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.

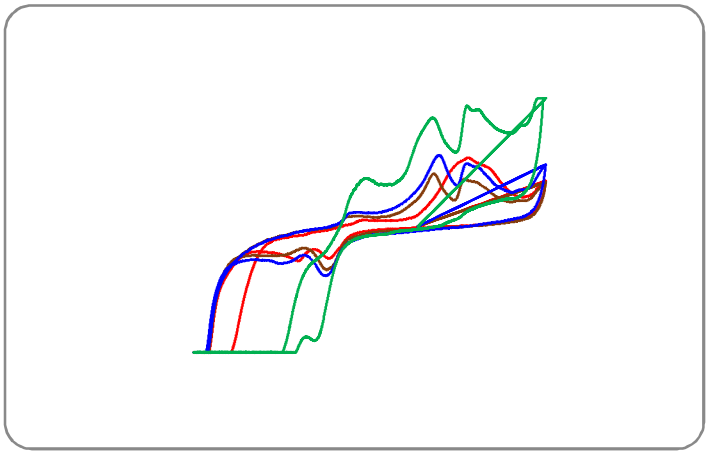

Figure 1:*Cyclic voltammograms of CTAFC inCH_3CN at different Scan Rates.*

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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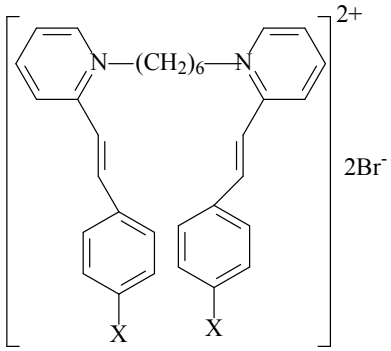
Abstract: Two bischoromophoric α-styrylpyridiniumdyes with hydroxy (OH: **1**) and N,N-dimethylamino (NMe_2: **2**) substituents with flexible spacer have been synthesized (Figure 1). Their solvatochromic behavior in 13 solvents of various polarities has been studied. Both the dyes clearly sense the 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

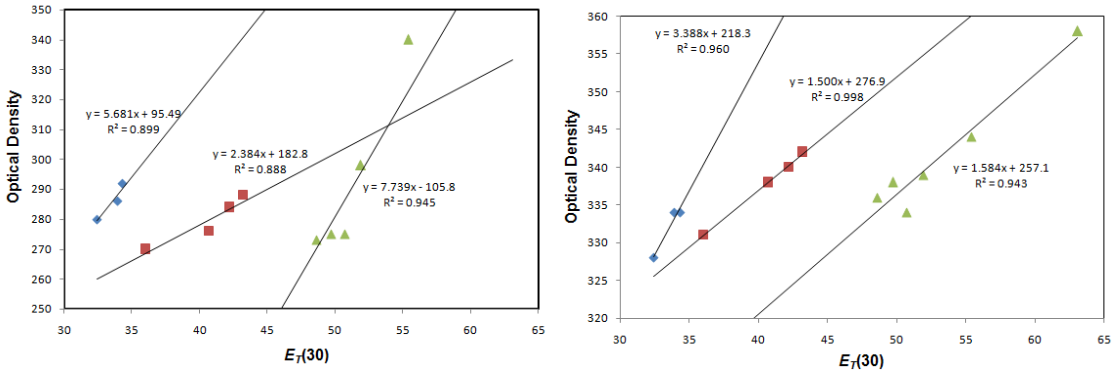


Figure 2

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^{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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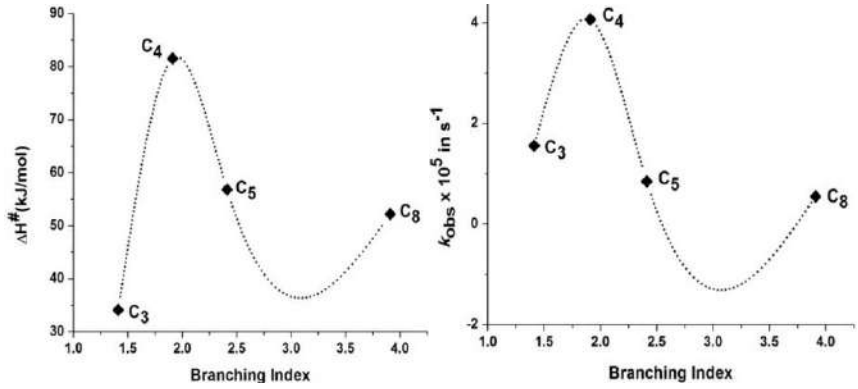
Abstract: Oxidation kinetics of various alcohols having varied hydrocarbons has been studied using cetylpicolinium dichromates (CPDC), a class of novel phase transfer oxidants, in DCM medium. The rate of reaction is first order with respect to oxidant and fractional order with respect to the substrates. 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_{CHCl3}/k_{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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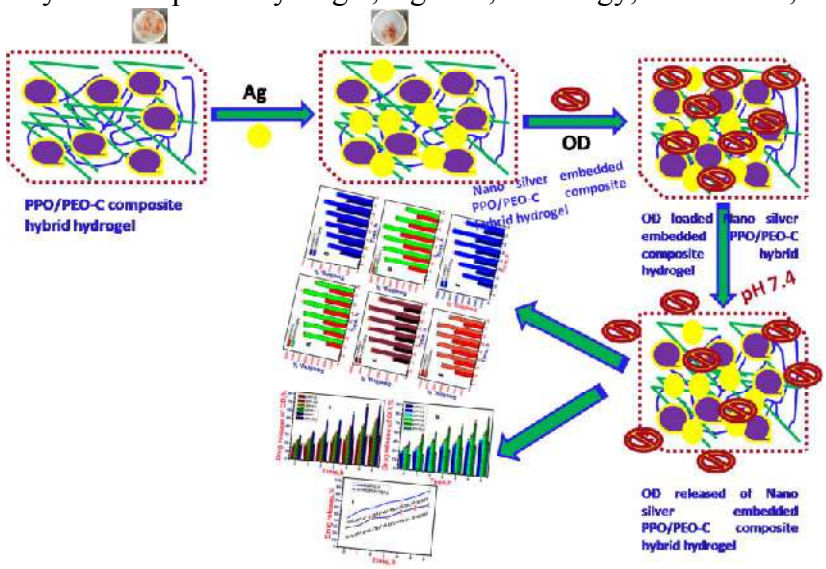
Abstract: In this work, nano silver embedded polypropylene oxide/poly ethylene oxide-cellulose (PPO/PEO-C@Ag) biodegradable nanohybrid composite hydrogel are synthesized by *in situ* polymerization technique for the *in vitro* release of ornidazole drugs.The change in structural, morphological and functional 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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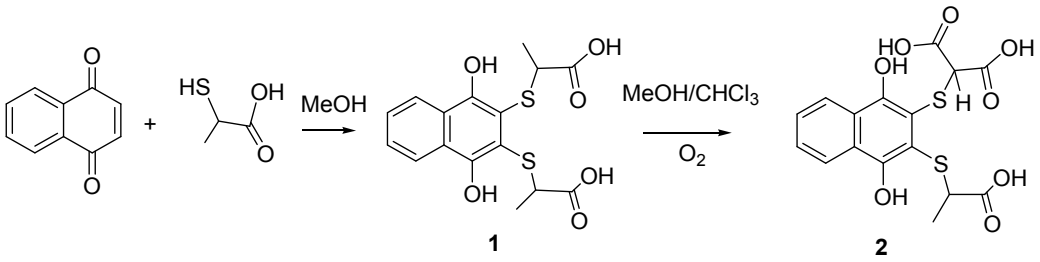
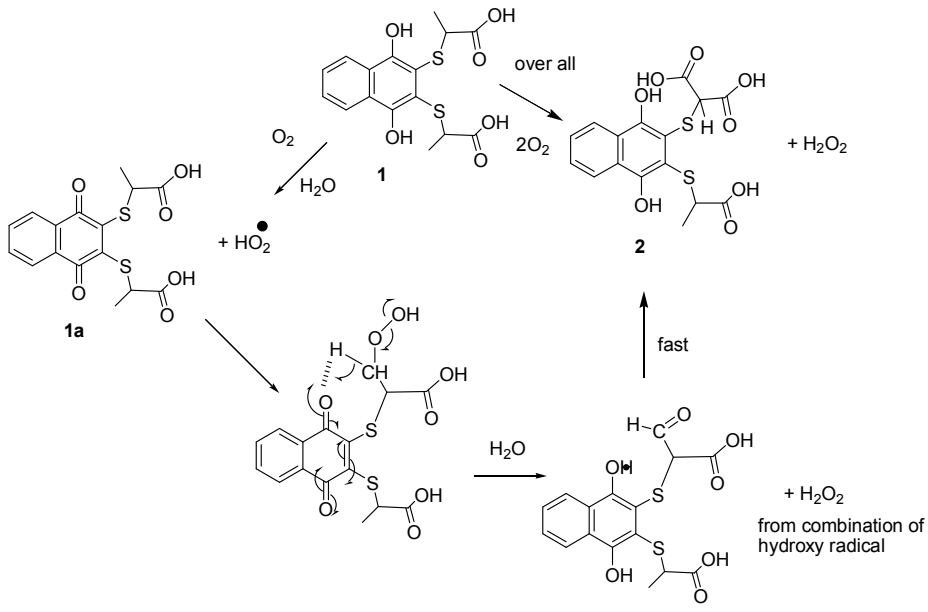
Abstract:2,2'-(1,4-dihydro-1,4-dioxo-naphthalen-2,3-diylthio)dipropanoic acid undergoes oxidation under ambient condition to form 2,2'-(1,4-dihydro-1,4-dioxo-naphthalen)-3yl-thiomalonicacid, 2-propanoic acid.
Keywords: Naphthoquinone; Thiolactic acid; Side chain oxidation; C–H activation.
General Reaction:



Mechanism:



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Poster Presentation-54

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

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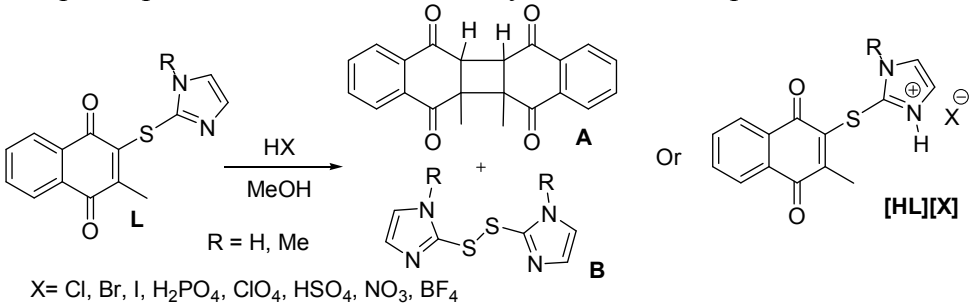
Abstract:Phosphoric acid (H_3PO_4) promoted [2+2] cycloaddition of 2-methyl-1,4-naphthoquinone derivatives *via* C-S bond cleavage was synthesized and characterized by physicochemical and spectroscopic tools. The effect of binding interaction of Bovine Serum Albumin (BSA) and Human Serum Albumin (HSA) 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.

Reference:

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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^oC. 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^oC. 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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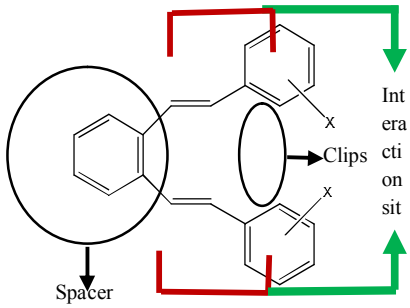
Abstract: The present work describes the synthesis, characterization and sensing properties of some xylene based polymethine molecules, which act as molecular tweezers towards foreign guests. The molecules were synthesized by the condensation of xylene and substituted benzaldehydes in 1:2 ratio in presence 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).



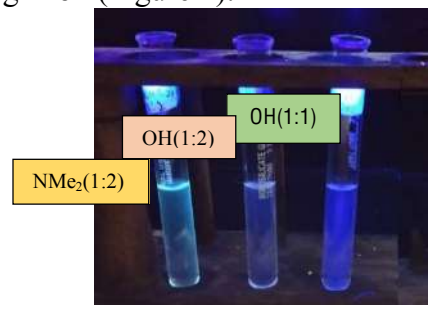


Figure 1:*Structural Representation of Xylene based Tweezer* **Figure 2:***Fluorescence Intensities of Clefts with Various Clips*

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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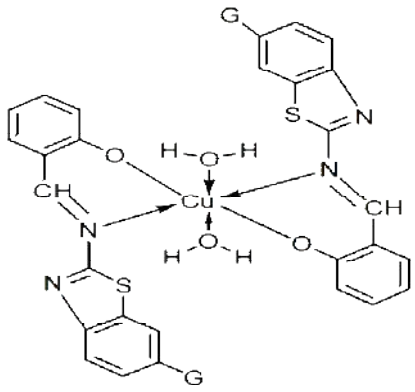
Abstract: The concentration of different toxic metals has increased beyond environmentally and ecologically permissible levels due to the increase in industrial activity. More than 1 billion people of the world are affected by drinking ground water contaminated with arsenic copper, cadmium and other 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 p^H. 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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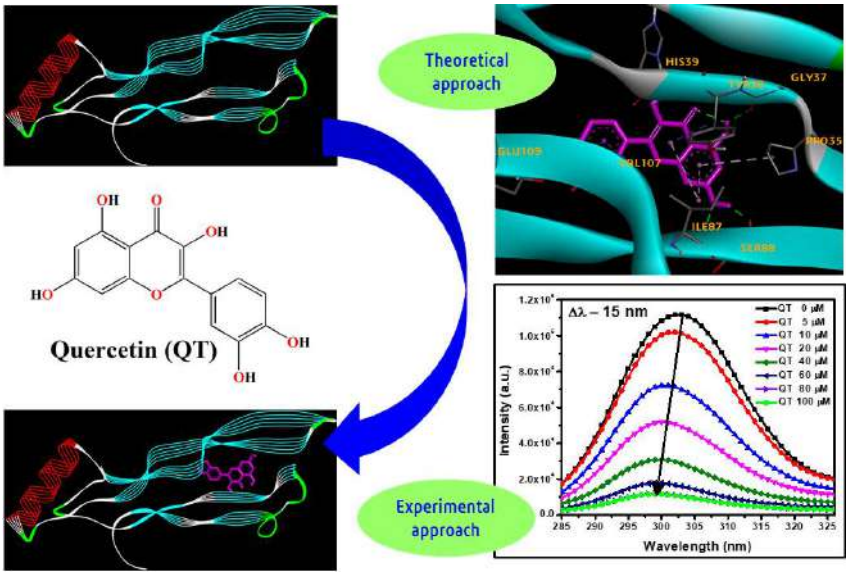
Abstract: Bone morphogenetic proteins (BMPs) are multi-functional growth factors that belong to the transforming growth factor beta (TGF-β) superfamily. We investigated the binding interaction between quercetin and BMP-2 by various spectroscopic, calorimetric and theoretical studies. Interaction profile 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.

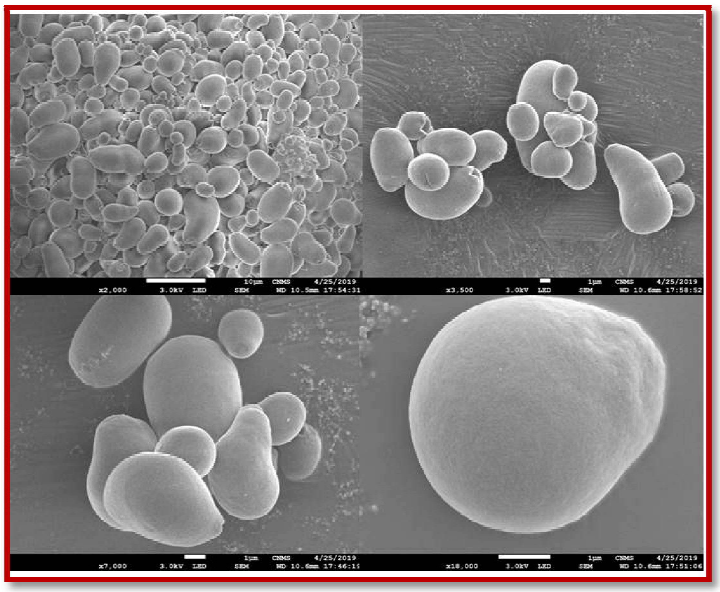

Figure 1: *Morphological Characterization of Plam Tuber (Phoenix Dactylifera) Starch Granules*

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

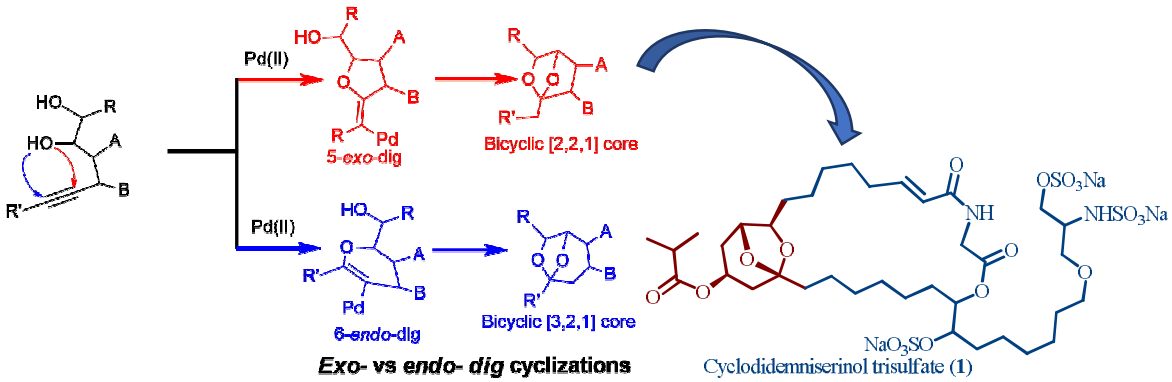

Figure 1:*Pd-mediated Cycloisomerization and Its Application in the Synthesis of Cyclodidemniserinol Trisulfate.*

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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.