2-yl)-3-(4-nitrophenyl)thiourea (**L1**) and 1-(4-methylthiazol-2-yl)-3-(4-nitrophenyl)thiourea (L2) towards environment polluting ions such as mercuric, fluoride, bromide and solvents provide scope to study various self-assemblies formed under different conditions and allied applications. The solid state structures of **L1** and **L2** revealed that both adopt the imine form. However, the number of symmetry independent molecules in asymmetric units as well as the

packing patterns of these two compounds have distinguishable features. The asymmetric unit of **L1** has three symmetry non-equivalent molecules. The packing patterns of these two positional isomers differ as **L1** has two arrays of dimeric self-assemblies in contrast to the single array found in the packing of **L2**. The reactivity of **L1** and **L2** with solvents was explored through crystal structure elucidation. The compound **L1** forms solvates with N,N′-dimethylacetamide or dimethylsulphoxide. The structural analysis of solvates of L1 provided avenues to study conformational adjustments. An unusual example of a metastable solvate of L1 with N,N′-dimethylacetamide was isolated. A ring-opening reaction of 1,8-diazabicyclo [5.4.0] undec-7-ene with **L1** has been observed. The compound **L2** underwent hydrolysis cum bromination with hydrobromic acid in dimethylsulphoxide. The reactivities of **L1** and **L2** towards mercuric and fluoride ions contributed to chemodosimetric signal transductions. The study establishes the impact of subtle changes in structure, reaction and crystallization conditions, which can influence pre-designed crystal engineering.



Scheme 1: *Reactivity of **L1** and **L2** towards Different Solvents.*

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Poster Presentation-76

Zeolite and Its Applications

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Abstract: Zeolites are hydrated aluminosilicate minerals of the family of microporous solids. Zeolites, also called molecular sieves, are traditionally referred to as a family of aluminosilicate materials consisting of orderly distributed micro pores in molecular dimensions. They have been widely used as highly efficient catalysts, adsorbents, and ion exchangers in petrochemical industries and in our daily life. Beyond these traditional applications, zeolites are playing an increasingly important role in many sustainable processes. In particular, zeolites have found promising applications in the fields of renewable energy and environmental improvement, such as biomass conversion, fuel cells, thermal energy storage, CO_2 capture and conversion, air-pollution remediation, and water purification, etc. These applications make zeolites potential candidates as solutions to the sustainability issues in our society. In this contribution, an overview of the current and potential applications of zeolites as a resource material is presented.

Keywords: Zeolite, Aluminisilicate material, Catalysis, Adsorbent, Fuel cell

Poster Presentation-77

Smart Materials and Environment

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Abstract: A smart material should possess a chain of capabilities exhibiting a number of properties and that exciting new materials with such characteristics will be needed in new advances in synthetic polymer chemistry. A large number of innovative methods are developed for the reduction of hazardous wastes like carcinogenic organic solvents, hazardous materials, and nuclear contamination, which has very disastrous effect on environment. For these, polymeric smart materials are finding useful applications in polymer catalysts, which are very useful in waste reduction, catalyst recovery, and catalytic reuse. The polymeric smart coatings have been developed that are capable of detecting and removing toxic nuclear contaminants. Such applications of smart materials involving catalysis chemistry and chemistry for reduced contamination methodology are especially applicable to environmental problems.

Keywords: Smart materials, Hazardous waste, Nuclear contamination

Poster Presentation-78

Synthesis, Characterizationof Chitosan-grafting-Poly(acrylonitrile)/Zn-Al Layered Double Hydroxide/Cu nanocomposites for packaging applications

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Abstract: In the large field of nanotechnology, polymer based nanocomposites have drawn serious attention both from industry and academic sections of current research and development. The present work deals with the application of a relatively new class of hybrid filler such as nano copper doped Zn-Al layered double hydroxides (LDHs) for synthesizing polymer based nanocomposites.We have synthesized nano copper doped Zn-Al layered double hydroxide reinforced CS-g-PAN nanocomposites bya simple and environmentally friendly *in situ* polymerization technique. The nanocomposites are characterized by FTIR, XRD, TGA, FESEM,HRTEM, EDS, and oxygen permeability Test. The interaction between hybrid filler and polymer is studied by FTIR. The XRD pattern indicates the presence of Zn-Al LDH, copper, chitosan and polyacrylonitrile in the nanocomposites. TGA reveals CS-g-PAN/Zn-Al LDH/Cu nanocomposites have more thermal stability over Chitosan, virgin PAN and CS-g-PAN copolymers. The surface morphology of copper nanoparticles was confirmed from the FESEM and the HRTEM images. The presence of nano copper and Zn-Al LDH in nanocomposites improves the antibacterial properties. The synthesized nanocomposites have appreciable thermal stability in combination with reduction in oxygen permeability and antibacterial activities by which the material is suitable for packaging applications.

Keywords: LDH, Cu nanoparticles,Nanocomposites, Chatacterization

Popular Article

Popular Article

SUSTAINABLE CHEMISTRY

Dr. Sarat Chandra Das

Former President, Orissa Chemical Society

Science is the gift of nature. Chemistry is a part of the gift. Why the question of sustainability of chemistry comes ? With the enormous enhancement of science and all its allied subjects individuality has merged into mass. Now a days chemistry as an independent species does not exists. If we look back for a couple of years Nobel prize in chemistry is shared by eminent scientists worked on biological science, life sciences. It is a good signal chemistry is becoming multi dimensional in its applications. Basic chemistry learning and research is now supposed to reach at a saturation point. People feel the concept and definitions have become obsolete now a days . There is no fume and smell in a chemical laboratory. Computer simulation says the environment of a chemical reaction. Recently I had the opportunity of visiting few top chemistry department of the world in USA. I could guess no dynamism in chemistry research in the laboratory. Few scientists spoke about its applications and utilisations in the society. If this trend goes the sustainability of chemistry will be in fix.

Currently there is attack on all sides with plastic industry. It has become a question of environment issues. Since plastics have replaced over steel, stone, cement and many hard materials it is widely accepted as economic, user friendly material. When it became non degradable the question of environment issues came to the front. Why chemistry will not find any solutions for it. Why our chemists shall not design all degradable plastics so that even after its use it will be recyclable. This is the job of the chemists and chemical technologists. The developed countries those who shout about the environment concern for the use of plastics they consume maximum amount of plastics and polythene per head per annum in comparison to other countries. Let the chemists solve this problem

Paints and coatings play an important aspect of modern chemistry with rapid urbanisation of many developing countries. A handful of companies are engaged in this field of research. Hardcore chemists can solve this problem in designing the molecular structure of organic dyes so that it shall have more durable and anti corrosion quality when it is applied to our buildings or even in our day today use.

Role of chemistry in the field of agriculture is now more challenging before a chemists. Whether it is an application of pesticide or fertiliser or even watering the field, chemists shall have to resolve these issues which is currently neglected in many countries. Farmers does not have any qualitative idea of using pesticides or insecticides in the field. Only quantitatively he applies in the field for more products As a result of which he performs hard work but its expenses he gets less yield. Applications of chemistry is now essential in the field of agriculture keeping in mind of latest technology and production in general. Farming with nano technology should be explored by our chemists.

In automobile industry the role of chemists is equally important. Many developed countries they adopt it. Still we lack to a substantial amount in this field. Moulding of material, light weight equipments, heat resistant structures are the main concerns before a chemists. We are to design the chemical structure of the light material which shall have wide applications in automobile industry. Basic research is needed in this field. Modifications of crystalline structure of a material to meet the need of the industries is essential.

Pharma industry is another branch where chemists are engaged for high level research. Since it is directly related to life cycle of human beings as well as plant and animals chemistry has an important role for it. Many multinational companies are the pioneer in this field of research. Still it should come down to base level pharma companies who can go for an intensive investigation in this field. Chemists has a major role to play for it. Choosing the right composition of a drug depending upon its multifacial applications in the job of a chemists. Hardly this is done in many places. This field can be explored by the chemists.

Now time has come let the chemistry research should go green in our laboratory also in our environment. Recently a research article published in Organic letters a journal by American chemical society which tells about the synthesis of many life saving drugs by using green catalysts. This is used in place of reactive, corrosive and many explosive chemicals which are replaced by green catalysts that helps chemists to synthesise new compounds. An important aspect is that it is working out at room temperature using water as solvent. Chemistry research and subject preparation should be angled towards green level now a days. When substantiality comes we the chemists should give importance to basic concepts and its implementation at grass root level of the subject.

Orissa chemical society constitute an elite and enlightened mass of the chemistry and chemical technologists. They shall focus more at base level of chemistry teaching, learning and research. When we think our self to be compared with other fellow chemists of different countries let us introspect our self what & How we have contributed to our own people and state for the sustainable chemistry and its research.

Jai Jagannath

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