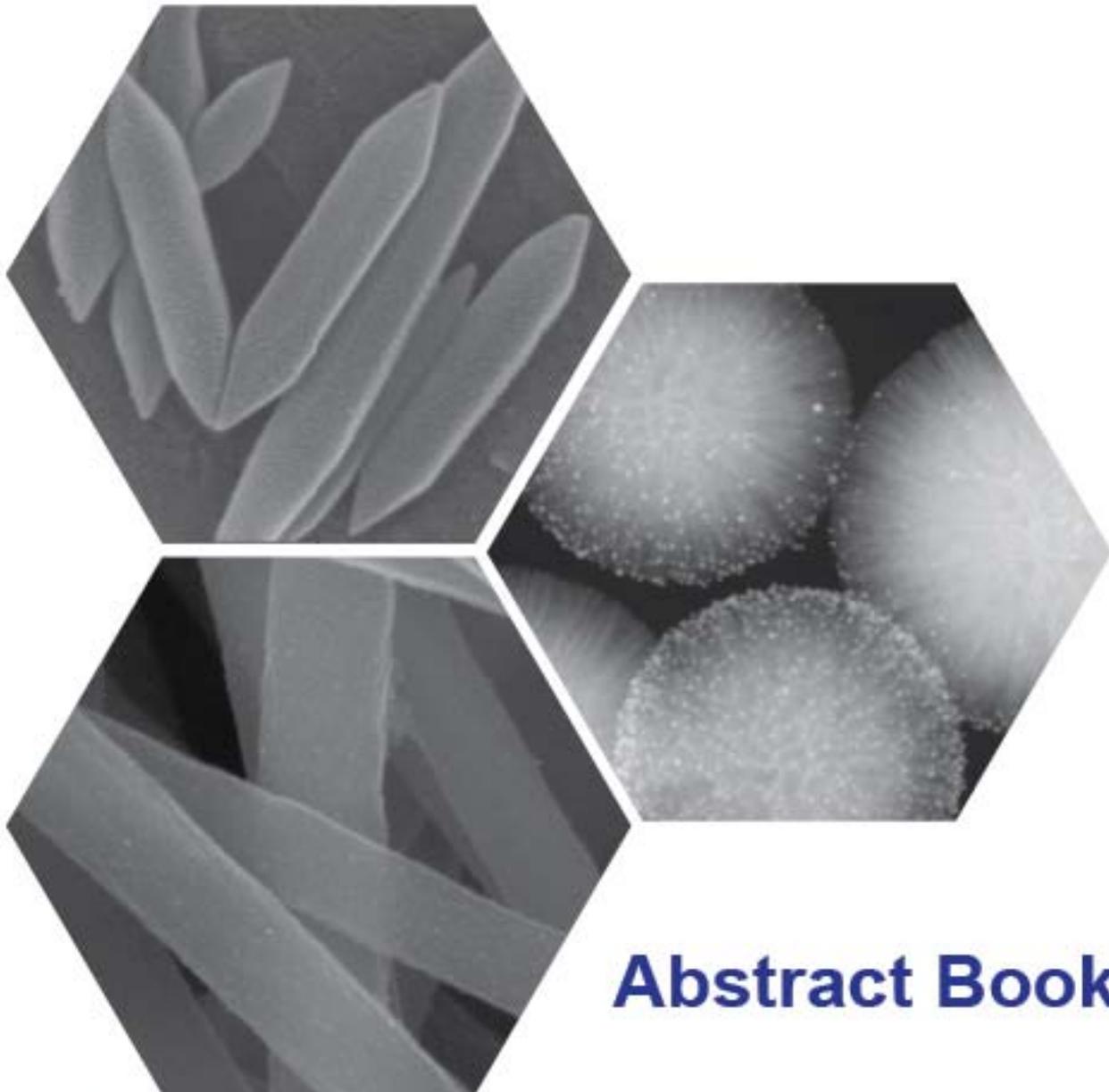




2nd INTERNATIONAL CONFERENCE ON
NANOSCIENCE & NANOTECHNOLOGY

2019

November 1 - 2, 2019



Abstract Book

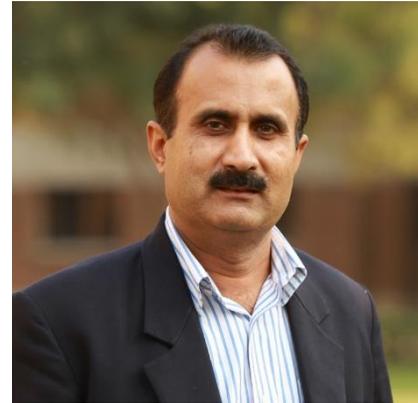


LUMS

Lahore University of Management Sciences (LUMS)

Welcome to ICONN-2019

On behalf of the organizing committee, I am delighted and honored to welcome all the guests, speakers and the participants of 2nd International Conference on Nanoscience & Nanotechnology (ICONN-2019). ICONN is a joint venture of Department of Chemistry & Chemical Engineering, SBA School of Science & Engineering, Lahore University of Management Sciences (LUMS) and School of Chemical and Materials Engineering (SCME), National University of Science & Technology (NUST), Islamabad. The first conference (ICONN-2018) of this series was successfully held at NUST on Nov. 1-2, 2018. This year, we are also collaborating with Prof. Walther Schwarzacher from Bristol University (UK) and Professor NM Butt (Fellow, Pakistan Academy of Sciences & former Chairman Pakistan Science Foundation) from Preston Institute of NanoScience & Technology (PINSAT), Preston University, Islamabad.



The major focus of ICONN-2019 is to highlight the important developments made in nanomaterials research especially the theoretical and experimental aspects to control the size, shape and surface chemistry of nanomaterials, and their applications in biomedical sciences, renewable energy technologies and environment. In addition to the keynote/invited speakers from Pakistan (16) and abroad (07) and LUMS students, over 200 participants have been registered for this conference from academia and industry, and British Council has sponsored 08 British PhD students to attend this event. Furthermore, a poster session is being organized to offer a platform to the students/young researchers to show-case their research in the field of Nanoscience & Nanotechnology. It will, therefore, provide an ample opportunity to the young researchers for networking and possibly developing research collaboration with the national/international leading research groups that may enrich their professional network to collectively explore exciting research ideas in the multidisciplinary field of Nanoscience & Nanotechnology.

Organizing an international event like this requires huge efforts and I thank the LUMS organizing committee/staff/students and our partners from NUST, Preston University and Bristol University, for their sincere and coordinated efforts to plan and organize ICONN-2019 at LUMS. On behalf of the organizing committee, I also acknowledge the support from various sponsors especially LUMS, British Council, Pakistan Academy of Sciences, Pakistan Science Foundation, Pakistan State Oil, Innovative Power Engineering, Prime Scientific Engineering, Kamstech, Professional Systems and QTech. LUMS Society of Chemical Sciences & Engineering (LSCSE), a students' society, is leading the efforts to arrange a cultural night and a food street to offer yet another opportunity to the participants to socialize, and their efforts in this regard are also highly appreciated.

We wish all the delegates to have an amazing learning experience and a comfortable, enjoyable and a memorable stay at LUMS.

Irshad Hussain

Principal Organizer

Organizing Committee of ICONN-2019

Department of Chemistry and Chemical Engineering, LUMS, Lahore.



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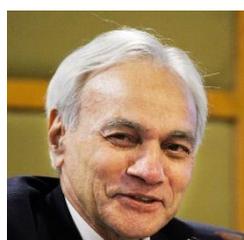
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Sequence-specific “Peptoids” for bionano science and engineering

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Analogous to biopolymers such as peptides and DNA, biomimetic “peptoids” are synthetic polymers that exhibit complex self-assembly properties and bioactivity encoded by the specific order in which simple monomer residues are arranged in linear sequences. In contrast to biopolymers, peptoids are resistant to enzyme degradation and have simplified intermolecular interactions. This talk highlights our recent efforts in “engineering” the sequence of solid-phase synthesized peptoids for applications beyond their conventional use in combinatorial drug discovery. We demonstrate a series of novel properties, including the shortest peptoid motifs found to self-assemble into nanospheres and nanofibrils, “stealth” surface-grafted peptoid brushes that resist biofouling, as well as the modification of known sequences to retain antimicrobial activity for biomedical surface applications. Our preliminary results also show that self-assembled peptoid nanosheets can influence protein expression of stem cells under culture.

Nanotechnology: Key to synthetic fuels for a sustainable energy transition

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Worldwide energy consumption in the last 50 years has grown from around 40K TWh to more than 150K TWh. At the same time, the unprecedented increase in the emissions of greenhouse gases and other pollutants, resulting in smog, has hard-pressed the society to look for cleaner energy and mobility scenarios. Society will continue to need more energy while demanding reduction in emissions and if it is to succeed in this formidable challenge, it must strike the right balance between cost, efficiency, scalability, and environmental impact. To attain these ambitions, the energy supply scenario will remain a complex mix with increasing share of intermittent renewable energy. This intermittency in power generation due to renewable power and in power demand mainly due to emerging electro-mobility will put stringent pressure on our energy supply-demand patterns.

With this background, the lecture will outline the keys to a secure and sustainable future energy supply: energy storage, grid balancing and sector coupling. To implement these, technologies for power-to-chemicals including synthetic “E”-fuels and electrolytic hydrogen as the building blocks will be needed. The lecture will explain how nanotechnology is one of the essential enablers of the technologies. The challenges and the current progress in nanotechnology for water electrolysis for green hydrogen and co-electrolysis for the production of synthetic hydrocarbon will be detailed. As the market adaptation of these technologies is driven by the cost of the produced fuel, the technological development towards lower cost will be discussed. In the end, the prototype plants of German Aerospace Center for water and co-electrolysis coupled with Fischer-Tropsch-Synthesis will be presented.

Porous hyper crosslinked polymer-TiO₂-graphene photocatalysts for visible-light-driven CO₂ conversion

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Significant efforts have been devoted to develop efficient visible-light-driven photocatalysts for the conversion of CO₂ to chemical fuels.^{1,2} The photocatalytic efficiency for this transformation largely depends on CO₂ adsorption and diffusion. However, the CO₂ adsorption on the surface of photocatalysts is generally low due to their low specific surface area and the lack of matched pores.³⁻⁵ To overcome this limitation, a well-defined porous hypercrosslinked polymer-TiO₂-graphene (HCP-TiO₂-FG) sandwiched structure is reported with relatively high surface area i.e., 988 m² g⁻¹ and CO₂ uptake capacity i.e., 12.87 wt% (**Fig. 1**). Meanwhile, the HCPs obtained by this strategy are comprised of ultrathin layers with a thickness of 3~8 nm wrapping around TiO₂ crystals, which facilitates the diffusion of CO₂ molecules from the adsorptive sites on HCPs layers to the catalytic sites on TiO₂ photocatalysts (**Fig. 2**). Due to the improved CO₂ adsorption ability and shortened diffusion length, such well-defined HCP-TiO₂-FG sandwich photocatalyst is expected to enhance the reactivity of CO₂ molecules, which will facilitate the CO₂ conversion especially for CH₄ production (**Fig. 3**).

This sandwiched structure shows high photocatalytic performance especially for CH₄ production, i.e., 27.62 μmol g⁻¹ h⁻¹, under mild reaction conditions without the use of sacrificial reagents or precious metal co-catalysts. The enhanced CO₂ reactivity can be ascribed to their improved CO₂ adsorption and diffusion, visible-light absorption, and photo-generated charge separation efficiency. It can be concluded that the in-situ knitting of porous HCP-TiO₂-FG sandwich structure are very effective to dramatically enhance visible-light-driven CO₂ conversion efficiency, which could be mainly ascribed to the well-defined sandwich structure from the following two aspects: (1) high CO₂ uptake ability and short distance between the adsorbent and the catalyst facilitating the CO₂ adsorption and diffusion; (2) broad light absorption of HCPs layers and fast charge mobility of graphene improving the visible-light absorption and charge separation efficiency (**Fig. 3**). This strategy provides new insights into the design and synthesis of well-defined porous photocatalysts for CO₂ uptake and conversion, and highlights the importance of microporous organic polymers in combination with photocatalysts for solar energy conversion.

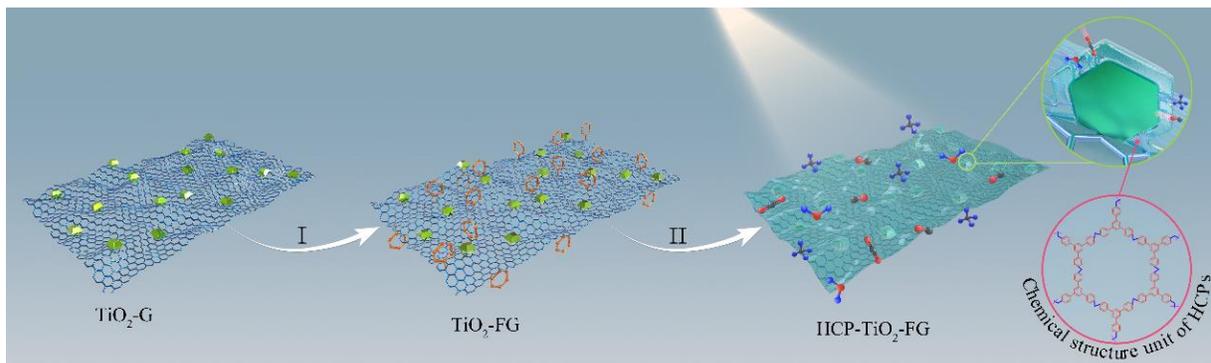


Figure 1. Construction of a well-defined porous HCP-TiO₂-FG sandwich structure.

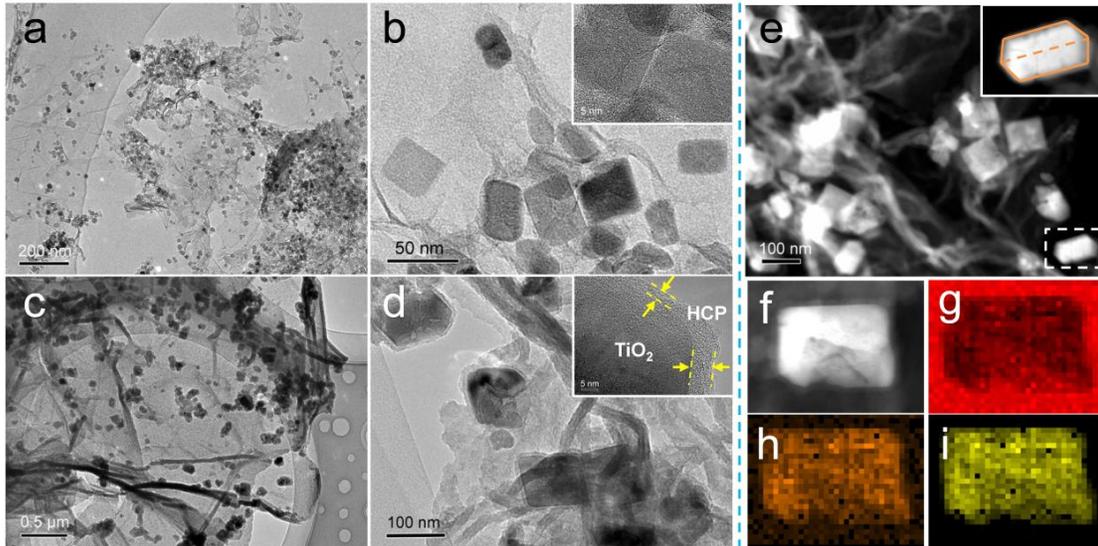


Figure 2. Morphology and elemental mapping of various photocatalysts. TEM images of TiO₂-G (**a, b**) and HCP-TiO₂-FG (**c, d**) at different magnification. The insets in **b** and **d** are the corresponding HR-TEM images. STEM images of HCP-TiO₂-FG (**e, f**). EDX mapping images of C (**g**), O (**h**), and Ti (**i**) for HCP-TiO₂-FG.

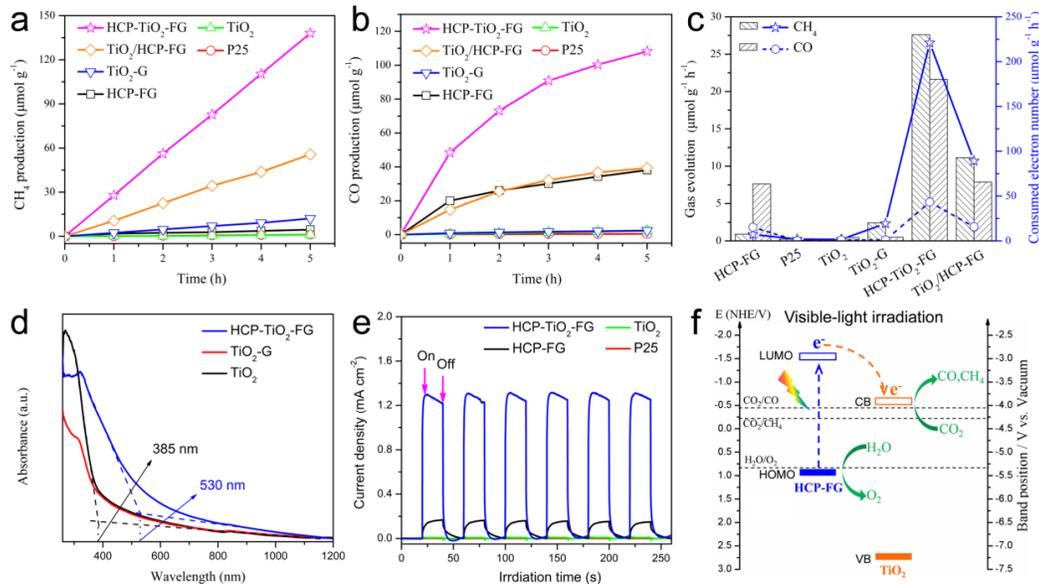


Figure 3. The photocatalytic performance of CO₂ reduction, optical and photoelectrical properties, and mechanism of charge transfer pathway. Time-dependent production of CH₄ (**a**) and CO (**b**) in photocatalytic CO₂ reduction with different catalysts under visible-light ($\lambda \geq 420$ nm). (**c**) Average efficiency of photocatalytic CO₂ conversion with different catalysts during 5 h of visible-light ($\lambda \geq 420$ nm) irradiation. (**d**) UV-Vis absorption spectra of TiO₂, TiO₂-G, and HCP-TiO₂-FG catalysts. (**e**) Amperometric I-t curves of samples under visible-light ($\lambda \geq 420$ nm) irradiation. (**f**) Proposed mechanism of charge separation and transfer within the HCP-TiO₂-FG sandwich photocatalyst under visible-light ($\lambda \geq 420$ nm) irradiation.

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Classical nucleation theory and electrodeposition

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Nucleation is a nanoscale process that plays a key role in controlling material properties. In this talk, I shall briefly cover the basics of classical nucleation theory using the nucleation of ice from liquid water as an example. I shall discuss what makes an effective heterogeneous nucleating agent for ice and why this is an important scientific problem. I shall then present some of our recent work using bio-nanoparticles as model iced nucleating agents. I shall finish by presenting an example of classical nucleation theory applied to electrodeposition as a warning that not every article published in a high impact factor journal should be believed. In this talk, I shall briefly cover the basics of classical nucleation theory using the nucleation of ice from liquid water as an example. I shall discuss what makes an effective heterogeneous nucleating agent for ice and why this is an important scientific problem. I shall then present some of our recent work using bio-nanoparticles as model iced nucleating agents. I shall finish by presenting an example of classical nucleation theory applied to electrodeposition as a warning that not every article published in a high impact factor journal should be believed.

The nanotechnology gold rush

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Computers have shaped our modern world more than any other invention. They became a realistic possibility only through the advent of microtechnology, which enabled the cheap mass production of integrated electronic circuits with previously unimaginable data processing power. Since computation speed and information density depend crucially on the level of integration and the feature size of the circuitry, further miniaturization has been the mantra of the industry from its beginnings, naturally leading to the concept of nanotechnology. Extrapolating from the opportunities afforded by microtechnology, extraordinarily high expectations have been associated with nanoscale manufacturing, and vast sums of money have been invested in it over the past three decades. In this lecture, I will examine from the point of view of a colloid chemist, why these expectations have not been fulfilled, and which alternative opportunities have been created instead, notably in the life sciences and in medicine. In this context, I will discuss our research on the use of gold nanoparticles for both analytical/diagnostic and therapeutic purposes. Photoacoustic methods of tracking gold nanorod-labelled stem cells within a murine model, and photodynamic approaches to the generation of singlet oxygen as a cytotoxin to kill cancer cells will be presented.

While microscale manufacturing is firmly based on top-down engineering principles and homogeneous and stable materials, nothing can be envisaged on the nanoscale without considering the graininess of matter along with the dynamics and instability inherent to assemblies of such small size. These are typical properties found in biological systems, which are also organised on the nanoscale but, in addition, depend on the ability to self-repair and on an existence far from chemical equilibrium. Unlike manufactured nano-systems, they are indeed processes, and not objects. Again, using gold-based assemblies as an example, I will present and discuss approaches to making artificial nanostructures more process-like and conceptually more similar to biological phenomena. In particular, I will present gold nanoparticles that act as ion transporters across membranes and can maintain ion fluxes between emulsion droplets that are not in chemical equilibrium with each other.

The effect of confinement on the crystallization of soft-materials

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Nanoporous hard templates provide a two-dimensionally confined space in which self-organization processes such as crystallization, protein secondary structure formation, and phase separation can be fundamentally different from those obtained in thin films and in the bulk. A particular advantage of hard templates is that they provide a range of parameter space (pore diameter, curvature and nature of pore walls etc.) that can induce or manipulate nucleation and crystal growth. Nowadays, a broad range of soft materials can be formed into nanotubes by means of nanoporous hard templates containing arrays of self-ordered cylindrical nanopores. Understanding the crystallization, thermodynamics and dynamics of soft materials under confinement allow for their rational design as functional devices with tunable mechanical strength, processability, electronic and optical properties. The principal focus of this lecture will be to find the basic underlying principles that give rise to nucleation and crystal growth in a range of soft materials (crystallizable polymers, amphiphilic molecules, liquid crystals, low-molecular weight liquids and biopolymers) under hard-confinement.

Bulk crystallization of polymers proceeds usually via heterogeneous nucleation and gives rise to structure over multiple length scales: from the crystalline unit cell (1-2 nm), to alternating crystalline/amorphous lamellae (50-100 nm) and to spherulitic superstructures (>500 nm and up to cm). This is the dominant nucleation mechanism in bulk polymers. Important studies of polymer crystallization confined to droplets and within the spherical nanodomains of block copolymers emphasized the interplay between heterogeneous and homogeneous nucleation and explored the kinetics of homogeneous nucleation observed at high supercooling. Some authors have even reported only homogeneous nucleation of polymers confined to AAO nanopores. This finding is surprising and leads to several questions about the type of nucleation under hard confinement typical for AAO: Is the crystallization process always homogeneous within the small AAO nanopores? Do surface effects always dominate? And even more, can hard confinement completely suppress polymer crystallization and if so, what is the required size? Providing answers to these questions is of technological relevance for the understanding of nanocomposites containing semi-crystalline polymers. We will try to explore these issues both by comparing the recent studies and by presenting research activities of our group.

In order to better understand the nucleation mechanism, we employed self-ordered nanoporous aluminum oxide (AAO) made by the electrochemical anodization of aluminum substrates as the inorganic model matrix that provides the required uniformity in diameter/length, thermal stability and resistance to organic solvents. In addition, the parallel arrangement of the pores in AAO allows to study anisotropic properties of crystal textures and even crystal dynamics parallel and perpendicular to the pore walls. In recent years it was shown that a size limitation in the nanometer scale can affect the energetics involved in crystal nucleation, growth and orientation. In this talk, we will mention the controlled crystal orientation in semi-crystalline polymers, liquid-crystals and even water molecules in nanoconfinement.

Fabrication of triboelectric nanogenerators using template assisted synthesis

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Triboelectric nanogenerator (TENG) is used to convert mechanical energy into electricity by means of triboelectric effect and electrostatic induction. There are four basic working modes of TENG, which includes contact-separation mode, sliding mode, single electrode mode, and free-standing mode. Triboelectrification occurs when two different materials with distinct electron affinity are brought in physical contact with each other that generate the triboelectric charges on the surface of these materials. Then by the separation of these two surfaces to a particular distance, the phenomenon of electrostatic induction occurs and the two charged surfaces can be discharged by flowing current in an external circuit. The output performance of TENG is based on the material selection, surface morphology of the active layers, and physical structure of TENG. In this research, we demonstrated two types of dielectric-to-metal based TENG working in vertical contact separation mode to harvest the mechanical triggering into electricity. Both nano generators (TENG A & TENG B) were fabricated using template assisted synthesis. For fabrication of TENG A, periodic array of microdomes of PDMS in the form of discs each with diameter of 50 μm were formed. The patterned PDMS sheet was used as an active triboelectric material for static charge generation when it was brought in physical contact with nanopatterned Al foil. The nanostructures on the surface of Al was formed by etching of oxide layer formed during anodization of the Al foil in 0.3M oxalic acid. The combination of micro and nanopatterned surfaces of two different materials 'having distinct electron affinity' increase the charge generation and enhance the TENG efficiency. The nanopatterned Al has dual functions that is used as second triboelectric layer and as top electrode for making the TENG device. When the micropatterned PDMS was brought in physical contact with the nanopatterned Al surface the triboelectrification was occurred between the surfaces of Al and PDMS that resulted the generation of triboelectric charges on these two surfaces with opposite polarities. By applying some mechanical force on TENG to compress and release it periodically, it worked as an active power source with maximum output voltage of 80 V.

The TENG B was fabricated using PDMS nanowires, which were formed on copper substrate using anodic aluminum oxide (AAO) membrane template. The Al substrate was then used as other triboelectric material for making top electrode to form TENG B. When the patterned PDMS were brought in physical contact with the Al surface the triboelectrification was occurred between the surfaces of Al and patterned PDMS that resulted the generation of triboelectric charges on these two surfaces with opposite polarities.

Applications of multinary metal oxides nanocomposites

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Different methods have been used to synthesize the multinary metal oxides nanocomposites containing more than two rare earth-transition metal oxides to achieve enhanced activities for their applications in degradations of textiles pollutants, pesticides, organic pollutants, and explosive materials etc.

In this regard, we have successfully synthesized more than 50 nanocomposites with variety of metals. Various factors e.g. change in precursors, pH, temperature, feed rate, surfactants, solvents, methods of preparation, and the concentration of precursors influenced the red shift as well as blue shift.

The structural investigation, thermal degradation, crystallite size, morphology, electrical, optical, surface and photocatalytic properties of synthesized samples were studied by using different characterization techniques i.e. thermogravimetric analysis (TGA), fourier transform-infrared spectroscopy (FTIR), particle size analyzer (PSA), Powder X-ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmission electron microscopy (HR-TEM), photoluminescence (PL) spectroscopy, RAMAN spectroscopy and ultraviolet-visible absorption spectroscopy. The activities of nanocomposites as photocatalysis were also investigated under the illumination of UV and sunlight and degraded products were evaluated by TLC, HPLC, GC-MS.

Other applications like hydrogenation reactions, slow release fertilizers, forensics and nanofiltration, catalysts for synthesis of organic reactions were also studied and will be discussed in this lecture.

Tailoring and tuning of optical properties of wide band gap semiconductor nanostructures

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Wide band gap semiconductor nanostructures have recently been the center of attraction for their use in a variety of applications ranging from electronic to photonic devices. Introduction of luminescence point defects has been the focus of a large amount of literature available. Some notable materials are ZnS, ZnO, In_2O_3 , TiO_2 , etc. which offer huge opportunities to play with defects and dopants to tailor their electronic and optical properties. In this talk, self-doping of ZnS nanowires and, as a result, tuning of the optical properties of these nanostructures will be discussed. It will be shown that the energy band gap states can be altered by the growth conditions and by the dopant choice. It will also be demonstrated that these defect states act as reservoirs of carriers and can be activated at high temperature. The storage of charge can lead to better characteristics that can be exploited for various applications.

Carbon dioxide capture from methane using mixed matrix membranes

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Methane is an increasingly utilized source of energy, both domestically and industrially, due to its lower CO₂ emissions and high thermal efficiency. In this lecture, effects of titanium dioxide (TiO₂) and nickel ferrite (NiFe₂O₄) nanoparticles on the permeation properties of carbon dioxide (CO₂) and methane (CH₄) in cellulose acetate/polyethylene glycol (CA/PEG) membranes will be discussed. CA/PEG and CA/PEG/metal nanoparticles membranes were fabricated by using solution casting method. Concentrations of TiO₂ and NiFe₂O₄ nanoparticles in CA/PEG based membranes were varied from 0 wt% to 20 wt% and 0 wt% to 2 wt% respectively. Scanning electron microscope (SEM), tensile testing analysis, X-ray diffraction (XRD) and thermal gravimetric analysis (TGA) were used to characterize synthesized membranes. Permeation study of these membranes has shown that in 5 wt%TiO₂ MMMs, the permeability of CO₂ and CH₄ is increased up to 5.75 and 3.75 times respectively as compared to pure polymer membrane. By adding 1.5 wt% NiFe₂O₄ in the polymer matrix, the permeability of CO₂ and CH₄ has improved up to 3.46 and 2.1 times respectively as compared to pure polymer membrane. It has been observed that the addition of metal nanoparticles in polymer matrix not only enhances the permeability of gases but also offers a great potential for CH₄/CO₂ separation.

Advanced functional nanoscale materials: Thin-films, electrocatalysis, sensing, solar and chemical energy conversion applications

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For many catalytic processes and solar and chemical energy conversion schemes under the umbrella of “Artificial Photosynthesis & Synthetic Fuels”, thin-film molecular and advanced functional nanoscale materials and their surface assemblies are becoming increasingly significant. In this regard, developing robust and high activity electrocatalytic materials that are obtained from thin-film molecular and functional nanoscale materials and their synergistic interfacing with efficient light-harvesting modules is imperative for electro- and photo-electrocatalysis applications. We have developed and simplified many methods such as electrodeposition, anodization, low-temperature spray pyrolysis, colloidal thin films, molecular precursors technique, CVD for making easily accessible thin-film materials both on conducting and non-conducting substrates. Next, we exploited various functional thin-films and nanoscale materials for catalytic water splitting, CO₂ reduction, and recently for biomass catalysis, solar energy conversion and for electrochemical sensing schemes. Now we implement several molecular materials, metal nanoclusters, thin-film inorganic nanomaterials and metal-oxides displaying great potential to be used in surface chemistry and electrocatalysis. Their effective interfacing with semiconductor photo-responsive materials can provide a potential platform to make renewable energy supplies for a renewable and sustainable future.

Inorganic materials for electrochemical and catalysis applications

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In this talk, applications of inorganic materials for the fabrication of electrochemical sensors and heterogeneous catalysis will be presented. Polymers are utilized widely in electrochemistry and materials science. Applications of electroactive polymers in electrocatalysis, electrochemical sensing and energy storage are enriched by the chemical and electrochemical modification of polymer backbones with pendant groups. Understanding of the behavior of high molecular weight redox active polymers under mild electro-forces has important ramifications for the preparation of innovative and microscale electrochemical devices based on controlled and tunable layering of electro-active materials at the substrate electrode.

Synthesis of nanostructured materials in large quantities is a major challenge for the industrial, biological and medicinal applications. New methods for the development of innovative nanocomposite materials and their applications in green energy production and environment friendly heterogeneous catalysis will be presented. Finally, latest results on the reticular synthesis of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) with their potential applications for petrochemical catalysis will also be presented.

Metallic nanoparticles and de-oxy sugar containing pro-angiogenic synthetic grafts to accelerate healing in burns and diabetic foot ulcer wounds

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Angiogenesis is an absolute requirement for wound healing. With extensive burns and diabetic ulcers neovascularization is very difficult to achieve due to the loss of blood vessels (with burns) or damage to blood vessels (in diabetes). In case of diabetic wounds this leads to significant number of amputations. Research has shown that growth factors stimulate endothelial cells to migrate, proliferate and form new blood vessels. However, the most commonly used proangiogenic growth factor-vascular endothelial growth factor (VEGF) while central to angiogenesis *in vivo* has not proven an effective therapy when delivered directly to wound beds. Recombinant VEGF and its relatively poor stability make it unlikely to be adopted by countries lacking financial resources for advanced wound healing biomaterials. Also, very high local levels of VEGF have been found to lead to the sort of vasculature associated with tumors. In the body, VEGF is produced and released in a highly regulated manner. In the current study, we explored the ability of a variety of zinc-based nanoparticles and D-sugar, a simple small organic molecule, to stimulate new blood vessels. These angiogenic agents can be loaded into a number of clinically acceptable commercially available carriers. These materials were tested in the chick chorionic allantoic membrane (CAM) assay to investigate their role in angiogenesis and D-sugar containing dressings were further tested on a full thickness diabetic wound model in rats. These materials showed excellent wound healing properties in diabetic rats. The proangiogenic activity may be due to indirect activation of the VEGF angiogenic pathway – this needs further investigation. However, D-sugars potency and stability are extremely promising and a biotechnology company, Cannenta Australia, has now been established in Australia to bring affordable, effective advanced wound care products to emerging markets around the world.

Multi-dimensional materials in health-related applications

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The material science in the modern world of research has produced a variety of materials with a range of applications. The properties are enhanced when moving from micro-sizes to nano-sizes and many of the applications of nanoscale materials are based on their unique characteristics. The biomedical area of research has benefitted from the fabricated materials, particularly the nanomaterials. This lecture will encompass the health-related applications on real samples like human serum and urine. These samples cannot be directly worked on because of their complexity. Useful information can only be retrieved if classes of biomolecules are segregated to individual levels. The nanomaterials need to be engineered in terms of their sizes and more importantly with regard to the chemical functionalities made available for specific enrichments from biofluids. The enriched biomolecules can be a source of information related to disease process, helping in earlier diagnostics. The process involves three-way strategy using nanomaterials, specific biomolecules and sample preparation methodology. The most-sensitive detection is made by mass spectrometry where biomolecules can successfully be detected with prior desalting of bio-samples. Samples are desalted through functionalized nanomaterials by incorporating hydrophilic and hydrophobic moieties. Structural biology with modern name of Omics Sciences is engaging nanomaterials for exploring the structural parameters of biomolecules in the areas of proteomics and metabolomics. The beneficial results are only possible when nanomaterials offer the highest possible selectivity, specificity and sensitivity. The enriched biomolecules are studied in relation to their sequences. The interference offered by matrices in case of the detection of small biomolecules are made by matrix-free mass spectrometry. The materials include carbon-based, metal oxides, polymers, cellulose and metal oxides. The nanomaterials are also employed in nano-cosmetics as sunscreens to minimize skin damage. The engineered nanomaterials with chemical functionalization can enrich specific biomolecules from diverse bio-samples like egg yolk, non-fat milk, human serum and HeLa cell extract, and their role in this regard will also be discussed.

Fused ring small molecule acceptors for high-performance fullerene-free polymer solar cells

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Solution-processed organic solar cells offer promising renewable energy conversion, due to low cost, low weight, and flexibility. Development of new materials and optimization of donor and acceptor interface of organic solar cells has driven efficiencies beyond 10% for single junction solar cells with bulk heterojunction architecture. Due to these arising issues of using fullerene derivatives as acceptors such as; difficult synthesis, limited tenability of energy levels, high cost for purification, morphological instability and weak light absorption in the visible region.¹⁻³

Fused ring non-fullerene small molecule acceptors have become more attractive recently due to their benefits of being easier to synthesize than fullerene-based acceptors and ability to gain excellent purity compared to polymers, chemical modifications allow for easy tuning of optical and electronic properties, good absorbance, good morphology and suitable for flexible devices.⁴⁻⁷ Recently, we have reported a series of the non-fullerene acceptor (IDTBR) containing IDT as a central core with efficiencies reaching 11%.^{5,7} In this talk, I will discuss a systematic modification of IDTBR acceptor structure. We have modified alkyl chains on the electron donating part indacenodithiophene (IDT) and replacement of acceptor end groups. Substitution of acceptor end groups result in the shift of energy levels and a shift in the absorption spectrum. I will discuss in detail the impact of a change in alkyl chain length and outer peripheral acceptors end group of these new molecules on optoelectronic properties. These new modified structures of IDTBR acceptors have shown promising performance in single junction solar cells with different donor polymers, resulting efficiencies were above 12%. OPV device performance, photo physics and morphological studies of these blends will be presented.

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Graphene and other 2D materials; Fabrication & applications

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The isolation of two-dimensional graphene from the layered material graphite by using the simple and unusual method of repeated mechanical peeling by scotch tape has stunned the scientific world. Rapid progress in 2D material research and demonstration of proof-of-principle applications in short time has forced R & D organizations and industries to strongly focus on these low dimensional nanomaterials in variety of areas.

Atomic crystals in 2D family are layered materials and can be viewed as individual atomic planes. These planes can be pulled out of bulk crystals similar to unrolled single-wall nanotubes. By using micromechanical cleavage, we have prepared and studied a variety of 2D crystals including those ranging from conducting to insulating properties and their monolayers e.g., *h*BN, graphene and several dichalcogenides. These atomically thin sheets are fabricated at room temperature and are found stable under ambient conditions. High crystal quality is one of their distinct features, also continuous on a macroscopic scale. Attractive features of these 2D nanomaterials are their exotic properties as compared to their bulk counterparts. Aside from technological applications, many phenomena of quantum physics can be probed and studied in detail in the excellent quality of 2D crystals. The superior carrier mobility of graphene compared to other semiconductor materials is quite an attractive electronic feature. The work presented in this lecture will include fabrication and characterization of 2D crystals exhibiting conducting, semiconducting and insulating characteristics and their potential use in practical sense.

Synthesis of ion channel, an ideal candidate for the drug delivery system

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Tethered bilayer lipid membranes (*tBLMs*) have been developed in the past decade as a model system of the biological membrane. They provide a fluid, stable, and electrically sealing platform for the study of membrane related processes, specifically, the function of incorporated membrane proteins. The *tBLM* has been studied extensively but the corresponding monolayer of *tBLM* is less understood. We developed a synthetic methodologies to synthesize various anchor synthetic lipids for attachment to silicon or gold surface and used AFM to study the growth process of several self-assembled monolayers of time-dependent *in situ* AFM images of such samples immersed in ethanol solution of thiolipids, bilayer and protein, performed in a liquid cell or *ex situ* in air. These studies showed that before forming a complete monolayer, the thiolipids molecules were aggregated in the form of small islands, in which 2D aggregates of adsorbate molecules nucleate, grow, and coalesce on the substrate. With the proceeding of immersion, these islands gradually grew and merged into larger patches. Finally, a close-packed film with uniform appearance and few defects was formed. The same phenomena were observed for the bilayer as well. The incorporated supramolecules rearranged into nanopores, which were studied with the help of AFM. These nanopores can be used for the site-selective release of drugs.

Magneto-optics of 2D materials

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In this talk, I will introduce some of the fascinating classes of two-dimensional materials such as graphene, silicene, phosphorene and borophene. In particular, I would show the electronic band structures of these materials allows one to envisage different classes of topologically distinct materials. Due to spin orbit interaction, these materials are endowed with a rich valleytronic structure. The valley, along with the conventional charge, degree of freedom can be used as an exciting paradigm for quantum information processing. I will explain how light interacts with these materials, especially in the presence of magnetic fields. This allows extraordinary tunability of the magneto-optic response. Some examples of magneto-optic effects I will cover are Faraday and Kerr rotation, circular dichroism, photonic spin Hall effect quantized spatial beam shifts.

The role of calixarenes as nanorobotics in material science

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It is a matter of fact that the water polluting toxicants including toxic metal ions and anions that enter into the environment by different industrial sources are hazardous to human health. To get rid-off from these pollutants, a large number of strategies are extensively used. The supramolecular chemistry has provided various convenient approaches for the recognition of guest species at ionic and molecular level. However, the development of synthetic selective and efficient host molecules as nanorobotics for trapping the guest species is increasing due to expanding environmental and health problems. This has inspired chemists to synthesize such materials, which are selective for guest species that may be either charged or neutral. Among them, the “Calixarenes” are well known as an attractive and excellent class of macromolecules that can play an important role as nanorobotics due to their unique three-dimensional structure with almost unlimited derivatization possibilities. The calixarenes could be functionalized to design several efficient extractants at molecular level according to the choice of application in varying fields such as analytical, environmental, pharmaceutical and industrial or sensor technology.^[1-5] Thus, in this lecture I will discuss the strategic alternatives to all the techniques that may help in organizing the toxicants removal processes and may prove to be useful not only for the remediation of hazardous species but also advantageous for the recovery of costly chemicals that could be reused.

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Emerging 2D-MXene and black TiO₂ nanomaterials and their potential for biomedical applications

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Among the recently emerged nanomaterials, two dimensional (2D) Mxene and black TiO₂ nanomaterials have attracted much interest from researchers owing to their multifarious applications like energy, environment, biomedical, etc. In this talk, we will present in detail synthesis techniques, structure features, properties and application potential of various 2D MXene nanomaterials as well as black TiO₂. We will also discuss how 2D MXene nanomaterials are different from graphene and black and white titania. Particular attention will be focused on environmental applications of above said nanomaterials.

Chiral metamaterials for biological sensing: the role of optical chirality and interference

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Chiral plasmonic nanostructures enable the sub-pg detection and characterization of biological materials. The sensing capabilities are associated with the chiral asymmetry of the near fields, which locally can be greater than equivalent circularly polarized light, a property referred to as superchirality.

However, sensing abilities do not simply scale with the magnitude of superchirality. We show that chiral molecular sensing is correlated to the thickness of a nanostructure. This observation is reconciled with a previously unconsidered interference mechanism for the sensing phenomenon. It involves the “dissipation” of optical chirality into chiral material currents through the interference of fields generated by two spatially separated chiral modes. The presence of a chiral dielectric causes an asymmetric change in the phase difference, resulting in asymmetric changes to chiroptical properties. Thus, designing a chiral plasmonic sensor requires engineering a substrate that can sustain both superchiral fields and an interference effect.

Real time STM tip state recognition using neural networks

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One of the most frustrating and time-consuming challenges facing scanning probe microscopists is the constant need to detect and correct flaws of the scanning tip apex. While atomically sharp tips can be created *ex situ*¹, imperfections such as blunted or “double” tips change images non-linearly, resulting in a variety of image artefacts. Furthermore, different atomistic image resolutions/states can also be seen, depending on the specific surface being observed.² Indeed, certain tip shapes may be desired for tasks such as imaging, but not for atomic manipulation, for example. Accounting for all these factors is a manual, frustrating process that would benefit greatly from automation, despite the relative lack of historical attempts to do so (most notably Rashidi et al, 2018).³

In this lecture, I will demonstrate a convolutional neural network protocol that enables highly performant state recognition with *h*Si(100), Au(111) and Cu(111). We correctly distinguish the full set of tip states specific to the surface, but do so with even greater performance when distinguishing surface-specific tip states from general visual artefacts. Furthermore, we also extend this system to accurately assess live data in real-time by considering individual lines cans and methods analogous to video classification. We find in certain cases that this particular method improves performance, whilst requiring less data to make an assessment.

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Nanocolloids to understand the nature of the glass transition

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The glass transition has been described as "the deepest problem in solid state physics".¹ In this lecture, I will show how insight into this longstanding challenge may be obtained through the use of nanotechnology, specifically super-resolution "nanoscopy" of nanoparticles. The challenge of the glass transition is that, fundamentally, the reason for solidification of a liquid in the absence of crystallization is not understood, and competing, mutually exclusive theories give equally good descriptions of the experimental data available.² There is thus an urgent need for better experimental data, and in particular higher-order correlations than pairwise have been identified as a key requirement to unravel the challenge of the glass transition.³

Such higher-order data requires measurement of the coordinates of the constituent particles or molecules, which is not possible for molecular glass formers, but has been achieved for mesoscopic colloidal glass formers.⁴ However, mesoscopic colloids have dynamics that are so slow that the physics of the glass transition is not captured,^{2,3} so to truly understand this problem we need to use particles that are almost as small as molecules, i.e. nanoparticles. Our first steps in this direction have revealed deep insight into the role of fivefold symmetric structures such as icosahedra and the role of configurational entropy.⁵ Here we probe a deeper question as to the nature of interfaces between co-operatively re-arranging regions, which will be discussed in this lecture.

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First principles modeling of anisotropic thermoelectric materials

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We present a theoretical analysis of arsenic telluride using various theories pertaining to electrical and thermal transport properties. The objective is to develop a general method for evaluating thermoelectric properties of any material. The work was performed using computational models based on fundamental principles of quantum mechanics, whilst accounting for complexities such as layering or anisotropy. Important challenges have included the computational cost of modelling complex materials like arsenic telluride, and ensuring that the method is sufficiently general that it can cope with arbitrary material complexity.

TiO₂ based nanocomposite hydrogel for solar disinfection

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Sol-gel chemistry has been adeptly exploited to fabricate nanocomposite gels for solar disinfection to render clean drinking water, especially in the developing countries. The present research is a novel approach to acquire potable water by improving the adsorption or catalysis through exploiting the synergistic effect of three different notions; the high surface area and controlled porosity of xerogels, immobilization of photocatalytic titanium dioxide (TiO₂) nanoparticles and red shift of absorption edge alongside high electron transport properties of carbon. The characterization and analysis through UV-Vis spectroscopic studies concluded the reduction in the bandgap (from 3.2 eV to 2.9 eV) of TiO₂, hence, these nanocomposites possess light absorption ability in the visible region of the electromagnetic spectrum. Moreover, the morphology examined through FESEM and chemical linkages through FTIR confirmed the predicted profiles. Finally, the S_{BET} for surface area analysis and the reduction in dye concentration over time, validated that these nanocomposites are potential disinfectants for the antimicrobial activity due to large surface area for maximum absorption of organic pollutants. Noteworthy advantage of these nanocomposites is the green synthesis approach and this disinfectant can be sequentially used efficiently for several number of cycles.

Long wavelength lattice dynamics in morphotropic $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$: the road to large scale electronic structure calculations

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The $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$ (PZT) solid solution can be regarded as a randomly ordered isovalent B-site substituted compound in a matrix of either of the two-phase diagram end members PbTiO_3 (PTO) or PbZrO_3 (PZO). The former is a prototypical ferroelectric (FE) with $P4mm$ symmetry whilst the latter, though still topical, is considered an antiferroelectric (AFE) with $Pbam$ symmetry. These observations are supported using the soft-mode theory of lattice dynamics by considering the symmetry (and energy) lowering distortions of a high symmetry cubic phase as indicated by imaginary frequencies at certain wavevectors in the phonon spectrum. It is most common to study PZT around $x \approx 0.52$ in the region near the morphotropic phase boundary (MPB). This is a compositional boundary with complex lattice dynamics where a flat energy surface for polarisation rotation exists between the ferroelectric tetragonal ($\mathbf{P}||[001]$) and rhombohedral ($\mathbf{P}||[111]$) phases via intermediate monoclinic phases. It is this process which is thought to bring about the giant electromechanical response of the material which has long been exploited for use in ultrasonic transducers ceramic capacitors and actuators. More recently, it has been suggested for use in piezoelectricity-induced room temperature superconductors for the potential generation of a supercurrent along a metal/piezoelectric interface.

Using density functional perturbation theory (DFPT), it is found that for some arrangements of PZT that single, long wavelength modes of a dual antiferrodistortive & antipolar character are competitive in their instability with more commonly considered zone centre/boundary modes (e.g. Ferroelectricity and Glazer-type rotations of the BO_6 octahedra). Although the eigenvectors of the distortion are available via the plane-wave DFPT calculation, due to the long wavelengths of the distortions, many thousands of atoms are required to find the resulting stable structure and to explore its energetics. Such calculations are of extraordinary computational expense and even intractable for conventional plane-wave based methodologies due to well-known $O(N^3)$ scaling in compute time where N is the number of atoms in the simulation.

Along with a full comparative study of the lattice instabilities of PTO, PZO and PZT, we evaluate the applicability of large-scale electronic structure calculations to study the long wavelength distortions using compact basis sets of pseudoatomic orbitals (PAOs) as implemented in the CONQUEST code. We find that even for basis sets of a modest size, the method is able to accurately reproduce the phase transition energies and stable structures predicted by plane-waves. Since our findings suggest that our method is applicable even for the fine, shallow energy surfaces of the perovskite-oxides, this method could pave the way for a new paradigm for first principles calculations in a diversity of nano systems.

Tuning metal chalcogenide molecular catalysts for the hydrogen- evolution reaction: Electronic effects and mechanistic insights

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The production of hydrogen through water splitting using earth-abundant metal catalysts is a promising pathway for converting solar energy into chemical fuels. However, existing approaches for fine stoichiometric control, structural and catalytic modification of materials by appropriate choice of earth abundant elements are either limited or challenging. One promising strategy is the design of molybdenum sulfide nanoclusters, which mimic the catalytically active sites found in MoS₂. These molecules have the unique property of exposing a high degree of active edge sites leading to improved catalytic activity.

Here, we explore the implementation of new design principles for the development of efficient molecular HER catalysts. In this work, we prepared [Mo₂O₂(μ-S)₂(S₂)₂]²⁻, [Mo₂O₂(μ-S)₂(S₂)(S₄)]²⁻ and [W₂O₂(μ-S)₂(S₂)(S₄)]²⁻ by wet-chemical methods and investigated their HER electroactivity.¹ Specifically, we aim to investigate the effects of stoichiometric and structural control resulting from the appropriate choice of the chalcogen elements and their ratio (e.g. O²⁻/S₂²⁻, O²⁻/S₂²⁻/S₄²⁻) within the coordination sphere of earth abundant transition metals (e.g. Mo or W). We evaluate the performance of these molecular catalysts for the hydrogen evolution reaction while we propose potential mechanistic pathways in relation to the interaction between catalysts and substrate.

The use of gold nanoparticles as novel photodynamic cancer therapy sensitizers

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Gold nanoparticles (AuNPs) provide a new and exciting tool in cancer diagnosis and therapy. Their unique surface and optical properties can provide significant improvements over conventional treatments. Photodynamic therapy (PDT) combines a photosensitizer and light to generate reactive oxygen species within a tumor to destroy the cancer. It can provide exceptional dual selectivity as only cells which contain the photosensitizer and are exposed to light are damaged.

The use of AuNPs as a photothermal agent has been researched extensively, however this approach fails to utilize the photochemical properties of AuNPs, and due to fast heat diffusion it may also kill surrounding cells which do not contain AuNPs. Upon irradiation with light, AuNPs have been shown to generate singlet oxygen – a key active species in photodynamic therapy [J Phys Chem C 120 (2016) 10647]. This could make them an ideal photosensitizer which, combined with the modifiable surface chemistry of AuNPs and their high stability against enzymatic degradation, could provide a photosensitizer that overcomes many limitations of PDT using traditional photosensitizers.

This study shows that cells containing AuNPs can be killed upon irradiation with 532 nm light in conditions that are below the required heating levels to cause cell death via a photothermal route. The characteristics of cell death in these non-photothermal conditions provide significant clinical advantages over the use of AuNPs in photothermal conditions and, combined with active targeting, could provide a cancer therapy with exquisite selectivity towards cancerous cells.

This work not only shows that AuNPs are a promising sensitizer for photodynamic therapy, but also that in their application as photothermal agents gold nanoparticles generate significant amount of reactive oxygen which is masked by the photothermal mechanism.

Mesoporous zirconia nanostructures (MZN) for excellent adsorption of As(III) and As(V) from aqueous solutions

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Arsenic contamination in water has become a serious environmental and health problem due to its high carcinogenicity and toxicity. Still it is a challenging task to develop novel adsorbents with high adsorption capacity and excellent selectivity for As(III) as well as As(V) along with good regeneration-ability and field applicability. In order to address this environmental issue, mesoporous zirconia nanostructures (MZN) were synthesized by hydrothermal method to efficiently remove highly mobile and toxic arsenite (As(III)) and arsenate (As(V)) from aqueous solutions using batch adsorption experiments. The as-synthesized MZN were characterized by Brunauer–Emmett–Teller (BET), X-Ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmission electron microscope (HRTEM), and energy-dispersive X-ray spectroscopy (EDX) techniques. The batch adsorption experimental results showed that the As(III) and As(V) removal capacities of the MZN were 105.03 and 110.29 mg/g, respectively, under neutral pH conditions at room temperature, which were better than many recently reported adsorbents. The adsorption behavior of As(III) and As(V) on the MZN could be well described by pseudo-second-order and Langmuir isotherms models. Moreover, As(III) and As(V) adsorption on the MZN was spontaneous, endothermic and favorable with increasing temperature. Some of the common co-existing ions had slightly affected the arsenic removal proficiency of MZN. Fourier transform infrared (FTIR) spectroscopy and X-ray photoelectron spectroscopy (XPS) were used to investigate the adsorption mechanism of As(III) and As(V) on the as-synthesized MZN. The as-synthesized MZN demonstrated quite fast and good treatment of simulated real arsenic (As(III, V)) contaminated water. This study suggested that the as-synthesized MZN are potential candidate for practical applications of As(III) and As(V) removal from the aqueous solutions.

***In vitro* and *in vivo* characterization of PVA/starch/g-C₃N₄/Ag-TiO₂ nanocomposite hydrogel membranes for wound dressings**

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Burn wounds are sternly aggravated by bacterial invasions. Biopolymers blended with certain wound healing and antimicrobial agents have potential to facilitate cell growth and tissue repair. In this research, hydrogel membranes based on polyvinyl alcohol (PVA) and starch were developed. To enhance the physicochemical properties, graphitic carbon nitride (g-C₃N₄) was incorporated as filler and silver-titania nanocomposite (Ag-TiO₂) as antibacterial agent. Ag-TiO₂ nanocomposite was synthesized by green route, using *Dictyosphaerium* algal strain. Solution casting technique was adopted for the fabrication of hydrogel membranes. The prepared hydrogel membranes were then subjected to various characterizations, including mechanical testing, moisture retention, water and oxygen permeability, swelling and antibacterial activity. The results exposed that superabsorbent hydrogels were prepared, with excellent ability to swell in various simulated body fluids (SBFs) up to 144 hours. As compared to pristine PVA/starch film, the film with 0.14g g-C₃N₄ showed 62% improvement in tensile strength. Similarly, highly effective antibacterial effect towards skin pathogens, *Staphylococcus aureus* and *Escherichia Coli* was detected. The highest diameter of zone of inhibition, 33.25±0.54 and 37.33±0.61 mm was found against both strains, respectively at PVA/Starch/0.14g-C₃N₄/0.7Ag-TiO₂ composition. Furthermore, the permeability to water and breathability to oxygen was revealed by water vapor transmission and oxygen permeability tests. Finally, the full thickness wound healing ability was demonstrated using female albino mice as animal model. Macroscopic analysis revealed good inflammatory response, perceptible wound reduction and re-epithelization rate with complete healing accomplished on 7th day of injury. All these properties render the prepared ternary blend of PVA/Starch/g-C₃N₄/Ag-TiO₂ as ideal wound dressings.

Controlled development of electrode material for water splitting

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The demand and consumption of energy is expected to be doubled in the coming 50 years and meanwhile the energy cost is also expected to rise significantly. Fossil fuels, currently the leading source of energy, subsidize a lot of CO₂ to the environment causing many environmental issues including greenhouse effect. To address these challenges, 'H₂' based economy is one of the vital scientific and political debate being a cleanest of all the fossils fuels with highest mass energy density (120-140 MJ/Kg). Water, being a renewable source, is a promising candidate in this regard because of its ability for the production of H₂ (HER) and O₂ (OER). OER is a 4e⁻ multistep process with a demand of 240-600 mV extra energy, which makes it more sluggish kinetically. Until now, RuO₂ and IrO₂ are among the best electrocatalysts for OER with minimum overpotential. It is generally believed that molecular nanoclusters (MNCs) are the strongest candidate in this regard because of their unique optical, catalytic, magnetic and electronic properties. These unique properties of MNCs are due to various factors including electronic shell closing (Jellium model), geometric shell closing, high surface to volume ratio and super atomic behavior unlike their bulk counterparts and are thus worth exploring not only to enhance their electrocatalytic activity due to their synergistic effect but also their expected recycling potential. In this talk, I will present our recent results on the development of earth abundant and cost-effective transition metal/metal oxide nanoclusters based electrocatalysts and their hybrids, which have great potential to make water a sustainable source of energy.

Exploiting the structure-property relationship in Bragg stacks: A soft matter approach

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Structural organization found in many examples from nature provides an inspiring model of engineering to produce smart materials. This approach is based on exploiting the theme of structure-property relationship to design new materials in which the applications stem from their structural aspects. The work presented in this lecture highlights this idea by exploiting diverse properties of specially designed hybrid Bragg stacks built up from different constituent polymer and nanoparticles.

Phononic structures, the acoustic analogues of photonic crystals, have recently sparked interest in materials science because of their ability to regulate elastic wave propagation. Acoustic waves of certain frequencies can be restricted in one direction or more while travelling through a phononic assembly, creating a band gap. We report on one-dimensional periodic Bragg stacks of poly-(methyl methacrylate) (PMMA) and porous silica (SiO₂) exhibiting clear band gaps in the hypersonic region (GHz). The non-destructive technique of Brillouin light scattering (BLS) is employed to measure the large and robust band gap offered by these hybrids [1]. Manipulating the structural parameters such as the composition of the constituent polymer and nanoparticle layers enables a tuning of the position and width of the band gap, subtly changing the band diagram. Theoretical calculations of these composite Bragg stacks coincide neatly with the experimental data, enabling an insight into wave propagation through periodic structures [2]. An engineering of the band diagram becomes possible for the hybrids by structural modifications of the constituent polymer or the colloidal particles. This study is a breakthrough in the sense that it utilizes soft matter fabrication techniques, in contrast to the semiconductor methods, for fabricating highly organized phononic crystals.

The concept of a structure-property relationship found in many natural materials has also been extended to design high strength and tough hybrid assemblies. The second part of the work takes inspiration from nacre architecture and mussel adhesion to fabricate layer by layer assemblies. Nanoindentation studies show very high elastic modulus values (in GPa) with a highly cross-linked structure indicated by TEM, indicating the potential of using these hybrid films as high strength adhesive coatings.

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A facile synthesis of FeCo nanoparticles encapsulated in hierarchical n-doped carbon nanotube/nanofiber hybrids for overall water splitting

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Electrochemical water splitting for the production of hydrogen is considered as an important reaction for the renewable energy technology which requires the development of highly efficient and cost effective catalysts. In this work, a facile synthesis protocol for the development of FeCo bimetallic alloy nanoparticles (NPs) supported over multi-walled carbon nanotubes (CNTs) and carbon nanofibers is presented. The CNTs, not only prevent FeCo NPs from agglomeration by encapsulating them in their hard protective shell at the tip but also provide an efficient electron pathway. Impressively, based on the synergistic effect of highly conductive and homogeneously distributed CNTs and FeCo NPs over N-doped carbon nanofiber support (FeCo@CNT/NCNF), the material exhibited excellent performance in oxygen evolution reaction (OER) and decent activity in hydrogen evolution reaction (HER) with exceptional durability of 48 hours even on glassy carbon electrode. By optimizing the FeCo precursors dosage it is deduced that FeCo@CNT/NCNF with Fe:Co ratio of 1:2 showed best activity in OER, with 283 mV overpotential required to achieve 10 mAcm^{-2} and very low Tafel slope of 38mV/dec, which is better than most reported studies for similar materials. The Faradic efficiency of OER and HER was also tested by using water displacement method and it was found close to >99%. This simple and cost-effective synthesis approach is very promising for growing well-dispersed CNTs over N-doped carbonaceous support using bimetallic transition metal alloys for applications in renewable energy technologies, batteries, sensors, etc.

P-1

Graphene based nanomaterials, synthesis, characterization and applications

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Graphene, a 2D material with unexpected mechanical, optical and electrical properties has recently attracted enormous interest in photocatalysis and nanoscience. Graphene stands out among many promising candidate materials because of its low cost and favorable band gap to absorb photons in the visible light range. However, its properties are hindered by issues like, photogenerated charge carriers, short hole diffusion length and mobility of charge carriers. To address these limitations, nanostructured composites with a solid-state electron mediator graphene act as ideal material for photocatalysis. The enormous charge transport properties of graphene have been widely discussed and proved by the scientist globally. Graphene has been considered as support material to work as a mediator between two semiconductor materials to boost their optical and electrical properties. It has been experimentally observed as the most useful unit for the construction of numerous nanocomposite materials in environmental and energy applications.

P-2

Reduction of coomassie brilliant blue R-250 dye by silver magnetic nanoclusters

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This work is about the synthesis of silver nanoparticles coated on magnetic iron oxide nanoparticles (chemical reduction and co-precipitation method). Silver nanoparticles were coated on magnetic iron oxide nanoparticles to form Ag@Fe₃O₄ (MNCs). The MNCs were characterized by UV-Vis and FTIR spectroscopy. MNCs catalytic activity was studied by performing experiments on the reduction of para-nitrophenol. The catalytic activity was further applied for the reduction of coomassie brilliant blue R-250. Effect of time, catalyst dosage and concentration of dye were studied. It was found that the 20 minutes were enough for catalytic reduction of the dye by MNCs. Kinetic analysis showed that the pseudo-first-order was found to be linear. It concluded that it is an effective method for catalytic reduction.

P-3

Synthesis of polyaniline/graphene nanocomposites as catalysts for counter electrode of dye-sensitized solar cells

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With the rapid increase in energy demand and continuous depletion of fossil fuels, the renewable energy resources emerged as a sustainable energy generation source. The objective of our research was to enhance the photovoltaic performance of dye-sensitized solar cells (DSSC) by replacing an expensive counter electrode material platinum (Pt) with relatively low-cost graphene/polyaniline (PANI/GR) nanocomposites. The nanocomposites were synthesized in an oxidative environment via *in situ* polymerization and, varying graphene amount from 3 wt.%, 6 wt.% 9 wt%, 12 wt.% to 15wt%. The morphological, elemental percentage content and crystallographic properties of pure graphene, PANi together with PANi/GR nanocomposites were observed using scanning electron microscopy together with energy dispersive X-rays (SEM-EDX) and X-rays diffraction (XRD). The results showed a uniform coating of PANi on graphene sheets. counter electrode of the GR/PANI nanocomposite were deposited on the surface of conductive substrate by doctor blading during fabrication of DSSC. The fabricated cells were electrochemically characterized using I-V, EIS, CV and Tafel polarization. The efficiency of DSSC containing 9wt.% GR/PANI counter electrode was achieved 7.45%, that is near to platinum based DSSC 7.63% under same conditions.

P-4

Investigation of structural, morphological and optical properties of Fe-doped copper oxide nanostructures

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In this work, pure copper oxide and Fe-doped copper oxide nanostructures [Cu_{1-x}Fe_xO where 0 ≤ x ≤ 0.08 in steps of 0.02] were synthesized using co-precipitation method. Ferric nitrate nonahydrate and copper nitrate trihydrate were used as precursors and sodium hydroxide was used as precipitating agent. As prepared samples were characterized by X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy (EDX) and UV-Vis spectroscopy for their structural, morphological and optical properties, respectively. XRD results confirmed the single-phase monoclinic structure of CuO. The average crystallite of pure copper oxide was found to be 43 nm whereas average crystallite size of Fe-doped CuO was found to be in the range 41-44 nm. It was observed that average crystallite size was increased with increasing iron concentration in CuO. Scanning electron microscopy analysis showed the agglomeration of CuO nanoparticles and EDX confirmed the presence of iron and copper with proper composition. UV-Vis spectroscopy results showed that band gap was increased with increasing iron concentration.

P-5

Synthesis of metal oxide nanoparticle immobilized fertilizer as growth regulator for selected vegetables

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Metallic nanostructures (NCs) has been emerging as a new type of efficient materials. NCs are ultrafine particles whose dimensions are in the range between 1 and 100 nm. Due to their physical and chemical properties, nonmaterials are being studied for their use in several different fields of science and engineering. Increase in the context of sustainability, applying innovative nanotechnology in agriculture (including fertilizer development) is regarded as one of the promising approaches to significantly improve crop production and feed the world's rapidly-growing population. Applications of diverse conventional fertilizers at high rates and for a long period in the agricultural sector have caused serious environmental issues globally. For example, heavy uses of nitrogen (N) and phosphorus (P) fertilizers have become the major anthropogenic factors exacerbating world-wide eutrophication problems in surface freshwater bodies and coastal ecosystems and even effecting people's daily life.

We have synthesized Fe_2O_3 , TiO_2 immobilized fertilizer as growth regulator via reported procedure and characterized by different analytical instruments. After the successful synthesis and characterization, Fe_2O_3 and TiO_2 nanoparticles were used as growth regulator and to mitigate (reduce) heavy metal ions like cadmium (Cd) and lead (Pb) from coriander plant. Effect of time, dose and temperature on biomass and fruit production was monitored weakly basis. Simultaneously the conventional fertilizers (DAP, natural biomass and urea) were also used to evaluate the effect of nanoparticles.

It was concluded after complete growth and fruit production, the TiO_2 nanoparticles, NPK immobilized TiO_2 and Fe_2O_3 and biomass has shown better growth in shorter time as compared with conventional fertilizer (urea and DAP).

Plant extract-based synthesis of gold nanoparticles and their applications in sensor

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Recently, many studies have reported that the plant extracts act as a potential precursor for the synthesis of the nanomaterials in non-hazardous ways. The plants are used successfully in the synthesis of several greener nanoparticles such as cobalt, copper, silver, gold, palladium, platinum, zinc oxide and magnetite etc. The most common sources that have been used for green fabrication of nanoparticles are extracts of plants, leaves, fungi and microorganisms. Green synthetic methods are cheaper, environmentally sustainable, and can lead to the fabrication of nano objects with controlled size and shape. In the present study, AuNPs were synthesized by using Green Capsicum extract as reducing as well as capping agent after mixing with aqueous chloroauric acid (HAuCl₄) as precursor and sodium hydroxide used as accelerating agent to speed up the reaction. The extract with different concentration reduced HAuCl₄ aqueous solution at 100 °C. The color change, pH change and UV-Vis spectroscopic analysis reveal the surface plasmon resonance (SPR) of the final reaction product which confirms the reduction of Au³⁺ ion to gold nanoparticles. The surface plasmon resonance band was controlled at 519 nm. The synthesized gold nanoparticles were characterized by UV-Vis spectroscopy, FT-IR spectroscopy, AFM, ZPA, SEM and DLS to check the stability, morphology, crystallinity and size of nanoparticles. Synthesized nanoparticles were successfully applied as colorimetric sensor for detection of selected metal ions such as Fe²⁺. The linear range of ferrous ion was 3.3-8 ppb based on increase in absorption intensity with R² value of 0.987 using UV-Vis spectrophotometer. The sensor was successfully applied to real water samples regarding the detection of Fe²⁺. Now gold nanoparticles as nanosensor are developed for detection of iron in tap water and distilled water.

P-7

Synthesis and characterization of metal nanocomposite for degradation of organic pollutant; A waste water treatment

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To report an excellent material for application in catalysis, for enhancing adsorption capability of removing contaminants from water as well as for organic material transfer, we have prepared nanocomposites using cerium as precursor via sol-gel method. The synthesized material was dried and calcined at 600-700 °C then transferred it to closed vessels. Then material was characterized by most sophisticated available analytical techniques such as X-ray diffraction (XRD) to determine crystallinity and amorphous nature of material, transmission electron microscopy (TEM) for internal structure, Fourier transform infrared spectroscopy (FTIR) for functional group detection, field emission scanning electron microscope (FESEM) for topography and composition and ultraviolet- visible spectroscopy (UV/vis) for band gap determination. After characterization, nanocomposites were evaluated as catalyst for degradation of organic dyes such as methylene blue and nitrophenol and the performance monitored by UV/vis spectroscopy.

Chemically synthesized Ni nanoparticles by sol-gel method, their characterization and potential towards catalytic reduction and degradation

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Nanosized Ni particles (NiNPs) were chemically synthesized by sol-gel method. Metallic salt solution of nickel was titrated against NaOH and pH was maintained at 8. The crystalline nature and face of the synthesized particles was determined by X-ray diffraction (XRD) technique while moieties present were characterized by Fourier transform infrared spectroscopy (FT-IR). The size and morphology of NiNPs were determined by scanning electron microscopy (SEM). The chemically synthesized Ni nanoparticles were 20 to 30 nm in size. These oval shaped NiNPs served as a catalyst for the reduction of 4-nitrophenol into 4-aminophenol and the reaction was completed in 15 minutes. The catalytic reduction of 4-nitrophenol was monitored by UV/Vis spectroscopy at different stages. Structural interpretation of reduced 4-aminophenol was done by FT-IR spectroscopy. NiNPs also acted as a catalyst for the degradation of organic dyes into non-toxic derivatives and the degraded product was determined by FT-IR spectroscopy.

Polystyrene based core-shell composite microparticles for catalytic degradation of toxic dyes

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Industrial wastewater consists of various toxic chemicals including dyes that are hazardous to human health, aquatic life and environment. Therefore, the removal of toxic dyes from wastewater sources is need of time. For this purpose, polystyrene-poly(N-isopropylmethacrylamide-acrylic acid) [PSy-p(NipmAm-Ac)] microgel particles were prepared via precipitation polymerization method. Silver nanoparticles (Ag-NPs) were loaded in shell of core/shell microparticles using AgNO₃ salt as source of silver ions. Ag@PSy-P(NipmAm-Ac) core shell hybrid particles were used as catalyst to accelerate the degradation of toxic dyes such as congo red (CR) in presence of sodium borohydride (NaBH₄) reductant. Controlled reactions were also carried out to prove the high activity of core shell hybrid microgels catalyst for the degradation of dyes. Pseudo first order was adopted to study the kinetics of CR degradation. The values of apparent rate constant (k_{app}) for degradation of CR in presence and absence of catalyst were found to be 0.63×10^{-2} and $0.4 \times 10^{-4} \text{ s}^{-1}$, respectively. Thus, prepared Ag@PSy-P(NipmAm-Ac) composite catalyst enhanced the rate of reduction of CR and made the reaction kinetically feasible. Activity of composite microgel particles was maintained even after ten months of synthesis, which shows their high stability. Reduction of CR was evaluated on the basis of Langmuir Hinshelwood (L-H) mechanism. CR degradation was also done under varying reaction conditions such as catalyst dose, concentration of NaBH₄ and CR. Percentage activity of catalyst was maintained up to four reusability cycles for the degradation of CR.

P-10

The antidepressant effect of diosgenin encapsulated solid lipid nanoparticles

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Cancer and depression are complex multifactorial co-morbidities. Depression contributes towards poor quality of life, dismal prognosis, increase in mortality rate and risk of suicide in cancer patients. Depression being a multi-factorial disorder is strongly linked to inflammation and has been validated through various studies. Many anti-inflammatory compounds had been tested and being used as potent antidepressant due to their anti-inflammatory properties. Scientific data has shown significant anti-inflammatory effects of diosgenin pointing it out to be a possible antidepressant. Blood brain barrier (BBB) had played a significant role in lowering the effectiveness of almost all brain therapeutics including resistance to anti-depressants. There is always an ongoing quest to devise alternate drug delivery vehicles that can enhance the potency and efficacy of the antidepressants. Emergence of nanotechnology has paved way to overcome such obstacle through formulation of solid lipid nanoparticle as a carrier. In current study, we have investigated the potential enhanced antidepressant effects of P-80 coated stearic acid solid lipid nanoparticles encapsulated diosgenin *in vivo* using sickness induced mouse model.

Diosgenin encapsulated P-80 coated solid lipid nanoparticles (SLNPs) were formulated by hot injection and solvent evaporation with few modifications and characterized by SEM, HPLC, FTIR, ZETA potential and XRD analysis. Drug entrapment and release was evaluated *in vitro*. The cytotoxic effects of the SLNPs coated as compared to uncoated diosgenin were evaluated by *in vitro* cytotoxicity assays using U87 cell line. Antidepressant effects of encapsulated vs non-encapsulated diosgenin were comprehensively evaluated *in vivo* using sickness induced mouse model. Furthermore, drug levels in various organs were also measured to exactly know the potential influx of the coated drug compared to uncoated drug.

SLNPs encapsulating diosgenin size ranged from 20 - 200 nm were confirmed by the scanning electron microscopy. The encapsulation of drug in SLNPs was confirmed by FTIR and XRD while stability and size were confirmed by the Zeta potential measurements. The IC₅₀ value of the diosgenin was calculated using U87 MG cell line which came out to be 18.34 μ M and it was found that diosgenin encapsulating drug was less toxic to the cells as compared to the naked drug. *In vivo* tests were carried out on sickened mice models, which showed positive therapeutic effects on mice with comparison to other anti-depressants.

This study validates the effective nature of SLNPs drug transport to brain which suggests that it could be an efficient vehicle for delivering diosgenin to brain crossing BBB. Our study validates that SLNP with diosgenin together can prove to be an effective way to treat depression and gliomas without imposing toxicity.

P-11

Polymer microgel-based silver nanoparticles efficient for degradation of azo dyes

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In this study, the synthesis of multi-responsive copolymer microgel poly-(*N*-isopropylmethacrylamide-co-methacrylic acid) [p-(NIPMAM-MAA)] and their use as microreactor for fabrication and stabilization of Ag nanoparticles has been reported. Both pure and hybrid microgels were characterized using Fourier transform infra-red (FTIR) spectroscopy, Ultraviolet visible (UV/Vis) spectroscopy, dynamic light scattering (DLS) and X-ray diffraction (XRD). Catalytic activity of hybrid microgels was investigated using congo red (CR), methyl orange (MO) and alizarin yellow (Al-Y) through UV-Vis spectrophotometry under different operating conditions. The apparent rate constant of reaction was also found to optimize reaction conditions for rapid and economical degradation of these dyes. The value of k_{app} was found to increase by increasing the concentration of dye up to a certain value and then it decreases by further increase in the dye concentration. Hence, it follows the Langmuir–Hinshelwood mechanism. The value of apparent rate constant (k_{app}) increases gradually with increasing quantity of hybrid microgel used as a catalyst. By comparing k_{app} values of these dyes, it was found that Ag-p-(NIPMAM-co-MAA) hybrid microgel gives better result for MO dye than other dyes.

P-12

Encapsulation of TiO₂ nanotubes with Cs nano particles to enhance the performance of perovskite solar cells

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Perovskite solar cell is the most developed form of dye sensitized solar cells which have exciting properties but it has some stability issues like photo stability, moisture stability and thermal stability. Cs doped TiO₂ nanotubes have good photocatalytic abilities so these tubes were used to enhance the thermal stability. UV-Vis Spectroscopy confirms the absorption rate increase in the visible region as compared to the pure TiO₂ nanotubes. By SEM images it was clear that after thermal treatment, many pits and holes were observed on the surface of perovskite film, but Cs doped TiO₂ have better stability at low concentration. If the Cs concentration is increased, then stability becomes even worse than pure TiO₂. These pits and holes are produced due to the degradation of methyl ammonium lead iodide (MAPbI₃), that was mainly responsible for thermal instability and this degradation was reduced by Cs doping. So, by Cs doping the actual performance of perovskite solar cell have been enhanced up to 18.1 %. The elemental analysis and structural configuration was confirmed by EDX and XRD, respectively.

Design and construction of a solar water purification system with graphene-plasmonic nanocomposite

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Availability of clean drinking water is a great challenge for communities all over the world. Production of clean water by utilization of solar energy from sewage and sea water has been considered a great alternative solution. Conventional solar water purification system has very low efficiency and high cost. Here we have extended a state-of-the-art solar water purification system by using graphene and plasmonic nanocomposite as an optimistic component to enrich the efficiency. We have synthesized the graphene plasmonic nanocomposite by using sol-gel technique and obtained in powder form. Synthesized graphene-plasmonic nanocomposite has been utilized in polluted water to design the water purification system. The nanocomposite has been combined with water in the presence of sunlight. It captured the polluted components and pure water converted to vapors, which have been collected on another chamber. We have attained the rate of purification $2.7 \text{ kg h}^{-1} \text{ m}^{-2} \text{ g}^{-1}$ under the sunlight with 80% efficiency. Result shows that a suitable nanocomposite gives an ideal change in solar water purification system by using the simple technique. The chemical composition, structural morphology and crystal structure of synthesized graphene plasmonic nanocomposite has been studied by energy-dispersive X-ray spectroscopy (EDX) and field emission scanning electron microscope (FE-SEM) and X-ray diffraction (XRD), respectively.

P-14

Cellulose acetate antimicrobial membranes enabled by metal nanoparticles and thiazolodines for potential applications in food packaging

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The study is based on the fabrication of novel antimicrobial cellulose triacetate packaging membranes. These membranes are fabricated by the integration of nanoparticles of different materials, 2-aryl substituted benzothiazoles and 2-aryl substituted thiazolidine carboxylic acid in the polymeric matrix of cellulose triacetate. These membranes are characterized by SEM and FT-IR. These modified packaging membranes showed positive antimicrobial activity when tested against *Bacillus subtilis*, *Bacillus cereus*, *Escherichia coli*, and *Pseudomonas aeruginosa*.

Synthesis of graphene/SnO₂ passivation layer to enhance the charge collection in perovskite solar cells

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Perovskite solar cells have been focused and highly preferred by scientists because of their considerable progress due to low cost, easy fabrication and high-power conversion efficiency (PCE). TiO₂ nanoparticles are considered as most promising electron selective layer but SnO₂ has higher conductivity than TiO₂. In this report, we have used graphene-doped SnO₂ nanoparticles electron transport layer in perovskite solar cells and have compared them with TiO₂ nanoparticles. SnO₂ electron transport layer-based perovskite solar cells were highly-efficient and stable than pure TiO₂ nanoparticles. We have adopted sol-gel method for the preparation of SnO₂ nanoparticles. We have fabricated the graphene single and multi-layers on SnO₂ nanoparticles to enhance the efficiency of graphene/SnO₂ based perovskite solar cells. Furthermore, the surface morphology, elemental composition, structure and efficiency have been investigated by SEM, EDX, XRD, UV-Vis spectroscopy and IV measurements. Above mentioned method of adding graphene layer onto passivation layer of SnO₂ in a perovskite cell has increased the overall power conversion efficiency to some extent.

P-16

Cs/TiO₂/rGo hybrid nanocomposite-based photoanode for highly efficient perovskite solar cells

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Perovskite solar cells (PSCs) are the most prominent area of research in new generation due to its power conversion efficiency (PCE). PSCs have the potential to replace the silicon solar cells for commercialization. PSCs have high efficiency, lower cost, longer carrier lifetime and high absorption coefficients. Much of the recent work on PSCs is dominated by absorber materials. Application of perovskite absorber in solar cell started in 2006 and published in 2009. The factor to influencing the PCE of PSCs is unusually increased from 3.8% to 23.7%. Now the stability issue is the most important provocation in PSCs. For increasing stability and efficiency, we have studied the Cs/TiO₂/rGo perovskite solar cells. Cs doped TiO₂ has been prepared by sol-gel method whereas reduced graphene oxide has been prepared by Hummer's method. In order to investigate the Cs/TiO₂/rGO prepared sample, SEM, XRD, EDX and UV-Vis techniques have been used.

P-17

Strategic design of graphene plasmonic nanocomposite-based photoanode for highly efficient plasmonic dye sensitized solar cells

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Renewable energy resources play an important role in meeting the global increase of energy demand. This research has been performed to enhance the efficiency of plasmonic DSSCs by harvesting the maximum sunlight. In this research, a nanocomposite of graphene, Cu and TiO₂ nanoparticles have been used to fabricate the plasmonic dye sensitized solar cells (PDSSCs). Furthermore, simple DSSC with TiO₂ and PDSSC with Graphene/Cu/TiO₂ have been synthesized by using the sol gel techniques. The Graphene/Cu/TiO₂ nanocomposite have enhance the efficiency of PDSSCs due to the plasmonic effect. Different techniques such as X-ray diffraction and scanning electron microscope (SEM) have been utilized for the analysis of samples. Due to limited resources of fossil fuels it is necessary to find out other ways for utilization of renewable energy sources. Although DSSCs are widely used in solar energy applications the performance of these cells is low. Transformation of the electron is necessary to achieve high conversion efficiency. Efficiency can be increased by increasing optical absorption. Furthermore, higher efficiency can also be obtained by increasing electron injection by minimizing the large band difference between TiO₂ layers. The band gap of TiO₂ is larger, therefore, nanoparticles of certain materials are used to reduce it and to make DSSC more effective. To increase efficiency of DSSCs cells, graphene, Cu incorporated TiO₂ nanoparticles will be utilized. Efficiency have been increased due to plasmonic effect of these nanoparticles.

Synthesis and characterization of hydrogel embedded with cobalt nanoparticles for water decontamination

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This work deals with the synthesis of poly (N-isopropylacrylamide-co-2-Acrylamido-2-methylpropane sulfonic acid) hydrogel, fabrication of cobalt nanoparticles in the prepared hydrogel and evaluation of catalytic potential of the as-prepared hydrogel-cobalt nanocomposite. The hydrogel was prepared by using a facile route of free radical polymerization. The cobalt nanoparticles were prepared by in situ reduction of Co (II) ions inside the hydrogel network. The *in situ* formation of cobalt nanoparticles was carried out by loading the Co (II) ions in the hydrogel from aqueous medium followed by their reduction with sodium borohydride. The formation of hydrogel and presence of both the monomers in the obtained hydrogel was indicated by FTIR spectroscopic results. The prepared hydrogel was able to absorb water as much as 63 times of its weight in dried water. The water absorption was found to follow the non-Fickian mechanism. The presence of cobalt in the hydrogel-cobalt nanocomposite was identified by ICP-OES analysis. The morphology of hydrogel and its composite with cobalt nanoparticles was studied by SEM. The shape and size of the cobalt nanoparticles fabricated in the hydrogel was assessed by TEM and it was found that the nanoparticles were almost spherical in shape and most of them had diameters ~ 25 nm. The thermal behavior was studied via TGA and DSC which showed that both the hydrogel and its composite were thermally stable below 260 °C. The catalytic potential of the as-prepared hydrogel-cobalt nanocomposite was assessed in the reduction of 4-nitrophenol to 4-aminophenol. The effects of amount of catalyst, temperature and recycling on the rate of this catalytic reaction were studied. The thermodynamic parameters such as activation energy, activation entropy change, and activation enthalpy change were also measured. The maximum rate constant was found to be 4.67 min⁻¹. The catalyst was also recycled and reused for five consecutive cycles, however, the reduction rate was decreased gradually after each cycle and 68 % decrease in the reduction rate was observed at the fifth cycle.

In operando investigation of the interaction mechanism among heterostructured VO_xN_y nanoparticles supported in nitrogen-doped reduced graphene oxide aerogel and lithium polysulfides for stable sulfur cathodes

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Reversible redox of sulfur (S_8) to lithium sulfide (Li_2S) through a series of lithium polysulfides (LiPS) still pose a key challenge to appreciate high-performance sulfur cathodes mainly because of their shuttling phenomenon and sluggish kinetics. Certainly, one of the most important parameters for transforming nanoscience is to realize the near-market host materials for Lithium-Sulfur batteries that are stable and scalable. Advances have been through in realizing the nanomaterials, those can effectively suppress the lithium polysulfides shuttle and improve the cycle life and stability of sulfur cathodes. It is hypothesized that transition metal compounds can be tuned to augment the interactions among oxides and LiPS by forming surface bound active redox intermediates. But, in most cases, the strategies to achieve nanoscale materials severely hamper the ease of production and scalability. Herein, authors come up with a simple and novel one-go synthetic strategy to accomplish heterointerface vanadium oxide nitride (VO_xN_y) nanoparticles in nitrogen reduced graphene aerogel (VONNG) via concurrent in-situ nitridation and carbonization processes. Metal oxide nitride particles have been achieved without involving external ammonia source. For the purpose, polycondensation reactions involved in accomplishment of C_3N_4 have been exploited to generate on-site active nitrogen species to realize porous vanadium oxide nitride nanoscales particles in nitrogen doped rGO aerogel through topotactic transformation. Remarkable performances have been observed using VONNG as host material for sulfur cathodes that can be attributed to the interface between V-O and V-N linkages to offer stronger binding interaction and fast electrocatalytical conversion of LiPS. The assembled cells from VONNG/S cathodes exhibit the initial discharge capacity of 1400 mAh g^{-1} at 0.05 C , 1250 mAh g^{-1} at 0.1 C and maintained their reversible capacity to 690 mA h g^{-1} at 0.2 C for more than 200 cycles. The loss in capacity is recorded less than 0.03% per cycle for 850 cycles with Coulombic efficiency close to 99% even at 1 C . The interaction mechanism between VONNG and LiPS has been probed by in-operando Raman spectroscopy, XPS and electrochemical methods. By modifying the chemical environment of vanadium oxide, we are enabling to fine tune the redox potential to facilitate thiosulfate formation that in turn form polythionate complexes to deter the LiPS shuttle. Secondly, the V-N linkage offer an opportunity to improve the kinetics of the redox reactions along with strong binding interaction. Previously proposed mechanisms of polysulfides conversion and polythionate complexation have been witnessed at practical specific current by surveying the cathode surface.

P-20

Biological applications of the characterized silver nanoparticles (NPs) and modular synthesis of photo-active Janus Dendrimers and Glycodendrimers as a platform for encapsulation of NPs and mimics of the plasma cell membrane

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Green Synthesis of the silver NPs by using plant extracts of *Mentha longifolia* and *Mentha arvensis* from Lamiaceae family, well renowned for the presence of essential oils provided a robust approach for the reduction of AgNO_3 to Ag nanoparticles. Different physicochemical parameters such as temperature, pH, concentration of the AgNO_3 and of the plant extract have effects on the morphology and the yield of the NPs were confirmed. UV-Vis, AFM, SEM, EDX and DLS manifested the hidden nanostructure of the moieties. Biological applications explored involved the antibacterial, antifungal, antileishmanial, hemolytic and cytotoxic activities. Multi-step modulated synthetic process that involved to architect amphiphilic Janus dendrimers (JDs) and Glycodendrimers (GDs) showed attributes to self-assemble in the presence of the aqueous environment into various architectures usually spherical in shape. These monodisperse dendrimersomes represent the class of complex organic supramolecular structures that can mimic biological cell membranes and are spherical in nature, can be designated to multifunctional tasks. Each dendrimer in dendrimersomes have hydrophilic and hydrophobic dendrons that align themselves according to their surrounding solvent and molecular structures into different morphologies. A library of the 12 amphiphilic Janus dendrimers were synthesized and they were having ability to cleave into two halves at the central core by irradiating with the UV light. These dendrimersomes provided a great opportunity to encapsulate anticancer drugs and their release can be easily steered by the process of cleavage. Surface of the dendritic capsules can be functionalized that act as a ligand and attach to the specific receptor sites on cells to deliver their load. Surface of the vesicles have abilities to respond to external stimuli and to expel drugs outside in environment such as photo-active Janus dendrimers are sensitive to lights of different wavelengths and can release drugs in the presence of a stimuli.

In Glycodendrimers the dendrons are extended to attach with sugar moieties that represent the carbohydrate ligands on the cell surface and are called as glycans, provided the breakthrough in glycoscience and protein research for the glycan and lectin interaction studies. Three additional Janus compounds were synthesized having a design of twin-mixed and decorated with sulfatide groups of two different types, varied in the chain length named as sulfatide type I and sulfatide type II and a new addition was made into sulfo-glycans by synthesizing sulphur containing lactose named as Sulfo-Lac II or SuLac. These glycodendrimersomes represents the cells of the neurons and the immune cells that have sulphur containing glycans and interact with lectins to decode the message found in the cells. The glycan lectin interaction plays a very important role in cell signaling, routing of the cells, immune responses, receptor-mediated attachment and the distinction of cells from adjacent cells.

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Future perspective of this work involves the synthesis of the hybrids of the dendrimers and NPs to increase the EPR effects, use of photoactive dendrimersomes for encapsulation of NPs and drugs alone and in conjugation, encapsulation of antimicrobials and their effects on increasing the efficacy and potency. The use of the GDSs as a platform and mimic of the cells to study the binding pattern of nanoparticles.

P-21

Design and development of Zr/TiO₂ nanocomposites for efficient breast cancer treatments

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Cancer accounted for about 17% of all deaths in 2019 and breast cancer is a public health problem all over the world. Moreover, breast cancer cells have a great resemblance to a high occurrence of bone metastasis. In this work, we have designed and developed Zr/TiO₂ based nanocomposites in order to use such affinity in the diagnosis and treatment of breast cancer. The application of Zr/TiO₂ nanocomposite could be in drug formulations. Nanocarriers such as nanoliposomal doxorubicin (Doxil) interact with the cancer cell membranes and they can selectively degrades and it is of clinical benefits for cancer patients with the passage of time. Here, we report a non-aggressive quantitative positron emission tomography (PET) technology that is predictive of therapeutic outcome in individual and double layer particles. In a breast cancer mouse model, we demonstrate that co-injecting DOX and a Zr/TiO₂ allows precise doxorubicin (DOX) quantification. In addition, Zr uptake also correlates with other types of nanocomposite' tumor accumulation such as Zr/TiO₂. We subsequently demonstrate that mice with >25mgkg⁻¹ DOX accumulation in tumors had significantly better growth reserved and enhanced survival.

P-22

Synthesis of optoelectrically active functionalized graphene materials and their applications

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Graphene is an allotrope of carbon consisting of a single layer of carbon atoms arranged in a hexagonal lattice. It is the strongest material ever tested, conducts electricity capably and is nearly transparent. Atoms at the edges of a graphene sheet have special chemical reactivity. Graphene is a transparent and flexible conductor that holds promise for various material/device applications, including solar cells, light-emitting diodes (LED), touch panels and smart windows or phones. In this study, graphene is prepared directly from graphite using microwave-assisted method. The prepared graphene was first exfoliated with aniline and then polymerization of aniline was carried out on the surface of graphene. By introducing graphene intercalated with aniline separately, the more compact graphene network structures were formed. The prepared graphene composite was thoroughly characterized via SEM, EDS, XRD, AFM, Raman, DSC and FTIR spectroscopy for morphology and composition. The synthesized graphene-based composite was deposited on glass substrate in different amounts using spin, spray and dip methods of coating. The transparency of prepared samples was checked using UV-Vis spectrophotometer. The effect of amount of material and method of coating on transparency of graphene composite was optimized. Four-probe DC conductivity technique was used to measure the conductivity of the prepared samples.

P-23

Design and development of Cs-doped TiO₂ nanoparticles to enhance the stability of solar devices

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DSSC is one of the most promising candidates for achieving efficient solar energy conversion because it is flexible, inexpensive and easy to manufacture. DSSCs are known to functioning well in low light or diffuse light conditions. Therefore, they might be interesting for indoor use, where the ambient light may have different spectra. DSSC provides a technically and economically credible alternative concept in the present days. The effect of additive on the performance of the dye-sensitized solar cell (DSSC) has been studied. Dye-sensitized solar cells based on titanium dioxide (TiO₂) are highly efficient, longer carrier lifetime to conventional solid state photovoltaic (PV) devices based on materials such as cesium. Doping of Cs has increased the stability and surface area in DSSC. Dye-sensitized solar cell employing Cs-doped TiO₂ has increased efficiencies and stability. Cs doped TiO₂ nano-particles has been prepared by sol-gel method. The compound samples have been characterized by X-ray diffraction (XRD), EDX, SEM, and UV/Vis. The XRD patterns have indicated that the crystal structure still remains as anatase phase for the doped samples.

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Silica nanoparticles doped polyurethane membranes for reverse osmosis applications

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Polyurethane (PU) is an exclusive class of polymers with special significance in membrane technology. In this work, a series of pure PU membranes were prepared and then doped with silica nanoparticles (SiNPs). The effect of doping of SiNPs (0.01-0.03 wt.%) was investigated in terms of structural, thermal, morphological, antibacterial and permeation properties of PU membranes. The FTIR spectral band at 944 cm⁻¹ confirmed the impregnation of SiNPs in PU matrix. The water content measurements revealed improved hydrophilic character of doped membranes. The SEM analyses exposed a uniform dispersion of SiNPs in PU matrix up to 0.02%, while aggregation was perceived at higher content. The PU membranes with highest SiNPs content (0.03%) showed highest thermal stability. The systematic study of desalination demonstrated the RO capability of prepared membranes. The membrane with 0.02% loading of SiNPs supported for highest salt rejection and water flux at effective pressure of 20bar. Hence, these results recommend the PU membrane doped with 0.02% SiNPs as a promising candidate for reverse osmosis applications.

P-25

Synthesis of colloidal-silica/transition metal oxide composite and its interaction with dye

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Colloidal silica is an important material due to its biocompatibility and wide range of applications. In the present study, sodium silicate, which is a low-cost precursor for silica synthesis, was used in the synthesis of colloidal-silica/transition metal oxide composite. Dyes have low photostability and silica can help to improve its photostability. Metals have the ability to alter the physiochemical process of dyes and so can either quench or enhance the fluorescence intensity of the dye. Interaction of dye with composite was investigated using UV visible and fluorescence spectroscopy. The parameters which were studied using these techniques are fluorescence intensity, wavelength shift and absorption.

Ag-doped TiO₂ nanotubes synthesized via anodization method for enhancing performance of solar cells

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Perovskite material for solar cells is a good candidate to overcome the energy crisis due to the mobility of the charge carriers and excellent absorption of light resulting in high efficiency of the devices and considerable possibilities to develop economic and scalable technology. A new technique was used to fabricate TiO₂ nanotubes by a modified electrochemical anodization method. For the fabrication of silver nanoparticles, we used a very simple and low-time consuming sol-gel method at room temperature for the construction of particles at a very big scale. Under the incipient humidity technique TiO₂ nanotubes were functionalized with Ag nanoparticles by utilizing ethanolic-palladium chloride solution. Perovskite cells with the highest energy conversion efficiency were consisting of carbon-counter electrodes and had been manufactured under circulatory air. TiO₂ nanotubes and Ag nanoparticles in perovskite solar cell was used to increase the proficiency of electron-inoculation. The result was ascribed to the strong Ag nanoparticles effect by surface plasmon resonance in nano-TiO₂ in the form of electron-transporting layer. The performance of PSCs was enhanced with increase in electron injection. The surface morphology, elemental composition, optical properties, and crystal structure of Ag/TiO₂ nanocomposite were characterized by scanning electron microscope, transmission electron microscope, energy dispersive X-ray spectroscopy, X-ray diffraction and UV/vis spectroscopy.

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Titania-supported silver/strontium nanoparticles (Ag/Sr-NPs@TiO₂) for photocatalytic H₂ generation from water splitting reactions

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Here we demonstrate a new strategy to boost the photocatalytic activity of titania supported silver/strontium nanoparticles (Ag/Sr-NPs@P25) for photocatalytic H₂ generation from water splitting. The Ag/Sr-NPs are in-situ prepared on the surface of titania via chemical reduction method. The impact of Ag and Sr nanoparticles in the photocatalytic reactions are further revealed. Strontium in the form of strontium oxide promotes electron transfer from the semiconductor surface to palladium nanoparticles by increasing the Fermi level of the titania support. The structural and morphological characterizations of the Ag/Sr-NPs nanocomposite are carried out using UV-Vis DRS, XRD, PL, TEM, and XPS techniques, based upon which the mechanistic insights are discussed.

P-28

Synthesis and catalytic applicability of Pt-Pd ITO grown nano catalyst: An excellent candidate for reduction of toxic hexavalent chromium

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In this study, we report the synthesis of indium tin oxide (ITO) decorated Pt-Pd nanoparticle by a simple and facile liquid phase deposition protocol and their application as a heterogeneous catalyst for the reduction of toxic hexavalent chromium. Different characterization techniques were used to confirm the synthesized nanoparticles are honeycomb-like structure. The average size of nanoparticles was found to be 2-5 nm and uniformly distributed over ITO surface. During this study, the parameter was optimized such as the effect of different reducing agent and their concentration, effect of microwaves radiation and dose of nanoparticles. It was observed that the kinetic mechanism was best described by the pseudo-first order. The synthesized Pt-Pd nanoparticles were successfully applied as an excellent heterogeneous catalyst for reduction of Cr (VI) to Cr (III) in water. The synthesized nanocatalyst was good in terms of fast kinetic, high catalytic efficiency, excellent recyclability, and analytical applicability for fast and efficient reduction of toxic hexavalent chromium as compared to conventional methods of nanocatalysts.

P-29

Green synthesis of silver nanoparticles for specific detection of Hg²⁺ ion

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This study demonstrates a simple, cost effective, rapid, environmentally friendly and highly sensitive colorimetric method for quantitative analysis of toxic metal ion Hg²⁺ using plant extract capped silver nanoparticles. A green route for preparation of highly stable and widely applicable silver nanoparticles (AgNPs) using aqueous leaf extract of Citrus Japonica for the first time was employed as bio-reductant which acts as the reducing and capping agent to synthesize more stable AgNPs. The formation of AgNPs shows yellowish-golden color appearance after 30 min of heating with Surface Plasmon Resonance (SPR) band at 403 nm in the visible region. Different parameters controlling the morphology of AgNPs were optimized, including pH, reaction time, and concentrations of silver salt, sodium hydroxide, and leaf extract. The fabricated green extract based AgNPs were characterized by UV-Vis spectroscopy, FT-IR spectroscopy, SEM, XRD, AFM, DLS and Zeta-Potential analysis. The AgNPs synthesized by Citrus Japonica leaf extract proved to be highly sensitive and selective colorimetric sensor for Hg²⁺. They showed visible color change from yellowish golden to light brown in aqueous medium. On the basis of the linear relationship between SPR band intensity of AgNPs and different concentration of Hg²⁺ a colorimetric method was developed on UV-Vis spectrophotometer for the specific detection of Hg²⁺. The linear range of the developed method was found as 9.4-90 μM with an R² value of 0.997 and limit of detection (LOD) and limit of quantification (LOQ) of 3.0 and 9.4 μM, respectively. The selectivity of prepared AgNPs for Hg²⁺ was also studied in the presence of Ni²⁺, Zn²⁺, Cu²⁺, Co²⁺, Pb²⁺, Cd²⁺, Cr²⁺ and Fe²⁺. The obtained results did not show any significant interference by competitive ions. No color change was observed in AgNPs when they were allowed to incorporate with other metal ions.

P-30

Synthesis of biocompatible material for effective delivery of CoQ10

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CoQ10 is classified as a fat-soluble vitamin. Chemically, it is a basic quinone skeleton containing compound having a 10 carbon isoprenyl side chain, exists naturally in oxidized quinone form, and chemically represented as 2,3-dimethoxy-5-methyl-6-decaprenyl-1,4-benzoquinone. Due to its isoprenoid side chain, CoQ10 is found to be extremely lipophilic. CoQ10 occurs in crystalline state. While crystalline form shows poor water solubility and associated with bioavailability problems. To improve its bioavailability, we prepared CoQ10-loaded nanoliposomes (NL) stabilized with graphene oxide by using sonication and magnetic stirring method. In this study, a liposomal formulation composed of soy lecithin (LC) and GO was utilized to encapsulate CoQ10 for its effective delivery. Latest technical developments reveal that encapsulation of CoQ10 in nanoliposomes results in a significantly enhanced bioavailability as phospholipids are a major component of all cell membranes, Graphene oxide have been extensively explored as some of the most promising biomaterials for biomedical applications due to their unique properties: two-dimensional planar structure, large surface area, chemical and mechanical stability, superb conductivity and good biocompatibility. These properties result in promising applications for the design of advanced drug delivery systems and delivery of a broad range of therapeutics. The phenomena of bioavailability enhancement by formulations comprising of phospholipids extracted from plant and stabilized with graphene oxide is a completely innovative strategy for improving the bioavailability of CoQ10. The liposomes were homogeneous, 7 nm in diameter and had a narrow size distribution. HPLC assay for the determination of CoQ10 was developed and checked the loading capacity and percent release which is 97.6% and 99%, respectively. Surface morphology was determined by using SEM technique and stability was determined by using zetasizer.

P-31

Synthesis of modifiable p(methacrylic acid-co-acrylonitrile) microgel fabricated with metal nanoparticles for simultaneous catalytic reduction of multiple water pollutants

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In this work, poly(methacrylic acid-co-acrylonitrile) p(MAc-co-AN) microgel were prepared by inverse suspension polymerization, and nitrile groups were converted into amidoxime groups to obtain more hydrophilic amidoximated poly(methacrylic acid-co-acrylonitrile) amid-p(MAc-co-AN) microgels. Amid-microgels were used as microreactors for *in situ* synthesis of copper and cobalt nanoparticles by loading Cu (II) and Co (II) ions into microgels from their aqueous metal salt solutions and then converted to corresponding metal nanoparticle (MNP) by treating the loaded metal ions with sodium borohydride (NaBH₄). The characterization of the prepared microgels and microgel metal nanoparticle composites was carried out by SEM, TEM and TG analysis. The amounts of metal nanoparticles within microgels were estimated by AAS measurements by dissolving the MNP entrapped within microgels by concentrated HCl acid treatment. Catalytic performances of the prepared amid-p(MAc-co-AN)-M (M: Cu, Co) microgel composites were investigated by using them as catalyst for the degradation of cationic and anionic organic dyes such as eosin Y (EY), methylene blue (MB) and methyl Orange (MO), and for the reduction of nitro aromatic pollutants like 2-nitrophenol (2-NP) and 4-nitrophenol (4-NP) to their corresponding amino phenols. Here, we also report for the first time, the simultaneous degradation/reduction of MB, EY and 4-NP by amid-p(MAc-co-AN)-Cu microgel composites. Different parameters affecting the reduction rates such as metal types, amount of catalysts, temperature and the amount of reducing agent were investigated.

Electrodeposition of 3D nanomaterials and their application in energy storage and sensing technology

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About 80 % of the world total energy production relies on the combustion of fossil fuels which has severe impact on world economy and environment due to CO₂ emissions which results in global warming.¹ From last few decades, scientists have started to find alternatives for energy production and energy consumption. Different strategies have been employed to store energy, but electrochemical methods for energy production/conversion are under serious consideration as an alternative energy source which is designed to be more sustainable and more environmentally friendly.^{1,2} From last few decades, nanostructures with two-dimensional (2D) and three-dimensional (3D) architectures have received great attention due to their large electroactive surface areas, excellent conductivity, and efficient electrocatalytic ability.³⁻⁵ Different approaches have been applied to produce these 2D and 3D nanostructures such as chemical vapor deposition (CVD), physical vapor deposition (PVD), galvanic displacement, and electrodeposition but the latter one is a highly competitive alternative technique to those described above, due to its simplicity, relatively low cost, and low power consumption.⁶ Additionally, a wide range of controllable parameters can be varied to produce the desired size of deposit. In this work, we have investigated the formation of 2D or 3D nanostructures with different shapes and geometries such as honeycomb like microporous structures, cauliflower- shaped nano deposits, metal-organic frameworks (MOFs) using single electrochemical step on commercially available cheap chip-based devices. We incorporate these nanostructures modified devices along with room temperature ionic liquids (RTILs) as an alternate electrolyte due to its unique properties such as wide electrochemical window, low volatility at high temperature and high chemical and thermal stability and then employed them for the application of energy storage and sensing technology.^{5,7,8}

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Fabrication of responsive hydrogel-nickel nanocomposite catalyst for rapid reduction of aromatic nitrophenols

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Poly (N-Isopropyl acrylamide - co - 2-acrylamido methyl propane sulfonic acid) hybrid hydrogel was prepared and used as matrix for nickel nanoparticles fabrication. The hydrogel was prepared by free radical polymerization and nickel nanoparticles were fabricated via *in situ* reduction of Ni (II) ions within the hydrogel matrices. The manufactured hydrogel and its corresponding composite with Ni nanoparticles were characterized by FTIR, XRD, EDX, TEM, and TGA. Thermal stability of hydrogel was found to be increased upon fabricating with nickel nanoparticles. The hydrogel was able to absorb water 63 times of its weight in dried form. The nickel nanoparticles were observed to be well dispersed, spherical in shape and most of them were having diameters around 12 nm. The as-prepared hydrogel-nickel nanocomposite was used as-catalyst for the reduction of 4-nitrophenol which is considered as a toxic pollutant. The catalytic activity was monitored through UV-Vis spectrophotometer. The effect of temperature on the reduction rate and recycling efficiency of catalyst were also studied. The maximum rate constant observed for catalytic reduction of 4-NP was 0.815 min⁻¹. The formation of well dispersed nickel nanoparticles in the prepared hydrogel reflects that this hydrogel system can act as efficient stabilizing agent and along with acting a reactor medium. The significant catalytic potential of the hydrogel-nickel nanocomposite catalyst in the reduction of 4-nitrophenol shows that this system can be used for rapid reduction of many aromatic water pollutants.

***In situ* synthesis of Cu nanoparticles in cross-linked polymeric network for catalytic reduction of organic pollutants**

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In the present work, a cross linked polymeric network was prepared from N-isopropylacrylamide and 2-acrylamido-2-methylpropanesulphonic acid by free radical polymerization and used as a template for the synthesis of Cu nanoparticles by in situ reduction of Cu (II) ions loaded in hydrogel. The network polymer and its composite with Cu nanoparticles were characterized by infrared spectroscopy (IR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron diffraction X-ray (EDX), X-ray diffraction analysis (XRD) and thermal gravimetric analysis (TGA). The copper nanoparticles were almost spherical and found evenly distributed without any aggregates. The diameters of most of the copper nanoparticles were in the range of 80-100 nm. The amount of metal nanoparticles in hydrogel was analyzed by inductively coupled plasma (ICP). The copper nanoparticles containing composite was used as a catalyst for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in aqueous medium. The reusability of the composite up to five cycles and effect of temperature was also investigated on the reduction of 4-NP. Pseudo first kinetics was applied to study the kinetics of this catalytic reaction and to measure the catalytic efficiency of the prepared catalyst.

New binary and ternary nanocomposite materials having dual functionality (electrode and single layer) in solid oxide fuel cells

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The binary $\text{Li}_{0.02}\text{Ni}_{0.98}\text{O}/\text{Al}_{0.02}\text{Zn}_{0.98}\text{O}$ (LNO/AZO) and ternary $\text{Li}_{0.02}\text{Ni}_{0.98}\text{O}/\text{Al}_{0.02}\text{Zn}_{0.98}\text{O}/\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{1.9}$ (LNO/AZO/SDC) nanocomposite materials were synthesized by conventional solid-state reaction method. From XRD analysis, the average crystallite size was found to be 32 and 36 nm for binary and ternary nanomaterials, respectively. The SEM results showed that particles were homogenous and well distributed. The conductivity of the material was increased with increase in temperature showing semiconducting material. The impedance plot shows that materials were mixed ionic and electronic conductors. Similarly, the cyclic voltammetry results showed that materials were possessing both oxidation and reduction potential. LNO/AZO nanocomposite material was used as electrode (anode & cathode) in 3-layer composition having maximum open circuit voltage (OCV) and power density of 1.06V and 842 mWcm^{-2} at 550 °C. The ternary nanocomposite (LNO/AZO/SDC) was used as single layer fuel cell (SLFC) having maximum OCV and power density of 1.01 V and 595 mWcm^{-2} at 550 °C. The durability of single layer fuel cell was tested at constant current density and temperature and the corresponding results demonstrated that material is stable up to 16 hours.

Non-phosgene route for synthesis of hexamethylene-1,6-diisocyanate by thermal decomposition of hexamethylene-1,6-dicarbamate over $\text{Co}_3\text{O}_4/\text{ZSM-5}$ catalyst

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Hexamethylene-1,6-diisocyanate (HDI) is one of the most widely used aliphatic diisocyanate because of its unique properties and highly demanded in industries for various application.¹ Conventionally, HDI is produced by phosgenation of amine at industrial scale.² Thus, it is highly desired to explore and develop phosgene-free and green route for the production of isocyanates, due to harmful and uncontrolled effects of phosgene route. It has been reported that thermal decomposition of carbamates can be employed for the isocyanates synthesis which seems to be phosgene-free and green route.³ Recently, our group develops a method for thermal decomposition of carbamate to isocyanate using chlorobenzene as low boiling point solvent. This method reveals the advantage of relatively low reaction temperature, low viscosity, high dispersion and avoiding polymerization of isocyanate.⁴ However, isocyanate yield is low because of unconverted intermediate and undesired byproducts. This issue can be overcome easily if a heterogeneous catalyst is utilized along with low boiling point solvent. ZSM-5 modified with transition metal ions has received increasing significant attention as promising catalysts for a variety of important reactions, due to its unique channel structure, thermal stability, acidity and shape-selectivity. Among the transition metal ions, cobalt showed high activity towards many reactions. In this work, we wish to report a green route for synthesis of HDI by thermal decomposition of hexamethylene-1,6-dicarbamate (HDC) over $\text{Co}_3\text{O}_4/\text{ZSM-5}$ as heterogeneous catalyst. High HDC conversion and HDI yield were achieved.

The ZSM-5 zeolites ($\text{SiO}_2/\text{Al}_2\text{O}_3 = 25, 38, 60, 170$) were purchased from the Catalyst Plant of Nankai University and XFNANO Advance Materials Supplier and were used as support. The $\text{Co}_3\text{O}_4/\text{ZSM-5}$ catalysts were prepared by incipient wetness impregnation (IWI) method, deposition precipitation with ammonia evaporation (DP) method and PEG additive (PEG) method as reported in the literature, respectively. The theoretical loading of Co was 20 wt%. All catalysts were dried and calcined at 600 °C for 6 h in static air.

The thermal decomposition reaction was carried out in a 1 L stainless steel autoclave. In a typical reaction, HDC (10.0 g) and chlorobenzene (333.0 g) were charged into the autoclave containing $\text{Co}_3\text{O}_4/\text{ZSM-5}$ (0.55 g) catalyst. The reaction mixture was then heated to 230 °C with continuously mechanical stirring for 3 h. During the reaction, the methanol was continually removed from the reaction system using a N_2 flow at 800 ml/min and pressure of the autoclave was 0.68 MPa with corresponding to reaction temperature. The samples were analyzed by Shimadzu GC-2010.

The performance of the $\text{Co}_3\text{O}_4/\text{ZSM-5}$ as a heterogeneous catalyst for synthesis of HDI by thermal decomposition of HDC was assessed (Scheme 1). In this work, the thermal decomposition

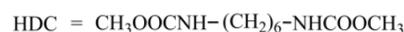
reaction was carried out under the reaction conditions mentioned in experimental section and results were listed in Table.1. A blank experiment was conducted without catalyst, which revealed 82.1% of HDC conversion. However, the HDI yield was only 28.4% and most of products were unconverted intermediate hexamethylene-1- carbamate-6-isocyanate (HMI) and undesired byproducts. The results show that bare ZSM-5₂₅ gave higher catalytic activity in thermal decomposition of HDC than the blank experiment. These results indicate that cobalt metal oxide supported on ZSM-5 might not only reveal much better catalytic activity in thermal decomposition of HDC, but can also give high yield of HDI.

The catalytic activities of Co₃O₄/ZSM-5 with different SiO₂/Al₂O₃ ratios were then investigated in the thermal decomposition of HDC under the similar reaction conditions. The HDC conversion reached 100% with the HDI yield above 70% in all Co₃O₄/ZSM-5_{25-170-IWI} catalysts. In particularly, Co₃O₄/ZSM-5_{25-IWI} catalyst revealed the highest catalytic activity with HDI yield of 82.3%, most probably caused by the appropriate amount active sites on catalyst which could lead the HDI yield. For Co₃O₄/ZSM-5 catalysts, the preparation methods can seriously influence its catalytic activity and selectivity. Therefore, Co₃O₄/ZSM-5_{25-DP} and Co₃O₄/ZSM-5_{25-PEG} were prepared and employed in the thermal decomposition of HDC as heterogeneous catalyst under same reaction conditions. For Co₃O₄/ZSM-5_{25-DP} catalyst, the HDC conversion could reach 100% while the HDI yield decreased to 73.4%, which can be caused by inappropriate deposition of metal particles into zeolite channels and decreased the catalyst selectivity to HDI. However, Co₃O₄/ZSM-5_{25-PEG} catalyst not only revealed better selectivity to HDI, but also reduced the reaction time. It was observed that the reaction could afford 100% HDC conversion in 2.5 h of reaction time over Co₃O₄/ZSM-5_{25-PEG}, with HDI yield of 92.4% being obtained.

Table 1. Catalyst screening for thermal decomposition of HDC

Entry	Catalyst	HDC Conversion (%)	HDI Yield (%)
1	None	82.1	28.4
2	ZSM-5 ₂₅	92.8	54.2
3	Co ₃ O ₄ /ZSM-5 _{25-IWI}	100.0	82.3
4	Co ₃ O ₄ /ZSM-5 _{38-IWI}	100.0	76.1
5	Co ₃ O ₄ /ZSM-5 _{60-IWI}	98.7	77.5
6	Co ₃ O ₄ /ZSM-5 _{170-IWI}	100.0	72.8
7	Co ₃ O ₄ /ZSM-5 _{25-DP}	100.0	73.4
8	Co ₃ O ₄ /ZSM-5 _{25-PEG} ^a	100.0	92.4

Reaction conditions: Conc. of HDC in chlorobenzene, 3.0wt%; temperature, 230°C; time, 3 h, 2.5h^a; catalyst, 0.55g; nitrogen flow rate, 800ml/min; pressure, 0.68MPa.



Scheme 1. Thermal decomposition of HDC to HDI over Co₃O₄/ZSM-5 catalyst

We have successfully developed a green route for the synthesis of HDI by thermal decomposition of HDC over Co₃O₄/ZSM-5 catalyst using low boiling point solvent. Among the various Co₃O₄/ZSM-5 catalysts, Co₃O₄/ZSM-5_{25-PEG} catalyst reveals high catalytic activity and gives 100% HDC conversion with 92.4% HDI yield. We currently focus on the reaction condition optimization, catalyst reusability and pathway for the synthesis of HDI by thermal decomposition of HDC over Co₃O₄/ZSM-5_{25-PEG}.

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Synthesis of naringenin loaded lipid based nanocarriers and their anti-inflammatory potential in arthritis induced animal model

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Rheumatoid arthritis (RA) also known as inflammatory arthritis, is a chronic inflammatory disease that results in progressive destruction of articular cartilage and bones. Naringenin is naturally occurring flavonoid that displays anti-inflammatory, anti-oxidant, antidiabetic, anticancer and antihyperlipidemic properties. In this study, focus was on anti-inflammatory potential of naringenin loaded lipid nanoparticles on arthritis induced with Freund's Complete Adjuvant (FCA). This study was planned to formulate biocompatible lipid based nanocarriers for the effective and efficient delivery of hydrophobic anti-inflammatory drug to the targeted site. For this purpose, different biodegradable lipid based nanocarriers were tested for the encapsulation of naringenin. XRD, SEM, UV-Vis spectrophotometer and DLS characterization were used for further analysis. A loading efficiency of 85% was found in the lecithin and chitosan nanocarriers, 81% in Lauric acid and stearic acid nanocarriers and 78% in stearic acid nanocarriers. Encapsulation of naringenin was further confirmed by FTIR spectroscopy. Average size of nanocarriers was < 200 nm. Thirty healthy eight weeks old male albino rats were used. Animals were randomly divided into six groups (n=5). All the animals except normal control group received the 0.1 mL FCA once in the sub-planter region of the left hind paw and were waited for seven days for the induction of arthritis. Group 1 was considered as normal control. Group 2 of animals was considered as arthritic control. Group 3 was considered as standard group and received pure naringenin 25 mg/kg orally for 14 days. Remaining three group i.e. group 4, group 5 and group 6 treated with naringenin loaded stearic acid nanoparticles, naringenin loaded stearic acid and lauric acid nanoparticles and naringenin loaded lecithin and chitosan nanoparticles respectively after the induction of arthritis. Statistical analysis was conducted by one-way analysis of variance (ANOVA) followed by Tukey's post hoc test at 5% level of significance (P<0.05). Results demonstrated an effective reduction in Interleukin (IL-6), Cyclooxygenase-2 (COX-2), tumor necrosis factor (TNF- α), and rheumatoid arthritis (RA) factor. Histopathological results also showed normal trend toward the recovery as compared to arthritic control.

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Formulation, characterization and pharmacokinetics of transdermal patch of gentamicin loaded poly lactic co glycolic acid nanoparticles

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Transdermal drug delivery is considered an important alternative to other routes for achieving systemic therapeutic benefits. Gentamicin (GM), an aminoglycoside, is the drug of choice for several diseases. Currently, its few topical preparations are available but they are not meant for systemic drug delivery. The current study aimed to develop transdermal patch for systemic delivery of GM. Gentamicin loaded poly lactic co glycolic acid nanoparticles were prepared by using solvent evaporation method. The NPs were characterized by zeta size, polydispersity index (PDI), entrapment efficiency, scanning electron microscopy, Fourier transform infrared spectroscopy (FTIR) and thermo gravimetric analysis (TGA). The NPs were incorporated to the baking layer of various polymer combinations. Transdermal patches were characterized further for various physico-chemical parameters. *In vivo* pharmacokinetics were studied in rabbits. Nanoparticles exhibited size of 219.2 nm with spherical surface morphology. Maximum entrapment efficiency was 90 % while no polymer-polymer or drug-polymer interaction was observed in FTIR studies. TGA confirmed the thermal stability of transdermal patch. Various pharmacokinetic parameters were studied like half-life, clearance, area under curve, time to maximum concentration and maximum concentration. Promising results regarding PK parameters were observed. It is concluded that GM-PLGA NPs patch have potential for systemic absorption of gentamicin and can be used for achieving therapeutic benefits. However, further studies are required for dose optimization of the formulations.

P-39

Conductive Nanocomposite Materials derived from SEBS-g-PPy and Surface Modified Clay

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Conductive nanocomposites were synthesized from surface modified clay and polypyrrole grafted triblock copolymer, polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene (SEBS-g-PPy). The grafting of PPy was carried out on SEBS using FeCl₃ as an oxidant and the formation of subsequent materials was monitored by IR, ¹H NMR spectroscopy and Gel permeation chromatography (GPC). Surface treatment of the clay was carried out by ion exchange method using the cationic salt of 2,2-bis[4-(4-aminophenoxy) phenyl]propane for better adhesion with the polymer matrix. Thin composite films containing 1–8-wt.% organoclay were investigated by FTIR, XRD, TEM, tensile testing, TGA, DSC and electrical conductivity measurements. The molar mass as determined by GPC was around 37,000. XRD pattern and TEM images described good dispersion of clay platelets in the nanocomposites. Tensile testing revealed improvement in mechanical properties up to 3-wt.% of organoclay. The bulk electrical conductivity was increased up to 7-wt.% with increase in resonance of delocalized electrons of stretched PPy chains due to hydrogen bonding with organoclay in the nanocomposites. Thermal decomposition temperatures of the nanocomposites were in the range 435–448 C. The decomposition of the nanocomposites was observed at higher temperatures relative to the pure polymer matrix with increasing clay loading. The weight retained after 900 C was approximately equal to the amount of organoclay added in the composites. These composite materials exhibited improvement in glass transition temperature as compared to SEBS-g-PPy.

P-40

Hepatoprotective effect of curcumin loaded chitosan nanoparticles in cypermethrin (CYP) induced liver toxicity in albino rabbits.

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Presently exposure to synthetic pesticides is increasing since its prevalent use in different field e.g., agriculture, horticulture and in domestic for pests' control and serious concerns are arising for potential risks imposed to human and animals. Frequently used pyrethroid is Cypermethrin, a type II insecticide because it has good efficiency, stability and persistent in air for long duration. Cypermethrin induced hepatotoxicity increases the ROS level leading to cell damage and immunosuppressive action. Liver malfunctioning is life threatening condition and different methods are used to protect it, one of them being nutraceutical. Current study was planned to evaluate hepatoprotective effect of curcumin in cypermethrin induced hepatotoxicity in rabbits. Curcumin was encapsulated in chitosan nanoparticles to improve its solubility and for better therapeutic goals. Nanoparticles were characterized for zeta size, zeta potential, encapsulation efficiency and FTIR analysis. A total number of 20 rabbits were divided into 4 groups (n=20). Cypermethrin was orally administered for alternate 28 days to induce hepatotoxicity in rabbits. Nanocurcumin formulation was orally administered to albino rabbits for 28 days to observe hepatoprotective effect against cypermethrin induced liver toxicity. Treatment of nanocurcumin plus cypermethrin was given. Blood samples were collected at 0th, 7th, 14th, 21th and 28th days. After completion of trial duration, the hepatoprotective effect of curcumin loaded chitosan nanoparticles was evaluated by studying the different parameters comprises the liver functioning test (AST, ALT, ALP & Total Bilirubin), hematological & histopathological analysis. Curcumin loaded chitosan nanoparticles were capable of lowering hepatotoxicity induced by concomitant administration of cypermethrin as proved by noteworthy decrease in Liver enzymes levels and improvement in hematology and histopathological features. Hence it is proved that curcumin encapsulated in chitosan nanoparticles has hepatoprotective action in cypermethrin induced hepatotoxicity in rabbits and they can be a potential target for hepatoprotective regimens.

P-41

Development of biopolymer- silica nanoparticle-based pH-sensitive hydrogels for application of periodontal disease

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Nanoparticles (NPs), novel in size, shape, and surface chemistry offer a wide range of biomedical applications ranging from drug-delivery to dental implant coatings. In this research project, we aimed to develop a system that could support regenerative processes within the periodontal pocket. Collagen, chitosan and silica NPs which are key representatives of a protein, polysaccharide and an inorganic material, are usually employed as biomaterials. Silica NPs have been used extensively in dentistry e.g. they are used as tooth polisher, in dental hypersensitivity and as dental filler.

Chitosan was blended with collagen and then PVA followed by the addition of different amounts of silica NPs in four different hydrogels or films. These films were also loaded with Cefradine. All the hydrogel samples were fabricated at same temperature and stirring rate. The characterization of the samples was performed by Fourier transform infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM) and Swelling tests. The swelling tests were performed in water, buffer solutions of pH (2,4,6, 7, 8) and ionic solutions of NaCl and CaCl₂ of different concentrations of 0.1, 0.3, 0.5, 0.7, 0.9 and 1M. The films showed maximum swelling in acidic medium (pH of mouth) and ionic solutions with lower concentration (0.1M) as the swelling decreases with increasing salt concentration. Drug release experiment was also performed in PBS solution and showed 97% release in 3 hours which was our requirement. All these results shows the potential of these hydrogels for their use in drug delivery and in the treatment of Periodontal disease as intra pocket drug delivery system.

P-42

Fabrication of TFN membranes integrated with UiO-66 for the removal of Cadmium from aqueous medium

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Environmental remediation of heavy metals from aqueous medium is getting popular area in the field of membrane technology. Cadmium (Cd) is toxic in nature and has the ability to bioaccumulate in water bodies. In the current study, zirconium-based Metal Organic Framework (MOF) UiO-66 with diameters of 200 nm were synthesized and integrated to form thin film nanocomposite membranes (TFN) via interfacial polymerization (IP). Fabricated TFN membranes exhibit higher selectivity and permeability for Cadmium as compared to thin film composite membranes (TFC). Zirconium based MOFs are highly water stable and due to smaller pore size enhanced hydrophilicity of TFN membranes. In addition, the effect of loading of different wt% was also investigated. The TFN membrane with 0.2 wt% loading of UiO-66 displayed the highest permeability of 11 LMH/bar and notable rejections of 90% towards Cd respectively. To our best knowledge, this is the first study of application of TFN membranes incorporated with UiO-66 for the removal of Cd from aqueous medium.

Advanced rGO-based nanocomposite approaches to highly optimized solar thermal generation of clean water

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Water pollution is destroying the natural resources and global water crisis is among the biggest challenges for the scientists. Clean water technology has a huge impact on the lives of 750 million people over the sphere, who don't have access to clean and potable water. Distillation of clean water from sea water and even from waste water by utilizing solar energy is a hot area of research. Cleaning water by using solar energy is eco-friendly, economical, and a long-term solution to water shortage and water pollution. Graphene oxide (GO) has recently attracted great attention due to its unique chemical and physical properties. Graphene materials meet the requirements of excellent porousness, brilliant light absorption and high photothermal transductions, which can be used to attain the maximum efficiency of producing clean water. Large-scale fabrication of graphene and reduced graphene oxide (rGO) is important for industrial and research applications. In this work, we have used an advanced graphene nanomembranes for efficient production of clean water by utilizing solar thermal energy. The GO nanomembranes were prepared by a chemical exfoliation technique, a best procedure included the chemical oxidation of the precursor graphite powder utilizing a concentrated blend of sulfuric acid and nitric acid. Oxidized graphite powder was thermally peeled at 1050 °C for 60 min to create graphene oxide (GO). Chemical reduction of GO with sodium borohydride/H₂O₂ led to the formation of rGO. Besides, scanning electron microscopy (SEM) results indicated that the rGO layer have the size of about 70 nm. X-ray diffraction and EDX investigations demonstrate the crystallinity and essential structure of the synthesized material.

P-44

A contrastive study of antioxidant potential using Flavonoids-based biocompatible nanomaterials of *Fagonia Cretica L*

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Nanomaterials find wide-spread applications ranging from drug delivery, bio-sensing, MRI contrast agent, and for the treatment of several diseases (acute & chronic) for instance, cancer, AIDS etc. The plants of Zygophyllaceae family have medicinal importance due to the presence of useful phytochemicals used in the treatment of diseases for digestive system and as vasoconstrictor and emmenagogue treatment of cancer. These phytochemicals are responsible for the synthesis of nanoparticles (NPs). The extract of plant was passed through column chromatography and 'Flavonoids' were separated and NPs were synthesized by using metal salts of transition metals. NPs were characterized by UV, FTIR, SEM and PXRD and were used as catalysts for the reduction of organic dyes.

P-45

Tuning the interfacial properties of cationic surfactants with modified counterions at air/water interface

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In this research, the interfacial properties of cationic surfactants were explored with modified transition metal based counterions. Zn (II), Cu (II) and Ni (II) were used to modify the surfactant i.e. cetyltrimethylammonium bromide (CTAB), where the modified surfactants formed were $[CTA]^+[ZnCl_2Br]^-$, $[CTA]^+[CuCl_2Br]^-$, $[CTA]^+[NiCl_2Br]^-$. The interfacial properties were characterized using automatic dynamic tensiometer, DCAT-25. The parameters determined were surface tension (γ), surface excess (Γ), surface area (σ), surface pressure (π) and critical micelle concentration (CMC). The study has shown that counterion modified surfactant can affect the thickness of the interfacial monolayer formed by CTAB and modified CTAB on the air water interface at nanoscale. This was probed by measuring surface excess (Γ) and other relevant parameters as mentioned earlier.

P-46

Synthesis of silver nanoparticles fabricated in poly(N-isopropylacrylamide-2-hydroxyethylmethacrylate-acrylic acid) microgel catalysts and their catalytic applications for reduction of 2,4-dinitrophenol

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Poly(N-isopropylacrylamide-2-hydroxyethylmethacrylate-acrylic acid) (p(NIPAAm-HEMA-AAc) microgels were synthesized by free radical precipitation polymerization in aqueous medium. Fabrication of silver nanoparticles (Ag NPs) within the framework of microgels was carried out through *in situ* reduction of introduced silver ions and Ag-p(NIPAAm-HEMA-AAc) hybrid microgels were obtained. UV-Vis spectroscopy and FT-IR spectroscopy were used to characterize both pure and hybrid microgels. The catalytic reduction of 2,4-dinitrophenol (2,4- DNP) was carried out in the presence of Ag-p(NIPAAm-HEMA-AAc) hybrid microgels to test their catalytic activity. Reduction reactions were also explored by varying concentrations of reacting species like 2,4-DNP, NaBH₄, and dose of catalyst. The kinetics data indicates that reduction reaction followed pseudo-first order kinetics. The variation in apparent rate constant (k_{app}) with respect to NaBH₄ concentration also discloses it to be following Langmuir- Hinshelwood mechanism. Catalyst concentration and k_{app} showed a linear relationship. Thus, data obtained also confirmed that Ag-p(NIPAAm-HEMA-AAc) hybrid microgels are potential micro-reactors for reduction of 2,4-DNP.

P-47

Green synthesis of iron nanoparticles from *Haloxylon recurvum* plant and their adsorption potential for removal of acidic dye

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Iron nanoparticles (FeNPs) are conventionally synthesized by using sodium borohydride as reducing agent, which is an expensive and environmentally toxic process. Here, we present the synthesis of FeNPs using a green method based on *Haloxylon recurvum* plant extract. These plant extracts contain a high concentration of polyphenols etc. which act as reducing agent. So obtained NPs were then used for the degradation of congo red dye. The synthesized NPs before and after the sorption of dyes were characterized by UV-Vis, FTIR, SEM-EDX, XRD and specific surface area (BET). Degradation of congo red dye over FeNPs showed a pseudo second order reaction kinetics. The studies exemplify that *Haloxylon recurvum* plant extract can be exploited for the synthesis of Fe NPS which find applications in the removal of the hazardous dye from aqueous medium.

P-48

Toxicity of nano metal oxides on Krebs cycle affecting succinate-fumerate system and its influence on metabolic pathways

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Succinic acid is involved in the tricarboxylic acid (ATP) cycle and has the ability to donate electrons to the electron transport chain (ETP). The aim of the current study is to investigate *in vitro* oxidation of sodium succinate in aqueous solution using potassium ferricyanide as an oxidizing agent and determine the toxic effects of nanometal oxides on Krebs cycle. By using the uv-vis spectrophotometer, various kinetic measurements were performed at λ_{\max} 420 nm. The effect of various nano metal oxides (MgO & CaO) was observed at $25 \pm 0.05^\circ\text{C}$ on oxidation of succinate. The hypodermal technique was used to prepare nano metal oxides and their characterization was done by using TEM, FTIR, TGA, SEM-EDX and PXRD. The results show that these NPs are potent inhibitors and hinder the conversion of succinate into fumerate. The pseudo first order rate constant values increase as the particle size of these nanomaterials was reduced. It is concluded from the current research that high concentrations of these nano metal oxides can badly affect the ATP cycle by impeding succinate oxidation which is an imperative step of this cycle and consequently it can lead to various metabolic disorders.

P-49

High performance electrode material for a hybrid supercapacitor derived from ZIF-67/graphene nanocomposite

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In recent few years, there has been rapid growth in the study of supercapacitors due to their fast charge/discharge rates and long-life cycles. Metal–Organic Frameworks (MOFs) are promising electrode materials for next generation supercapacitors due to their low density and high specific surface area available for charge transport. In this study MOFs were combined with graphene nanoplatelets (GNPs) to enhance the capacitance of the supercapacitors. It was observed that (GNPs) have enhanced specific capacitance values of 117.5 F/g, 83 F/g and 73.33 F/g at current densities of 1 A/g, 2.5 A/g, 5 A/g respectively. Similarly, specific capacitance of MOFs (ZIF-67) was observed as 756.11 F/g, 567 F/g, 525 F/g, 336 F/g and 256 F/g at current densities of 1 A/g, 3 A/g, 5A/g, 8A/g and 10A/g respectively. The nanocomposite of GNPs/ZIF-67 showed the highest specific capacitance values of 931 F/g, 570 F/g, 226 F/g, 204 F/g and 158.33 F/g at current densities of of 1 A/g, 3 A/g, 5 A/g, 8 A/g and 10 A/g respectively. The prepared nanocomposites showed excellent cycling performance (95% after 5000 successive cycles at a current density of 10 A/g).

P-50

Green Synthesis of CuO Nanoparticles Using *Achyranthes aspera* L.

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Achyranthes aspera (*A. aspera*) was selected for the synthesis of nanoparticles (NPs) because it has not been reported previously for the synthesis of any kind of NPs. CuO NPs were successfully synthesized by green method using *A. aspera* aqueous leaves extract and were characterized through UV-visible spectroscopy, FTIR, PXRD, AFM and TGA. Synthesized NPs were tested for their antibacterial activity by agar diffusion method. The results demonstrated that the CuO NPs showed appreciable antibacterial activity against Gram positive as well as Gram negative bacteria. Antioxidant activity of synthesized CuO NPs was also evaluated by Total phenolic content (TPC) and ferric-reducing antioxidant power (FRAP) methods. Better results were observed with 3 mg concentration of CuO nanoparticles as compared to 2 mg and 1 mg concentration. It can be concluded that the 3 mg concentration of copper oxide nanoparticles was very effective for antioxidant activity.

Key word: Green synthesis, CuO nanoparticles, *Achyranthes aspera*

P-51

Green Synthesis of Copper Oxide Nanoparticles using *Guaiacum officinale* L. Extract

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Nanoparticles (NPs) of copper oxide were successfully synthesized from *G. officinale* leaves extract. *G. officinale* belongs to family Zygophyllaceae. *G. officinale* was selected for the synthesis because it has not been reported previously for the synthesis of any type of NPs. Green synthesis of NPS by using plant extracts has emerged as an effective method for the synthesis of nanomaterials for biological and bio-medicinal applications. *G. officinale* mediated CuO NPs characterized by UV-visible spectroscopy, FTIR, XRD, AFM and TGA. A peak at 250-300 nm in absorption spectrum and at 568 cm⁻¹ in FTIR spectrum indicated the existence of CuO NPs. PXRD patterns confirmed the crystalline nature of CuO NPs. TGA showed that the synthesized CuO NPs were stable up to 200 °C. Synthesized NPs were tested for their antibacterial activity by agar diffusion method and showed clear zone of inhibition against all bacteria. Antioxidant activity of synthesized CuO NPs was also evaluated. TPC (Total phenolic content) and FRAP (ferric-reducing antioxidant power) were used for the evaluation of antioxidant activity. Total phenolic content (TPC) of different concentrations of CuO NPs ranging from 18.4 to 51.4 (mg/L GAE). The total phenolic content (TPC) of CuO NPs increased with increasing their concentration. FRAP values for 3, 2 and 1 mg of CuO nanoparticles were 1.8, 1.6, 1.2 mM FeSO₄.7H₂O, respectively. **Key words:** Green synthesis, CuO NPs, antibacterial activity and antioxidant activity.

P-52

Interfacial Engineering of Organic Solar Cells to Realize Highly Efficient and Stable devices

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The recent years have witnessed the remarkable progress in hybrid organic–inorganic solar cells (OSCs) with power conversion efficiencies (PCEs) reaching to 10-15%. Their facile fabrication process, panchromatic absorption, longer charge carriers diffusion length, excellent charge carriers' mobility and low cost make them attractive candidate of new class of solar cells. However, the instabilities associated with the OSCs hinder their widespread commercialization to translate the lab-scale progress towards the large-scale industrial production. While, tremendous achievements in the PCE of OSCs has been achieved, above 10% values only represent their initial performance– how the performance of the device degrades with time is of paramount importance. The stacked architecture of the OSCs consisting of organic-inorganic constituents makes it susceptible to several degradation factors affecting every layer of device. Although, the prime concern is to address the instability of the absorption layer affected by the intrinsic and extrinsic degradation factors; however, it is important to explore the other layers (*i.e.* hole transport layer or HTL) and interfaces within the device. In this context, rational interfacial material design and engineering are one of the highly regarded approaches to improve the device efficiency and stability. The performance of the PSCs is highly dependent on the hole extraction and electron blocking ability as well as the surface properties of HTLs. The present work aims to use 'Normal' configuration of OSCs as a device for study, to look for novel strategies/materials for increasing the device stability without compromising the PCE by employing the interfacial engineering of HTLs. The work aims to use benchmarked polymers (such as PEDOT:PSS) along with the novel composition/combination of materials such as; metal oxides and/or graphene oxide as well the design configurations to realize highly efficient and stable devices.

Keywords: Organic Solar Cells, Hole Transport Layer, Stability, Degradation

P-53

Optimization of bulk heterojunction organic solar cell for higher performance: A computational modeling approach

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Organic solar cells (OSCs) have attracted attraction because of their suitability for large-scale production using an industrially viable rapid roll-to-roll processing. Employing the GPVDM software, effects of three different metals, active layer film thickness and light intensity were simulated and analyzed on photon density, photon absorption, and other photovoltaic parameters of ITO/PEDOT:PSS/PTB7:PC₇₁BM/Metal (Al, Au, Ag) type organic solar cells. The results show that the device performance can be improved significantly by adjusting layer thickness. The highest performance was obtained for Al as the metal contact electrode, active layer thickness of 200 nm and at lower incident irradiance.

P-54

Synthesis of Polyaniline/Graphene nanocomposite via in-situ chemical polymerization, as a catalyst material for the counter electrode of Dye- sensitized solar cell (DSSC)

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In this work, low cost graphene/polyaniline (GR/PANi) nanocomposites were synthesized to replace Platinum (Pt), an expensive counter electrode material to improve the photovoltaic performance and efficiency of Dye-sensitized solar cells (DSSC). The GR/PANi nanocomposites with varying graphene content were synthesized by increasing graphene amount from 3, 6, 9, 12 and 15wt% in an oxidative environment via in situ polymerization. Pure graphene, polyaniline and GR/PANi nanocomposites morphological, elemental percentage content and crystallographic properties were studied using Scanning Electron Microscopy (SEM) together with Energy Dispersive X-rays (EDX) and X-ray Powder Diffraction (XPRD). The results showed that a homogeneous coating of PANi nanoparticles adhered to the surface graphene sheets. Counter electrode of the GR/PANi nanocomposite were coated on the surface of conductive substrate by doctor blading during fabrication of DSSC. The fabricated cells were electrochemically characterized using I-V, EIS, CV and Tafel polarization. The efficiency of DSSC containing 9wt.% GR/PANi counter electrode has achieved 7.45%, that is near to Platinum based DSSC 7.63% under the same conditions.

P-55

Synthesis and characterization of multi-walled CNTs-piprazinyl derivative and their potential as anti-bacterial agents

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The aim of presented study was to investigate the anti-bacterial effect of CNTs-piperazine derivative. Firstly, surface modification of multi-walled CNTs was done by introducing the carboxylic group followed by the synthesis of functionalized multiwalled carbon nanotubes (FMWCNTs)-piperazine derivative. The latter was achieved by developing amide covalent linkage between the carbonyl group of FMWCNTs and -NH group of piperazine. As compared to other solvents, for instance acetonitrile, FMWCNTs-piperazine derivative could be nicely dispersed in water. FMWCNTs-piperazine derivative showed high antibacterial activity against *E coli*, *S aureus*.

P-56

Biosynthesis of silver nanoparticles using *Alkanna tinctoria*: a novel approach to weed utilization

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Weeds are undesirable plants with robust growth. Of 30,000 species of weeds, 18,000 weeds are known to suppress native biodiversity and cause economic losses. Medicinal plants are promising source of bioactive compounds and have been used to treat various ailments since ancient times. Antimicrobial resistance (AMR) is a rising global health concern, where approximately 700,000 people die each year from AMR infections. Antimicrobial activity of *Alkanna tinctoria* weed and its biogenic silver (Ag) nanoparticles (NPs) has not been reported previously. This study aims to elucidate phytochemical properties of *Alkanna tinctoria* leave extract, and biogenic synthesis of Ag NPs against bacterial strains. Qualitative phytochemical analysis was performed using standard tests. The synthesized Ag NPs were characterized by UV–Vis spectroscopy and X-ray powder diffraction. Antibacterial activity of biogenic Ag NPs were tested against gram positive (*S. aureus*) and gram negative bacteria (*E. coli*) via Agar well diffusion methods, and Minimum inhibitory concentration was determined. *Alkanna tinctoria* leave was found positive for alkaloids, carbohydrates, saponins, amino acids, and fixed oil. Ag NPs significantly affect the growth of *E. coli* as compared to *S. aureus*. The MIC for *E. coli* was recorded as 62.5 μ L and 125 μ L for *S. aureus*. Search of naive plants as novel therapeutic agents can open new avenues in drug development to combat antibiotic resistance.

Key words: *Alkanna tinctoria*, Weed, Silver nanoparticles, Antibacterial Agent, Phytochemical analysis

P-57

Dye-doped graphene treated TiO₂ nanotubes for efficient solar water splitting

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Solar water splitting is a significant technology for solar energy conversion and storage. It has progressively been at the forefront of chemical research and also provides a promising path for sustainable hydrogen production. TiO₂ has wide range of applications and considered as one of the most auspicious semiconductor due to its photo-stability, low-price and chemical dullness. TiO₂ nanotubes were prepared by using electrochemical anodization method followed by the deposition of an organic dye. Surface morphology, elemental composition, structure and size of the nano crystalline TiO₂ nanotubes was examined by using TEM, SEM, XRD, EDX and UV/Visible spectroscopy. Dye-doped and graphene treated TiO₂ nanotubes showed enhanced activity for water splitting as compared to un-doped TiO₂ nanotubes.

Keywords: Graphene oxide, Reduced Graphene oxide, Titanium dioxide.

P-58

Preparation, characterization and in vivo wound healing study of topical formulations of curcumin and quercetin loaded PLGA nanoparticles

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Different drugs and drug delivery systems have been widely investigated aiming at wound healing. Agents commonly used to treat wound infection are limited by toxicity, incomplete microbial coverage, inadequate penetration, side effects and rising resistance, which set a path for the discovery of new therapeutics to meet the clinical challenges. Quercetin and curcumin are nutraceuticals with antimicrobial, antioxidant and anti-inflammatory activities which aids wound healing. Quercetin and Curcumin's poor aqueous solubility and rapid degradation are major limitations that can be overcome by encapsulating in nanoparticles. When quercetin and curcumin are used in combination, they show synergistic effect as well. In present study, we prepared curcumin and quercetin loaded PLGA nanoparticles in different ratios 50:50, 75:25 and 25:75 of curcumin and quercetin as T1, T2, T3 respectively. These preparations were characterised for particle size, zeta potential and polydispersity index. Size of prepared nanoparticles was <250nm which is recommended for effective drug delivery. Zeta potential was in range of -1.83 mV to -3.2 mV that indicate good stability of nanoformulations. Higher encapsulation efficiency from 64.84% to 88.48% in different formulations was achieved. The experimentally wounded rats were equally divided into five groups. Quercetin and curcumin nanoformulations and standard drug (T4) was topically applied on the wounds of group 1, 2, 3 and 4, respectively, once daily for 12 days while control group was left untreated. All combinations along with standard drug were compared for wound contraction rate and wound healing time. Two-way ANOVA followed by DMR was applied on data to see statistical difference between treatments. Results demonstrated that Wound contraction rate was in following order T2>T1>T3>T4>C. Wound healing time was 14 days in C, 8 days in T1, 7 days in T2, 9 days in T3, and 10 days in T4. Gross evaluation of wound revealed that topical application of 75:25 curcumin and quercetin caused fastest wound closure, as compared to other treatments in our study. So it can be concluded that PLGA loaded nanoparticles of curcumin and quercetin enhances the bioavailability of curcumin and quercetin and hence their wound healing potential.

Keywords. Nanomedicine, PLGA, Curcumin, Quercetin, Wound healing

P-59

Role of polyvinylpyrrolidone in developing interaction between multi walled carbon nanotubes and polymethylmethacrylate for composites with low percolation threshold and enhanced electrical character

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Polyvinylpyrrolidone (PVP) modified multi walled carbon nanotubes (*p*-MWCNTs) based polymethylmethacrylate (PMMA) composites (*p*-MWCNT/PMMA) were fabricated by using sonication method. The aim of this research work was to synthesize composites with enhanced electrical properties. The results of FTIR and UV-Vis spectroscopy confirmed physical interaction between *p*-MWCNTs and PMMA matrix. LCR meter was used to measure the capacitance and resistance of the composites at different frequencies ranges from 40 Hz to 1 MHz. Tangent loss, dielectric constant and conductivity was calculated with the help of these measured values of capacitance and resistance. Percolation threshold value in these composites was observed to be 0.1 wt%. The maximum conductivity value observed in these composites was 2.2E+01 S/m. The value of critical exponent of synthesized composites was 1.79 at 1 MHz and thus lies within the universal range of value of *t* reported in literature. Maximum dielectric constant value shown by these composites was 8.0E+01 at 0.3 wt%. The tangent loss value was approximately 5 times lower in magnitude then the reported tangent loss value of PMMA composites. Detailed investigation has been done on change in the value of conductivity, dielectric constants and tangent loss as a function of wt% of filler and frequency.

P-60

Structural, Optical and Transport Properties of $\text{La}_{2-x}\text{Y}_x\text{NiMnO}_6$

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We prepared a series of double perovskites $\text{La}_{2-x}\text{Y}_x\text{NiMnO}_6$ ($x=0, 0.5, 1, 1.5, 2$) by a sol-gel method and characterized by PXRD, FTIR, UV-visible spectroscopy, dielectric and electrical techniques. The doping effect of Yttrium at A-site in DPOs $\text{La}_{2-x}\text{Y}_x\text{NiMnO}_6$ system is discussed in this paper. The structural properties revealed by PXRD at room temperature are fitted by JANA 2006 software which showed monoclinic structure with space group $P2_1/n$ for all samples. We discussed optical properties of DPOs by FTIR and UV-visible spectroscopy. Room temperature FTIR measurements give IR spectra which is fitted by using Lorentz oscillator model, optical conductivity, oscillator strength and damping factors. UV-visible spectroscopy gives optical band gaps, indicating the semiconducting behavior of observed series. The transport characteristics of DPOs $\text{La}_{2-x}\text{Y}_x\text{NiMnO}_6$ have been found by electrical and dielectric measurements. The activation energy calculated by Arrhenius plots confirmed the semiconducting nature of all samples. It has been confirmed that there is small polaron hopping conduction mechanism in this system. The dielectric constant, tangent losses and ac conductivities as a function of frequency and temperature have been discussed.

P61

Biocompatibility and toxicity of gold nanoparticles biosynthesized using *Monotheca buxifolia* leaf extract

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In this contribution a complete green route was adopted for biosynthesis of gold nanoparticles (AuNPs) using *Monotheca buxifolia*. The synthesized NPS were characterized by UV, FTIR, XRD, ERD, SEM, TEM and TG/DTA. Biological activities were performed including antioxidant, antibacterial, antifungal, hemagglutination, cytotoxic, thrombolytic, hemolytic and Ames assay. The crystallite of AuNPs had different shapes. FTIR spectra indicated several functional groups primarily phenols as potential reducing and amide as stabilizing agents. AuNPs revealed highest free radical potential as compared to *M. buxifolia* extracts. *M. morganii* was found to be the most susceptible strain to AuNPs. Growth of Vancomycin Resistant *Staphylococcus aureus* was also inhibited. Furthermore, no mutagenic properties were shown by the biogenic AuNPs. Significant insecticidal activities were revealed for AuNPs and plant extract against all test insects. In addition, the biogenic AuNPs manifested significant cytotoxicity. AuNPs possessed no mutagenic potential against human DNA and revealed moderate thrombolytic activity. Aqueous extract was hemolytic at high concentration while AuNPs were slightly hemolytic. AuNPs showed cent percent mortality against insects. Results suggest broad applications of biogenically derived Au NPs.

P-62

Supported silica catalysts for hydrogen production and catalytic reductions

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Mesoporous silica (MCM-41), with its high surface area, tunable pores and tailorable surface properties, has been considered as excellent support for the dispersion of transition metal nanoparticles (NPs) to fabricate supported heterogeneous catalysts. However due to wettability issues, generation small sized and uniformly distributed metal NPs over silica is challenging. In this study, we attempted to generate ultras-small palladium (Pd) NPs over MCM-41 by utilizing loading and thermal decomposition of a palladium complex within the pores. So obtained catalysts were characterized by SEM, XRD, BET, FTIR and TGA. The fabricated catalysts were tested for the dehydrogenation of sodium borohydride (NaBH_4) and ammonia borane (NH_3BH_3). Effect of annealing temperature and atmosphere on the catalytic activity of the catalysts was studied. The catalyst pyrolyzed under air was found to be the most active for dehydrogenation of NaBH_4 and NH_3BH_3 providing activation energy of 14.3kJ/mol and NH_3BH_3 , 34.3kJ/mol, respectively. The same catalyst also showed superior activity for the reduction of 4-nitrophenol with NaBH_4 as compared to the commercial palladium catalysts (Pd/C , $\text{Pd/Al}_2\text{O}_3$).

P-63

One-pot synthesis of heterobimetallic Metal-Organic Frameworks (MOFs) for multifunctional catalysis

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Metal-Organic Frameworks (MOFs), crystalline nanoporous materials constructed from metallic nodes and multipodal organic ligands, find intensive applications in gas storage, separation, sensing, drug delivery and catalysis. Catalytic properties of MOFs can be modulated by a pre or post synthetic metal exchange at node. We present a one-pot synthesis of a bimetallic MOFs by the direct reaction of stoichiometric amounts of Fe and Co with 2-aminoterephthalic acid. Energy-dispersive X-ray (EDX) analysis confirmed the incorporation of both Fe and Co in spindle-shaped crystals, typically known for the Fe-MIL-88B structure and confirmed by PXRD. To test the catalytic potential of mixed-metal MOFs, reduction of nitroarenes was selected as a benchmark reaction. Incorporation of Co enhanced the activity of the catalysts as compared to the parent NH₂-BDC-Fe catalyst. These MOFs were also tested as electro-catalysts for Oxygen Evolution Reaction (OER) with best activity exhibited by the catalyst with equimolar ratio of Co and Fe (Catalyst B). The catalyst provided a current density of 10 mA.cm⁻² at 410 mV overpotential, which is comparable to the benchmark OER catalyst (i.e. RuO₂). Moreover, it showed long-run stability in 1M KOH typically unknown for MOFs. In a third catalytic test, dehydrogenation of sodium borohydride was attempted and again, a high activity (TOF: 87/min) and hydrogen generation rate (67 L/min/g catalyst) was provided by the catalyst B. This is the very first example of the synthesis of bimetallic MOFs as multifunctional catalysts particularly for catalytic reduction of nitroarenes and dehydrogenation reactions.

P-64

Controlled development of higher-dimensional nanostructured copper oxide thin film for electrochemical water oxidation catalysis

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The development of cost-effective and highly efficient electrocatalysts for oxygen evolution reaction (OER) is a great challenge in water splitting process for the neat and clean production of hydrogen in a viable way. Herein, we report the fabrication of thin film of CuO nanostructures with controlled morphologies i.e., nanosheets, nanocubes, nanoflowers, and nanoleaves without using any additives and surfactants at room temperature and controlled pH, and evaluation of their relative performance for water oxidation catalysis. CuO nanoflowers exhibit high catalytic activity with an onset potential of 1.48 V and a Tafel slope of 84 mVdec⁻¹ in 1 M KOH solution. Moreover, it needs an overpotential of 270 mV and 400 mV to attain a current density of 10 mAcm⁻² and 100 mAcm⁻² respectively. More promisingly, the catalytic performance was found highly dependent upon the morphology and subsequently the improved electrochemically active surface area (ECSA). Such morphology dependent OER performance and binder-free nature of catalyst may provide faster electron transport owing to the inherent catalyst-substrate electronic interconnection and thus making it more promising candidate as a future high-performance electrocatalyst for OER.

P-65

Microwave assisted growth of nanostructured NiS supported over carbon nanofibers for overall water splitting

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Electrochemical water splitting has attracted much attention to produce hydrogen and oxygen for energy storage and conversion devices. However, it is often impeded by the oxygen evolution reaction (OER) due to its unfavorable thermodynamics and sluggish kinetics. The precious metal oxide based electrocatalysts, such as RuO₂ and IrO₂, are the benchmark catalysts for OER. However, the scarcity and high costs of these precious metals limits their practical use. Thus, there is a dire need to develop cost-effective as well as efficient catalysts for water splitting to produce hydrogen. Recent focus has been on the development of metal alloys, oxides, carbides, sulfides, phosphides, and nitrides of earth-abundant transition metals. Metal chalcogenide based catalysts are promising but their long term stability, conductivity, and desirable redox properties are challenging to achieve. Tunable composition, morphology, and enhanced active sites can play a significant role in developing efficient noble-metal free electrocatalysts. In this study, NiS nanostructures supported over carbon nanofibers (NiS@CNF) were synthesized by microwave assisted method and their morphologies and elemental composition were optimized for overall water splitting. These catalysts were characterized by X-Ray Diffraction analysis (XRD), scanning electron microscope (SEM) and X-ray photoelectron spectroscopy (XPS). Their morphologies and composition were tuned to achieve enhanced activity for electrocatalytic activity. For OER, the overpotential was 270 mV for nanoflower-shaped and 300 mV for spherical shaped NiS at 10 mA/cm². The corresponding Tafel slopes were 51 and 143 mV/dec, respectively. Similarly, for HER, the overpotentials were 362 and 405 mV and Tafel slopes were 100 and 209 mV/dec, for nanoflower and spherical-shaped NiS, respectively. The bifunctional catalytic applicability of these materials for overall water splitting was demonstrated by a potential of 1.64 and 1.705 V at 1 mA/cm² current density which is excellent when compared to recently reported results.

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