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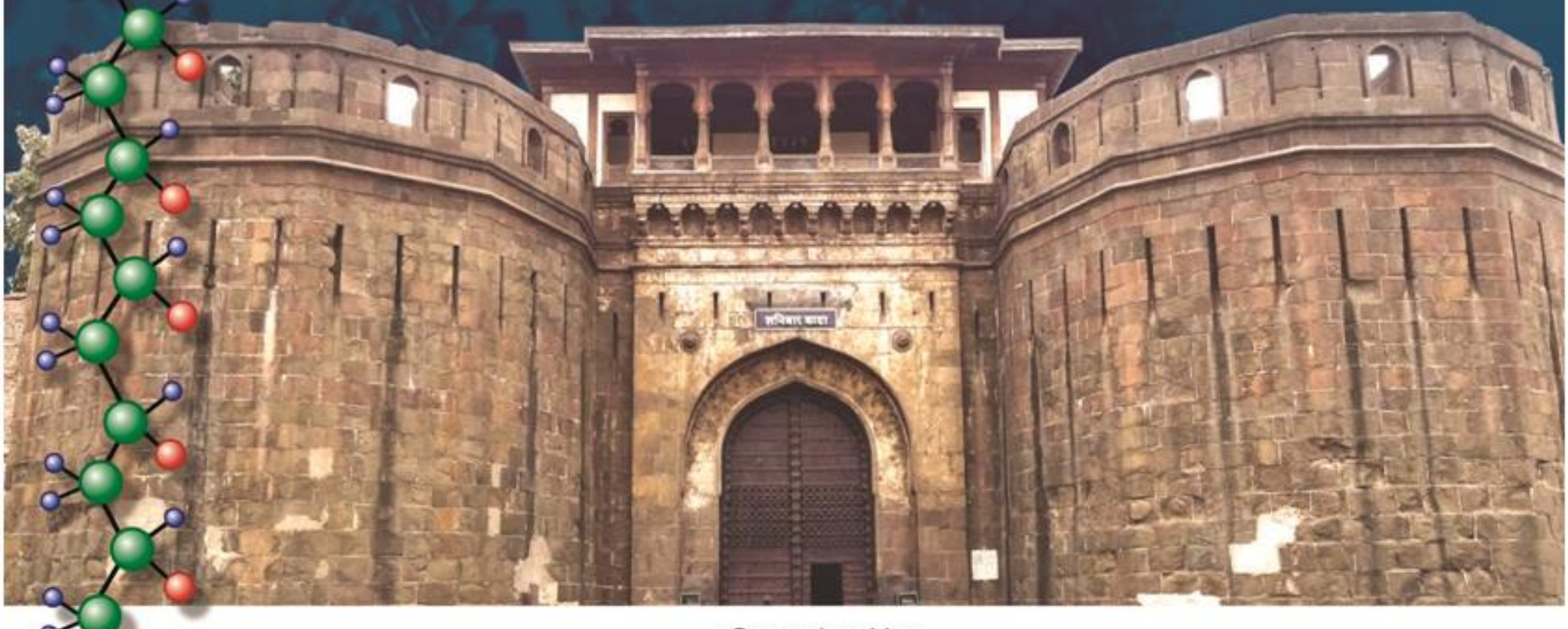

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S. Sivaram Endowment Lecture

C1 and C3 Polymerizations: Ways to Unprecedented Structures

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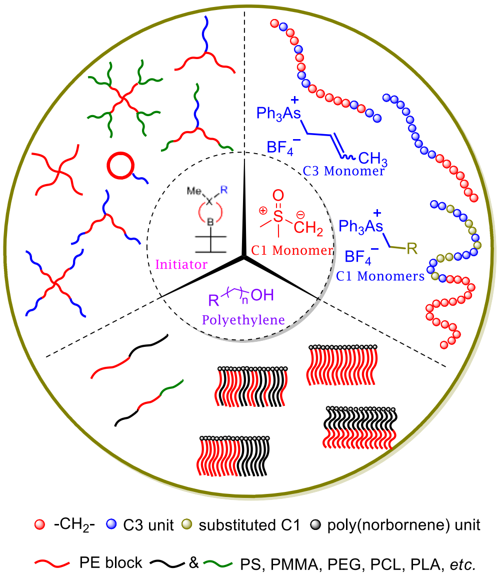
Abstract

In contrast to the well-known C2 polymerization of vinyl monomers (the chain is growing by two carbons at a time) and C4 polymerization of dienes (the chain is growing by four carbons at a time), the borane initiated polymerization of sulfoxonium and arsonium ylide monomers are leading to C1 (the chain is growing by one carbon at a time)[1] *and C3 (the chain is growing by three carbons at a time)*[2] *chains, respectively. By using appropriate ylides and trialkylboranes we were able to direct the polymerization either to C1 (dimethylsulfoxonium methylide) or C3 (methylallyltriphenylarsonium ylide) mode. These findings open new horizons towards the synthesis of polyethylene (PE)- and polymethylallyl-based unprecedented polymeric materials*[3-14]*. A few of them are given in Scheme 1.*



Scheme 1. PE-and polymethylallyl-based polymers with complex macromolecular architectures

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Santi Ranjan Palit Memorial Lecture

Anti-biofouling- How a Polymer Brush repels Proteins and our novel Integrated Design

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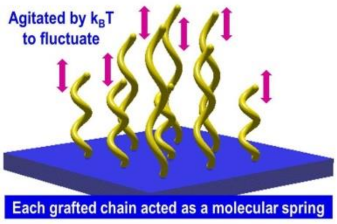
Abstract

Grafting a layer of chains on a surface to form a polymer brush has been considered as an effective approach to make it anti-biofouling (less protein adsorption). The anti-biofouling property has been qualitatively attributed to the hydration of such a polymer brush with a layer of immobile water molecules and the steric effect; namely, the adsorption decreases monotonically as the polymer grafting density () increases. However, there is no quantitative and satisfactory explanation why the adsorption starts to increase when is sufficiently high and why polyethylene glycol (PEG) still remains as one of the best to repel proteins. We have looked the captioned question from another angle: the entropic elasticity instead of the protein-surface interaction, i.e., the enthalpy change.

Considering that each grafted chain is confined inside a cylindrical “pore/tube” made of its neighboring chains, as shown in the right figure, we found its optimal length by minimizing its free energy (*A*) that contains the exclude volume interaction and the chain elasticity (both of them have an entropic nature) [1, 2];estimated how *A* depends on and the chain length (*L*); and calculated its thermal energy-agitated chain conformation fluctuation that slows down the adsorption kinetically. After comparing *A*with the thermal energy, we are able to predict how both *L*and affect the protein repelling and explain why PEG performs better than others. Our predictions are surprisingly and *quantitatively* comparable with those literature results [3, 4]. We will also illustrate how to develop some novel anti-biofouling coatings for shipyard/marine applications by using an integrated design that combines different existing strategies; namely, the self-polishing, the self-structure and the self-generated soft and dynamic surface [5, 6].



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Plenary Lecture-1

Supramolecular Polymerization of Linear π-Conjugated Molecules to Exotic Superstructures

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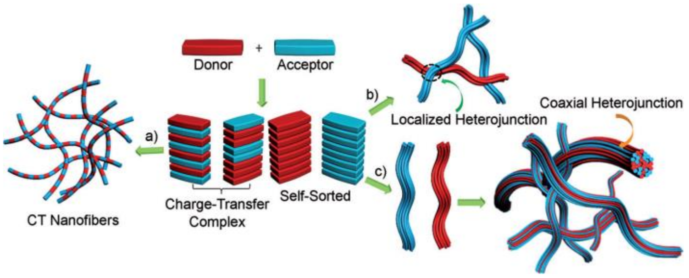

Supramolecular polymers are a class of nonconventional macromolecular architectures formed by the “bottom-up” self-assembly of organic molecules. While a large number of different molecular systems have been used as the building blocks, linear π-systems such as *p*-phenylenevinylenes, *p*-phenyleneethynylenes, and thienylenevinylenes are of interest due to the formation of supramolecular architectures of different size, shape and properties.[1] For example, nano to micro sized fibers, rods, tubes, toroids, vesicles, helices etc. could be designed using small molecular building blocks. The π-interaction in these system can be strengthened by incorporating H-bonding functional groups, leading to their spontaneous self-assembly to supramolecular polymers. However, control on the size and shape of these macromolecular architectures is a challenge.[2] In recent times several approaches have been reported for the controlled synthesis of supramolecular polymers. One of the approaches involves the use of directional H-bonding motifs to achieve shape control. For example, spontaneous assembly of linear 1D assemblies can be directed to circular assemblies using radially H-bonding functional groups.[3] Another strategy is the use of logistically designed donor-acceptor type molecular building blocks.[4] We have demonstrated this with gel forming thienylenevinylenes which result in fibrous structures with high conductivity. These donor gelators upon mixing with an acceptor, PBI, forms self-sorted assemblies at molecular level and self-aligned fibers at supramolecular level, resulting in co-axial heterojunctions with enhanced photoconductivity and charge carrier mobility (Figure). We have also used C_3-symmetrical H-bonding core groups attached to donor acceptor systems for the creation of supercoiled supramolecular polymers.[5] Details of these studies will be presented.

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Plenary Lecture 2

Rethinking the Coupling of CO_2 with Epoxides For the Synthesis of Aliphatic Polycarbonates

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Abstract

Carbon dioxide (CO_2) is an abundant, inexpensive, and non-toxic renewable C1 feedstock that is only used in a limited number of product-yielding reactions due to its low reactivity. After the discovery by Inoue *et al.* of the copolymerization of CO_2 and epoxides by diethyl zinc [1] a number of efficient transition metal catalysts functioning by coordinative chemistry have been developed: in the latter case the polymerization occurs by coordination and successive insertions of epoxides and CO_2 to produce aliphatic polycarbonate chains. [2-3a,b,c]. We show for the first time that CO_2 and epoxides can be copolymerized *anionically* using classical alkali metal *anionic* initiators or even metal-free *anionic* initiators, without resorting to the transition metal-based coordinative chemistry used so far. This opens up new horizons for the utilization of CO_2 in its *anionic* copolymerization with epoxides: [4a,b,c]

1) perfectly defined polycarbonate telechelics can now be prepared for further use as precursors of polyurethanes,[4a,b]

2) very high molecular weight polycarbonates samples can be generated due to the "living" nature of the copolymerization,

3) diblock and triblock copolymers can be easily obtained and thus thermoplastic elastomers generated by sequential addition of two different epoxides,

4) various functional polycarbonates can be derived by copolymerizing under "living" conditions functional epoxides with CO_2 . [4c]

So far CO_2 has been uniquely used in *anionic* polymerization for carbonation purpose of living carbanionic chains by R. Quirk[5]; we demonstrate here that it can be *anionically* copolymerized with epoxides, provided a Lewis acid is added to specifically activate the epoxide monomer.

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Plenary Lecture 3

Polymers at Synthetic and Biological Surfaces

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Abstract

Polymer science provides a diverse toolbox to modify and control the properties and function of both synthetic and biological surfaces.The first part of this lecture will discuss the use of surface-initiated, controlled radical polymerization (SI-CRP) techniques for the preparation of surface tethered polymer brushes. SI-CRP reactions are characterized by a number of unique features, which include the ability to (i) prepare polymer brushes with precise control over chemical composition and film thickness;(ii) to conformally coat both simple, planar substrates as well as complex, 3D structured or porous substrates and (iii) to tune the conformation of the surface grafted polymer chains by controlling the grafting density. We will present recent work that illustrates the use of SI-CRP to generate thin polymer films with sensory properties as well as for the generation of novel mechanically responsive surfaces. The second part of this talk will concentrate on biological surfaces and more specifically the membrane of living cells. Living cells are attractive as carriers to mediate transport of drug-loaded particles. The successful use of cells as carriers for polymers and polymer particles requires chemical approaches that allow to immobilize (and release) the polymer or particle payload from the cell surface, without compromising cell viability and function. This presentation will discuss various polymer cell surface modification strategies and compare these different approaches in terms of the possibilities they offer to modify cell surfaces as well as their impact on cell viability and function.

Plenary Lecture-4

Tuning cooperativity on the free energy landscape of protein folding

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A major goal of protein folding studies is to understand the structural basis of the coupling between stabilizing interactions, which leads to cooperative conformational change. In particular, the relationship between folding cooperativity and stability is poorly understood. The goal is challenging because of the difficulty in simultaneously measuring global cooperativity by determining population distributions of the conformations present, and the structures of these conformations. We have used native state hydrogen exchange in conjunction with mass spectrometry to explore the free energy landscape accessible to the small protein monellin, when the stability of the protein is varied. Mass distributions obtained in the EX1 limit of exchange have allowed a direct distinction between correlated (cooperative) and uncorrelated (non-cooperative) structure-opening processes. Under conditions where the native protein is maximally stable, a continuum of partially unfolded states is gradually sampled before the globally unfolded state is transiently sampled. Under conditions that stabilize the unfolded state of the protein, the slowest structure-opening reactions leading to complete unfolding, become cooperative. The data provide experimental evidence for a gradual uphill unfolding transition on a very slow timescale, in the presence of a large free energy difference between the native and unfolded states. The results suggest that the cooperativity that manifests itself in protein folding and unfolding reactions carried out in the presence of denaturant, might merely be a consequence of the effect of the denaturant on the unfolded state and transition state stabilities.

The segment-specific pattern of HX reveals that the backbone hydrogen bonding network disassembles in a structurally diffuse, asynchronous manner. A comparison of the site-specific transient opening rates of secondary and tertiary structure in the protein provides a structural rationale for the observation that unfolding is hierarchical and describable by exponential kinetics, despite being diffuse. Since unfolding was studied in native conditions, the sequence of events during folding in the same conditions will be the reverse of the sequence of events observed during unfolding. Hence, the formation of secondary structural units during folding would also occur in a non-cooperative, diffuse and asynchronous manner.

Plenary Lecture 5

Highly Defined Multiblock Copolymers:Testing the Limits of Living Polymerization

H. Frey,[1] M. Steube,[1] E. Grune,[1] P. von Tiedemann,[1] C. Wahlen,[1] T. Johann,[1] A. H. E. Müller,[1] M. Appold,[2] M. Gallei,[2] E. Galanos,[3] G. Floudas,[3]
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Abstract

The multiblock structure plays a key role in natural scleroproteins showing extraordinary mechanical properties, such as silk fibroin and collagen. They consist of alternating flexible and rigid, crystalline chain segments in repetitive sequences [1], which leads to high tensile strength. In contrast, only few cases of synthetic polymers consisting of well-controlled flexible and rigid chain segments are known that additionally show low dispersity.The living anionic copolymerization of isoprene and styrene in cyclohexane affords tapered block copolymers due to the highly disparate reactivity ratios of $r_I = 12.8$ and $r_S = 0.051$. Repeated addition of a mixture of these monomers was exploited to generate tapered multiblock copolymer architectures of the $(AB)_n$ type with up to 10 blocks ($1 \leq n \leq 5$), thereby subdividing the polymer chains in alternating flexible polyisoprene (PI) and rigid polystyrene (PS) segments. Three series of well-defined tapered multiblock copolymers with approximate molecular weights of 80 kg/mol, 240 kg/mol and 400 kg/mol were prepared on the 100 g scale. Via this synthetic strategy polymer chains were divided in di-, tetra-, hexa-, octa-, and decablock tapered multiblock structures, respectively. Due to the living nature of the polymerization, low dispersities in the range of 1.06 to 1.28 (decablock) were obtained. In order to ensure full monomer conversion prior to the addition of the isoprene/styrene mixture, kinetic Monte Carlo simulation was employed, permitting to simulate chain growth *in silico* by employing the known polymerization rates and rate constants k_p [2].Subsequently the question was addressed, to which extent the multiblock copolymers are capable of forming ordered nano-segregated morphologies. Detailed thermal, structural and rheological investigations showed that the tapered multiblock copolymers with a molecular weight of 240 kg/mol formed ordered phases with the expected lamellar morphology. However, X-ray scattering data and transmission electron microscopy (TEM) images of the octablock and decablock copolymers reflect weakly ordered structures at ambient temperature. The domain spacing, d, was found to scale as $d \sim N^{0.62}$, where N is the total degree of polymerization, suggesting stretching of chains and non-ideal configurations. The viscoelastic response of the tapered copolymers is controlled by the nanodomain structure, the degree of segregation, nanodomain-bridging configurations of blocks and also the proximity to the glass temperature of the vitrified PS domains. Tapered hexablock copolymers were found to best combine structural integrity and mechanical toughness, while maintaining a large strain at break (> 900%).The principle can be universally applied to a variety of combinations of diene

monomers and styrene derivatives, enabling precise control of block length, sequence and block number.

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Plenary Lecture-6

Material, morphology and device design for efficient polymer solar cells

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Abstract

Organic semiconductors continue to attract interest for application in organic optoelectronic devices. For solar cells, the organic semiconductors have to fulfil several chemical, optical electronic, and morphological requirements to provide high power conversion efficiencies in solar light. The chemical structure, molecular weight, processing conditions, charge transport layers and device architectures all exert important roles to reach the intrinsic limits of these materials. Recent progress in the field of donor and acceptor polymers and molecules will be discussed, resulting in high efficiencies as consequence of controlling chemical structure of donor and acceptor materials and length scales of their phase separation in mixed blends. We have studied morphology formation in real time during solvent evaporation to clarify the role of co-solvents and further analyzed and quantized the width of semi-crystalline polymer fibers by transmission electron microscopy in combination with automated image analysis. The fiber width is mainly determined by the solubility of the polymer in the co-solvent and the molecular weight of the polymer. Recent results on multi-junction polymer solar cells will be presented. We have been able to develop new semiconductor inks for the interconnection layers that allow versatile stacking of a large number of different photoactive layers combinations in tandem, triple and quadruple junction cells.

Plenary Lecture-7

Atypical Responses in Polymeric Nanoassemblies

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Abstract

Nature has designed complex molecular and supramolecular networks of interactions to offer systems that bridge molecular scale initial events to macroscopic final outputs. Thus, Mother Nature has evolved intricate networks of systems that can bridge chemical events across multiple length scales and timescales. Design know-hows for generating artificial systems with such capabilities are primitive at best. We are inspired by this challenge. As a part of addressing this grand challenge, we have developed molecular designs that afford tunable host-guest characteristics in supramolecular assemblies in specific response to a variety of stimuli. Such a capability endows these assemblies with functional capabilities that could find use in diverse applications. In this presentation, we will focus our discussions on supramolecular assemblies that are designed to respond to an atypical stimulus or feature atypical responsive characteristics.

Plenary Lecture-8

Polymerizable Porogens

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Abstract

Porous polymers have been extensively studied for the past half a century; these have been primarily used as separation media, as adsorbents, and, more recently, designer porous polymers have been tailored for more specific purposes, such as analyte detection, catalysis, stimuli-responsive gates, etc. The control of pore size, shape and their inter-connectivity are key parameters that govern the performance of the porous polymeric materials; these are controlled using *porogens*, which are often small molecules (or polymers) that serve as *place-occupants* during the polymerization. Two important approaches have been developed to create porous polymers – one is polymerization-induced phase separation (PIPS) and the other is polymerization-induced microphase separation (PIMS). Whereas in the former the porogen is not linked to the polymer matrix, in the latter the *porogen* becomes covalently attached to the matrix via RAFT-based chain transfer, and thus the size of pores becomes regulated by the *porogen* molecular weight; the degradative removal of the *porogen* leaves behind the porous matrix, which under appropriate conditions generates a continuously linked porous structure, a key feature for improved access to pores and high flux. To create an alternate single step process to porous crosslinked polymers wherein the internal walls of the pores are lined with desired functional groups, we embarked on the idea of developing *polymerizable porogens, wherein the covalent bond between the polymerizable unit and the porogen is thermally labile*; and thus, the *porogen* can be cleaved from the crosslinked matrix by a simple thermal treatment. By proper design of the thermally cleavable linkage, the desired functional group can be installed on the internal walls. I shall first describe some of the basic ideas associated with the formation of porous polymeric matrices using PIPS and PIMS methods. I shall then contrast our approach that uses a novel *polymerizable porogens* that also undergoes polymerization-induced microphase separation (PIMS), however with some differences. The thermally labile linkage that we first examined is the carbamate linkage, which under hydrothermal treatment *cleaves-and-reacts* to leave behind amine functionalities on the internal surface of the pores. Excellent control over the pore-size and surface area is demonstrated by regulating the polymerization-crosslinking process. The effect of various parameters, such as porogen size, polymerization-crosslinking rate, volume-fraction of the porogen and added non-polymerizable porogen, on the structure of the porous polymer will be discussed.

Abstracts for Joint Symposium Society of Polymer Science, India and Society of Polymer Science, Japan

Joint Symphosium: Invited Talk-01

New Hybrid Materials Based on Element-Blocks

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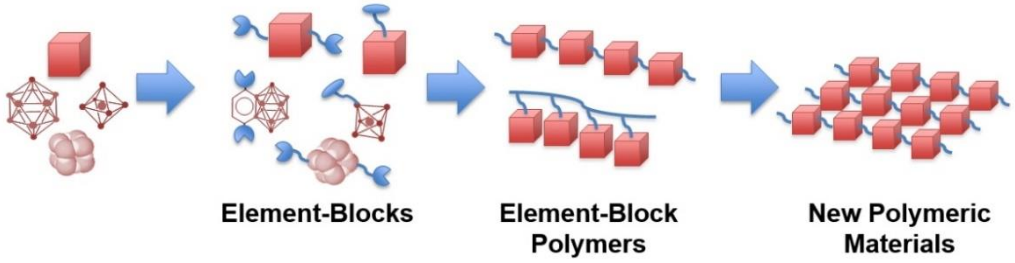
Abstract

A structural unit consisting of various groups of elements is called an "element-block." The design and synthesis of new element-blocks, polymerization of these blocks, and development of methods of forming higher-order structures and achieving hierarchical interface control in order to yield the desired functions are expected to encourage the creation of new polymeric materials that share, at a high level, electronic, optical, and magnetic properties not achievable with conventional organic polymeric materials as well as forming properties of molding processability and flexible designability that inorganic materials lack. Here, our recent research results concerning with these "element-block" materials are demonstrated. Such examples include "Luminescent Boron Complexes" and "Polyhedral Oligomeric Silsesquioxane (POSS)".



Scheme 1. The idea for the construction of polymeric materials based on element-blocks.

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Joint Symposium: Invited Talk-02

Self Assembly and Hierarchies of Perylenebisimide (PBI)- Poly(4-vinylpyridine) (P4VP) in Homo and Block Copolymers.

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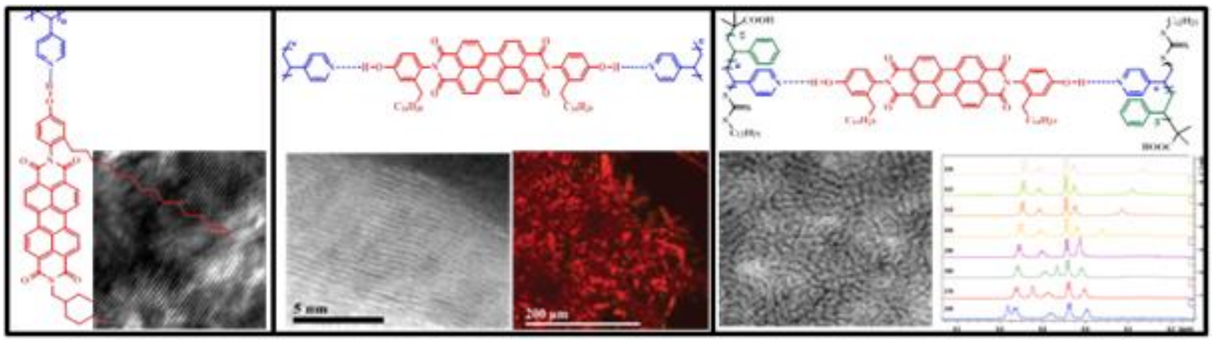
Abstract

The supramolecular comb complexes of P4VP or the comb-coil supramolecular complexes of PS-b-P4VP with small molecules like pentadecylphenol (PDP) has been well studied in literature for their well-defined nanostructures in bulk and thin films. The majority of the literature studies have focused on the bulk assembly of these systems by experimental techniques like the FTIR, SAXS, or microscopic techniques like TEM, AFM for understanding their morphologies. Our research group introduced the self assembly of the n-type organic semiconductor molecule, Perylenebisimide (PBI) with P4VP and established their self assembly in bulk by FTIR, XRD, TEM in addition to solution based studies involving absorption spectroscopy by virtue of the high absorption coefficient of the PBI chromophore.[1-3] The self assembly studies were further extended to the complexes of PBI with PS-b-P4VP having varying P4VP block length. My talk will elaborate on the hierarchical structure formation of a difunctional PBI molecule (PBI-PDP) with PS-b-P4VP in the bulk using XRD and microscopic techniques. Detailed NMR spectroscopic studies in deuterated THF as solvent revealed for the first time, unique information regarding the self assembly at the molecular level between the block copolymer and the small molecule that could not be extracted by any other analytical methods. NMR relaxation experiments gave insight into the environment of the complexed PBI derivative deeply embedded within the P4VP core or located at the periphery. This is perhaps the first direct experimental evidence for the retention of self organized structures in solution for supramolecular complexes based on PS-b-P4VP.



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Joint Symphosium: Invited Talk-03

Copolymerization of Norbornene and Styrene Derivatives withSingle-Site Catalysts

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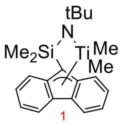
Abstract

Cyclic olefin copolymers (COCs) consisted of rigid alicyclic polymer-backbone, of which glass transition temperature (T_g) can be controlled by the comonomer composition in a wide range, are attractive materials because of their good heat and chemical resistance as well as their low dielectric constants, nonhygroscopicity, and high transparency. Despite the expectation for copolymerization of cyclic olefins with 1-alkene giving new COCs, the catalytic systems giving high molecular-weight copolymers with 1-alkene are very limited. We found that *ansa*-dimethylsilylene(3,6-di-*tert*-butylfluorenyl)(*tert*-butylamido)dimethyl-titanium complex (**1**)activated by $Ph_3CB(C_6F_5)_4$gave high molecular-weight norbornene (NB)/1-alkenecopolymers in high activity[1]. The catalytic system conducted NB/styrene (St)/ethylene terpolymerization[2]. The introduction of the St unit compensated the birefringence of NB unit to be realized zero birefringence polymer with the St content of 12 mol% and the $T_g$of 86 ˚C. The catalytic system also conducted NB/St copolymerization to produce the copolymers with highweight-average molecularweight (M_w, 30000 ~ 143000), but the St content (< 5 mol %) and the activities (1.4 ~62 $kg \cdot mol_{Ti}^{-1} \cdot h^{-1}$) were limited[3].We previously reported an anilinonaphthoquinone-ligated nickel complex (**2a**) activated by $B(C_6F_5)_3$ conducted coordination insertion polymerization of NB with high activity (2000 $kg \cdot mol_{Ni}^{-1} \cdot h^{-1}$) to produce a high molecular-weight polymer soluble in cyclohexane. We therefore applied **2a** and its derivatives, **2b** and **2c**, for NB/St copolymerization using modified methylaluminoxane (MMAO) or $B(C_6F_5)_3$ as a cocatalyst[4]. The catalyst conducted the copolymerization with higher activities (11 ~130 $kg \cdot mol_{Ni}^{-1} \cdot h^{-1}$) than **1**-$Ph_3CB(C_6F_5)_4$ and produced copolymers withhigh M_w values of 25000 ~ 148000 in a wide range of the St content (4~ 59 mol%). Accordingly, the $T_g$value of the copolymer was controllable from 128 ˚C to 329˚C. We also conducted the copolymerization of NB with a series of*p*-substituted styrene and investigated the effects of the substituent on the copolymerization and the properties of the copolymers produced.In this presentation, I will introduce novel COCs synthesized by theseNi-based catalytic systems.



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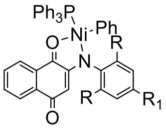

2a: R = iPr, R1 = H
2b: R = R1 = Me
2c: R = = H

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Joint Symphosium: Invited Talk-04

Exceeding Shockley–Queisser Limit with Singlet Fission

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Abstract

Multiexciton generation through singlet fission has the potential of exceeding Shockley–Queisser limit in photovoltaic devices. However, only very few materials suitable for singlet fission are available at present and the mechanism of inter- and intra-molecular singlet fission are not fully understood. Detailed knowledge regarding the processes is crucial for developing new materials. In this talk, I will present the molecular design and synthesis strategies to meet the exchange energy and morphology criteria for molecules to undergo singlet fission.

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Joint Symphosium: Invited Talk-05

Alignment Control of Liquid Crystals by Scanning Wave Photopolymerization

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Abstract

Macroscopic alignment control of liquid crystal (LC) films is key to the development of next-generation high-performance electronic, photonic, mechanical, and biomedical organic devices. Current methods achieve such large-area alignment of LCs, having intrinsic structural ordering over various length scales from nanometer to micrometer, by applying uniform external fields along one direction, such as mechanical stress, surface rubbing treatment, and electromagnetic or light fields. Among these more advanced 2D techniques, light-driven alignment control (photoalignment) might provide the greatest potential for fine control over molecular orientation, because of its remote and precise influence, and suitability for micro- or nanofabrication, which can enable many applications that require more complex alignment patterns. With conventional photoalignment methods, one typically irradiates an LC film containing added photoresponsive molecules with spatiotemporally uniform polarized light. We report here a new concept of scanning wave photopolymerization (SWaP) using spatiotemporal scanning of UV light to start photopolymerization and create a mass flow in the film, which results in LC alignment coincident with the incident UV light patterns.

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Joint Symposium: Invited Talk-06

Modelling the Universal Viscoelastic Response of Polymer Fibers

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Abstract

Polymer fibers, including natural silk and synthetic fibers exhibit universal viscoelastic response. On stretching below yield, they show logarithmic stress decay. On unloading fibers with a glassy amorphous phase, the stress recovers. A simple phenomenological model accurately describes data from independent mechanical experiments and provides insights into the microstructural origins of the fiber response. Counter to intuition, the model indicates that it is the crystalline regions, rather than the amorphous glass, that deform first on stretching fibers at high strain rates. On holding a stretched fiber, stress decays as a consequence of relaxations in amorphous regions. Finally, unloading the fiber transfers stress from the amorphous to crystalline regions resulting in stress recovery. Model parameters correlate well with the fiber microstructure. Crystal and amorphous moduli from the model match those from X-ray diffraction. Activation energies for the temperature dependence of the peak relaxation time are similar to those reported in the literature. Thus, a simple model that invokes only crystal-amorphous coexistence can successfully model the mechanical response of a wide variety of polymer fibers.

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Joint Symphosium: Invited Talk-07

Spider silk-mimicking polypeptideMechanism in nature & chemoenzymatic synthesis

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Abstract

In nature, high-performance biological polymers and composites consist of various organisms. The high-performance biopolymers in nature are mainly protein/ polypeptide, and have therefore been recognized as bioactive and functional material. However, use of those biopolymers as structural materials is still challenging in the human life. One of the major drawbacks of polypeptide-based materials is their limited synthesis method. My research group has successfully synthesized various polypeptides, even with unnatural amino acids or nylon units, via chemo-enzymatic polymerization. Those artificial polypeptides containing unnatural units achieve several properties that cannot be done by natural polypeptides. This synthesis method provides a new insight for material design of polypeptide. Novel multiblock polypeptides with a structure similar to the unique sequence observed in spider silk proteins were synthesized via a two-step chemical and enzymatic synthesis method. Resultant multiblock copolypeptides formed an antiparallel beta-sheet structure with a degree of crystallinity similar to that of spider silk, which resulted in a fibrous morphology. This study provides new examples of synthetic multiblock polypeptides mimicking the natural structural proteins as renewable materials. In my presentation, the new finding in spider silk spinning, which is important to design tough structural polymers, will be introduced as a molecular design strategy.

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Abstracts for Award Lectures

Santappa Award Lecture

Coulomb Interactions-Driven UCST Polymers

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Abstract

Thermoresponsive polymers have been extensively researched in the academic community and the major focus has also been on their wide range of applications in sensing and devices as well as in biomedical filed. The water-soluble polymers with lower critical solution temperature (LCST) are most widely studied in terms of their use in biomedical sciences. But, polymers with upper critical solution temperature (UCST) behaviors are less studied, though conceptually they are equally useful. The UCST-type phase transition is driven by either hydrogen bonding (HB) or Coulomb interactions among the polymer chains. Consequently, there has been major development in synthesizing new UCST polymers with HB interactive functional groups. But, the explorations of UCST polymers that are rely on Coulomb interactions are very less. Thus, our research is focused on the development of new electrostatically interacted UCST polymers. I will discuss several recent achievements of various ionic UCST-type polymers including their phase behaviors and responsiveness towards other stimuli in our laboratory. Specifically, the discussion focuses on the synthesis of amino acid-based poly(zwitterions), amino acid-based zwitterionic polysufobetaine, poly(zwitterionic ionic liquid)s and discussion of their UCST-type behaviors due to intra- and inter-molecular electrostatic interactions between the pendent zwitterionic groups of the neighboring polymer chains. The synthesis of other type of ionic polymers such as phosphonium and imdazolium poly(ionic liquid)s, their copolymers and cationic polypeptides as well as their UCST-type behaviors due to the electrostatic ionic bridging interactions in the presence of added anion will also be discussed.

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K. Kishore Memorial Award Lecture-01

Crystalline Polyperoxides from Fatty Acid Containing Styrenic Monomers

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Abstract

Vinyl polyperoxides, alternating copolymers of vinyl monomers and molecular oxygen, are highly viscous amorphous materials because of the flexible peroxy (-O-O-) bonds in their main chains.[1,2] Polyperoxides show highly exothermic degradation in contrast to common polymers which generally degrade endothermically, and finds applications in various areas as; polymeric radical initiators, curators in molding and coating applications, dismantlable adhesives, auto combustible polymeric fuel, drug carrier, plastic waste management, etc. Although this class of polymers is known since 1922, till date there is only one report, where crystallinity was found in poly(*α*-phenyl styrene peroxide) (PAPSP).[3] However, detailed mechanism of crystallization was never studied.

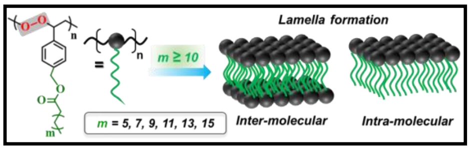

Figure 1. Crystalline domain formation in the side-chain fatty acid based polyperoxides.

Side-chain crystallization occurs from long *n*-alkyl side chains of polymers with C ≥ 12 of the side chain alkyl carbons.[4] Thus, to prepare crystalline polyperoxides side-chain fatty acid based vinyl monomers of appropriate fatty acid chain length could be used, to restrict the main chain flexibility from the side-chain crystallization of long fatty acid moieties. Therefore, we have polymerized styrenic monomers having fatty acid moieties with different chain lengths at the *para*-position of phenyl group *via* oxidative polymerization in the presence of a free radical initiator at 50 ^{o}C in toluene. Indeed, crystalline polyperoxide forms when C ≥ 12 of the side chain alkyl carbons in fatty acid moiety (Figure 1), as confirmed by differential scanning calorimetry (DSC), polarized optical microscopy (POM), powder X-ray diffraction (PXRD), transmission electron microscope (TEM) and density functional theory (DFT) calculations. Side-chain crystallinity imparts high thermal stability and powdery nature to these polyperoxides, despite their low molecular weight and highly flexible backbone owing to the main chain peroxy links.

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K. Kishore Memorial Award Lecture-01

Hierarchical Ordering of Poly(L-lactide) in Block Copolymers and Star-Shaped Polymers

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Abstract

Poly(L-lactide) (PLLA), the most common stereoisomer of the poly(lactic acid), is a widely used biobased polymer in degradable plastics. It is also used as a degradable biomaterial in many medical devices and tissue engineering. To overcome the limitations of polylactides and tailor its desirable properties, multiphase polymer systems have been developed [1-5]. The structural ordering process plays a key role in controlling the nanostructured morphologies of the multiphase systems. In the first part of the talk, the structural evolution of PLLA during heating of the amorphous ABA triblock copolymers will be discussed. For that purpose, two triblock ABA copolymers poly(L-lactide-b-dimethylsiloxane-b-L-lactide) and poly(L-lactide-b-ethylene glycol-b-L-lactide) containing poly(L-lactide) were synthesized. Upon heating of the glassy triblock copolymers, the amorphous PLLA transiently transformed to the mesophase just above the T_g of PLLA block before crystallizing into the regular □ form.[1-2] The formation of the mesophase was faster in miscible triblock copolymers due to the enhanced molecular mobility of the amorphous PLLA. In the second part of the talk, the role of polymer chain packing on the solid state emission properties of the star-shaped PLLA (Figure) will be discussed [3]. Using the blends of enantiomeric star-shaped polylactides, the structure formation process of stereocomplex will be discussed. Last part of the talk highlights the structure and morphology (superstructure) of the solvent-induced crystallized PLLA films in different length scales using wide-angle and small-angle X-ray scattering, atomic force microscopy, and polarized light microscopy.[4,5]

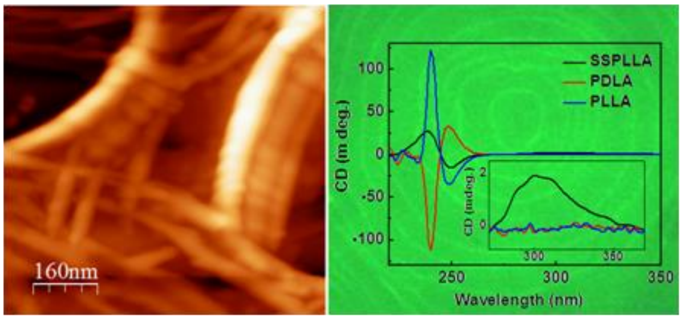

Figure 1: AFM height image of the drop-cast aggregates of star-shaped PLLA and circular dichroism spectra of PLLA (blue), PDLA (red) and star-shaped PLLA (black).

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Abstracts for Invited, Short and Oral Lectures Under the Theme Controlled Polymer Synthesis and Architectures (CPSA)

CPSA-IL-01

Strong underwater adhesion: maximizing adhesive and hydrophobic interactions with the surface

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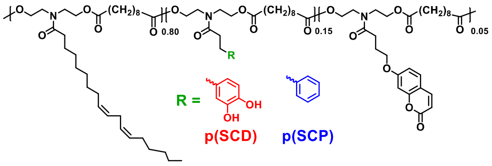
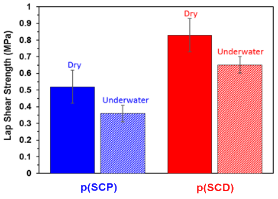
Abstract

Mussel adhesion has fascinated scientists for their ability to adhere to underwater substrates. They do this by the secretion of adhesive proteins underwater in a temporal fashion. The mixture of proteins secreted by mussels are tuned to provide both adhesive and cohesive interactions with the substrate. Synthetic adhesives in comparison are for the most part compromised in an aqueous environment due to their inability to prevent water penetration into the adhesive interface. We will present our work on the design and evaluation of synthetic polyesters that demonstrate strong underwater adhesion. The polyester is designed to flow at room temperature that enables application without any solvent. Catechol units of the polymer provide adhesive contacts with the substrate. The applied polymer is subsequently cured to a crosslinked polymer providing cohesive interactions. Lapshear measurements show strong adhesion even when the polymer is applied underwater. Our current results indicate that in addition to the role of catechol, a hydrophobic environment is necessary for synthetic adhesives to show good performance in wet environments. The nature of the adhesive interface has been characterized by sum frequency generation spectroscopy and JKR measurements, and these studies have provided mechanistic insight into the role of each functional group in maximizing adhesive and cohesive interactions.





CPSA-IL-02

Polymers and Chemicals Manufacturing via Continuous Flow Processes:
A New Paradigm in Process Intensification

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Abstract

Continuous flow manufacturing provides a potential alternative to batch manufacturing because of its inherent advantages such as very efficient heat exchange, high batch to batch reproducibility, fast mixing, high throughput, safety, and the ability to do multistep telescopic synthesis. Due to these advantages, these processes have been referred to as the most promising "Green Technology". In fact, continuous flow processes are projected to be the "CHEMICAL FACTORIES" of tomorrow. Continuous flow processes also provide "On-Demand" synthesis with complete control over reproducibility, size, shape and these parameters can be achieved at various scales (lab synthesis to pilot to bulk production) with excellent reproducibility. This opens up the opportunity for synthetic chemists to prepare materials with precise control over critical molecular design parameters. It also enables one to carry out chemical synthesis at higher temperatures which were outside the domain of an organic synthetic lab. Apart from this, continuous manufacturing opens up new domains in formulations and various downstream processes. It is also revolutionizing the domain of high throughput machine-assisted synthesis leading to development of Artificial Intelligence (AI) in various domains of chemical industries. In this presentation, I will review some of the recent advances in these directions and some results from our laboratory. An introductory tutorial (developed by us) can be found at YOUTUBE at following address:

https://www.youtube.com/watch?v=CYo85cdhEfc&feature=youtu.be

CPSA-IL-03

Insertion Copolymerization of Difunctional Polar Vinyl Monomers with Ethylene: A Comprehensive Account

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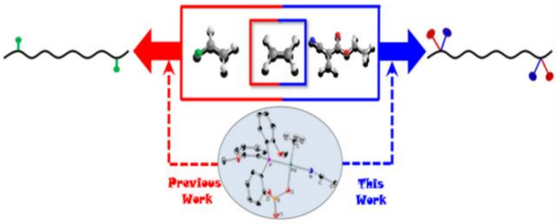
Abstract

Today we produce about 300 million tons of polymers every year and polymers have become indispensable in 21st century. Among these, polyolefins contribute more than half of the total volume of polymers produced. Most of these polyolefins are produced by a reaction called “Insertion Polymerization” or more popularly “Ziegler-Natta Polymerization”.[1]Despite the seeming maturity, the insertion polymerization reaction continues to surprise us with growing complexity and is young as ever. My talk shall take a stock of the remaining challenges in Ziegler-Natta polymerization; briefly discuss current solutions, and reiterate the enormous potential of this seventy year old reaction to meet contemporary demand. I will showcase our endeavor in insertion copolymerization of difunctional olefins with ethylene to prepare functional polyethylene.[2-4] Synthesis of acetonitrile ligated phosphine-sulfonate palladium complex, its application in the first insertion copolymerization of 1,1-disubstituted difunctional (such as super glue) olefin with ethylene, mechanism and structure-property-performance correlation will be disclosed.[5]



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CPSA-IL-04

Smart Functional Polyurethanes: Preparation and Properties

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Abstract

Polyurethanes (PU) are one of the most important class of versatile polymers. Since its first report at IG Farben in Leverkusen, Germany in 1930s, PU has been widely used as plastics, rubbers, fibers. The properties of PUs can be tuned by changing the nature of polyols, diisocyanates and chain extenders. In this investigation, we have prepared specialty PUs by introducing different functional groups by using different types of modified chain extenders. Incorporation of group furfuryl as well as functional nano-hybrid material like polyhedral oligomericsilsesquioxane (POSS) leads to self-healing as well as hydrophobic characteristics in PU. PUs are known to be good shape memory polymer which can recover into its original shape from a deformed state. It was observed that incorporation of ionic crosslinks in PU significantly improves its shape recovery and shape fixity making it an excellent shape memory material. This talk will delineate synthetic strategy of preparation and characterization of smart self-healable as well as shape memory PUs.

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CPSA-IL-05

Sustainable thermoplastic and thermosetting polymeric nanocomposites

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Abstract

Development of sustainable polymeric materials with high performance is the necessity of hours. In this milieu, a few sustainable thermoplastic and thermosetting polymeric nanocomposites have been fabricated using different types of nanomaterialsincluding carbon nanotubes, carbon dots, graphene derivatives, organoclay, metal and metal oxides, etc. Biodegradable polyesters, poly(ester amide)s,epoxies and polyurethanes with varieties of structures and compositions have been synthesized and used as matrices for such nanocomposites. Some of these raw materials were obtained from different renewable resources. The nanomaterials have been incorporated in the above matrices by following in-situ and solution polymerization techniques. These nanocomposites exhibited substantial increase in mechanical, thermal, chemical and other desired properties including optical and electrical properties from their respective pristine systems. As an example,citric acid derived polyester thermosetting nanocomposite with carbon dot-TiO_2 showed an excellent excitationwavelengthdependentphoto-luminescence,self-cleaning, anti-reflecting, etc. behaviors andability to separate crude oil from its mixture. along with desired mechanical properties. Similarly, castor oil modified silicone containing polyurethane-polystyrene interpenetrating thermoplastic elastomeric nanocomposites with multi-walled carbon nanotubes exhibited excellent shape memory, water repellence with static water contact angle up to 140°, and outstanding self-cleaning and anti-icing behaviors along with high mechanical attributes. All the studied polymeric nanocomposites showed biodegradability under exposure of specific bacterial strains anda few of thempossess biocompatibility. Thus these nanocomposites have great potential to be used as active surface coating binders and smart biomaterials including engineering materials.A brief overview of all these materialsfrom synthesis to applications will be discussed.

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CPSA-IL-06

Catalytic Processes for Novel Ultra High Molecular Weight Polyethylene

Raksh Vir Jasra

Abstract is waiting

CPSA-IL-07

Grafting of Glycopolymer Chains on the Nanoparticles Surface Using RAFT Polymerization

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Abstract

The weak binding between carbohydrates and proteins is a major constraint towards the development of carbohydrate-based therapeutics. To address this, we have developed a method for the synthesis of glycopolymer (GP) grafted nanoparticles by using Reversible Addition Fragmentation Chain Transfer (RAFT) polymerization through *in-situ*/*grafting from* approach using a multistep process.[1, 2] GP chains of various lengths with controlled molecular weight and narrow polydispersities were grown on the RAFT agent anchored nanoparticle surface using various type of glycomonomers. The mean diameter of the glycopolymer grafted nanoparticles (GP-*g*-NPs) can be readily tuned by altering the chain length, type of nanoparticles and the type of glycomonomers used in the polymerization feed.[1, 2] GP-*g*-NPs displayed stronger binding to the carbohydrate specific lectin such as *Concanavalin A* (Con A) owing to the larger positive binding entropic contribution (**Figure 1**) which resulted in an association constant that is 800 and 400-fold stronger than that of monomeric carbohydrate and linear GP chains, respectively.[2] These initial results opened up the huge scope for developing carbohydrate based vaccine based on glycopolymer coated nanoparticles.

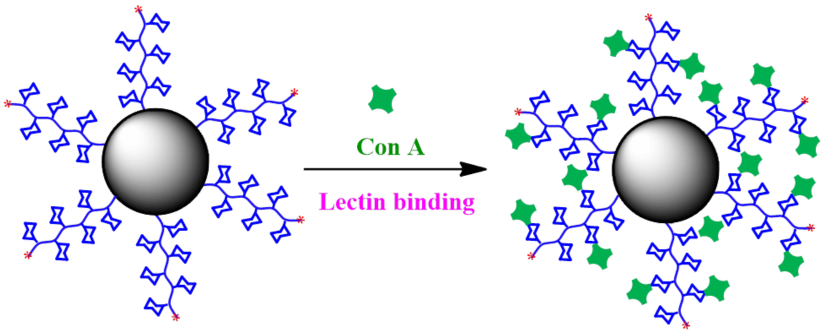

Figure 1. Schematic representation of binding between glycopolymer coated nanoparticles and specific lectin.

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CPSA-IL-08

Block Copolymer Resists

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Abstract

Studies of block copolymer (BCP) materials and their phase separation in bulk and thin-film form have exploded over the last few decades due to their multitude of applications in lithography, and drug delivery, and as biomaterials, rheological modifiers, and mesoporous materials. This is partly because BCPs provide a flexible size and shape tunable platform to create nanostructures over large areas in the 3 - 200 nm length scale, using inexpensive materials and processes. This requires addressing aspects, from synthesis of new block copolymers with high chi, chemistry and physics to enable their thin-film assembly, and technology to multiply the density of features. While new monomers are one route to access these high chi block copolymers, we have focused on existing monomers that are explored in traditional photoresist chemistry to create highly functional block copolymers that self-assemble into sub-10 nm features. This design allows us to simultaneously incorporate a number of requirements that are needed for their use in thin-films. Surprisingly, even chi has not been quantified for a wide variety of simple, well-known polymers. We describe ongoing research in the group on the design, synthesis and characterization of these new strongly phase segregating block copolymers[1-5].

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CPSA-IL-09

Sulfur to Sulfur Polymers & Composites: New Directions

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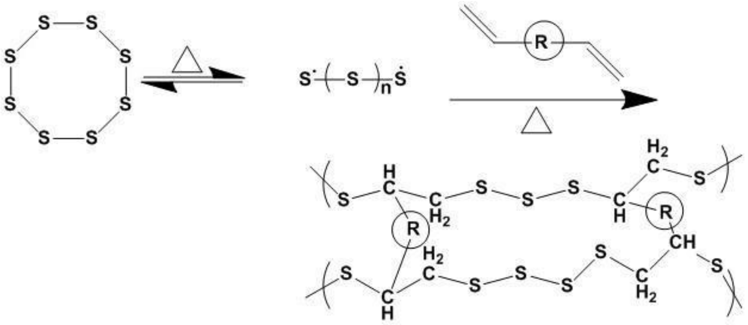
Abstract

More than 60 million tons of elemental sulfur are produced annually as a by-product of hydro-desulfurization process in refinary. It is used mostly for the production of commodity chemicals like sulfuric acid and fertilizers. Abundance of elemental sulfur coupled with possibility of developing innovative chemistry opened new directions for sulfur based high performance materials in recent years.

Elemental sulfur exist in the form of eight-membered ring (S_8) that undergoes solid-to-solid transition from orthorhombic to monoclinic crystal at 100-109°C. On further heating, it melts into a yellow liquid phase at 120–124°C with rings ranging from 8–35 sulfur atoms. Above 159°C, it offers the possibility of equilibrium ring-opening polymerization (ROP) of the S_8 monomer into a linear polysulfide with diradical chain ends. Polymeric form of sulfur is not stable and reverts back to S8 at room temperature. Di-radical polymeric sulfur can be stabilized by diene types of modifier which yield semi-interpenetrating network (**semi-IPN**) structure.



The present talk will discuss the synthetic strategy and characteristics of sulfur based IPN with different vinylic and allylic modifier. The use for copolymers from sealant to concrete based composites will also be presented.

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CPSA-IL-10

Synthesis and self-assembly of stimuli-responsive linear-dendritic copolymers

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Abstract

Stimuli-responsive polymeric nanostructures in solution are important tools in drug delivery and other applications. We have synthesized amphiphilic stimuli-responsive linear block copolymers and linear-dendritic copolymers incorporating one or more of pH- and photoresponsive (UV- and visible light-sensitive) groups, and temperature-responsive polymer chains such as poly(N-isopropylacrylamide) (PNIPAM). The self-assembly of these polymers in aqueous solution was investigated by TEM and DLS analysis. Dye encapsulation and stimuli-responsive dye release were shown. Polymers that were designed to be biocompatible were studied for cell uptake and controlled release of anti-cancer drug inside the cells was demonstrated. Dendron generation and linear block length were varied in some of the polymers to tune the size and shape of the self-assembly. Temperature-responsive change in morphology was shown for PNIPAM and poly(ε-caprolactone) containing linear-dendritic copolymers. Triazole-containing linear-dendritic amphiphiles were used to fabricate Cu and Ag nanoparticles in dilute aqueous solution and their efficiency in catalyzing reduction of p-nitrophenol was evaluated.

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CPSA-IL-11

Fabrication of Reactive Polymeric Coatings as Functional Interfaces

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Abstract

Polymeric coatings on various inorganic surfaces and nanoparticles have emerged as widely used component for a broad range of functional materials with biomedical applications ranging from sensing to targeted imaging and delivery.Oftentimes, the inorganic materials used for such applications are coated with a layer of polymeric material to impart properties that not only enhances their utility, but are crucial for the desired function. Today, polymeric coatings on inorganic surfaces play a role beyond their protection. They equip these materials with functional attributes necessary for the targeted applications. The polymeric coating provides an interface for communication between the material and biological world (Figure 1). For example, a judicious choice of polymeric coating on planar and nanoparticle surfaces provides the much needed resistance towards biofouling under physiological conditions. This is very important for applications like sensing where a high signal to noise can be achieved. For many applications, the surface coatings needs to be engineered in a manner that would allow attachment of specific ligands and biomolecules while exhibiting resistance towards undesired protein adsorption in the biological media. To date, in our research group, a variety of polymeric coatings ranging from ultrathin coatings and hydrogels to surface tethered polymer brushes have been utilized towards fabrication of functional inorganic planar surfaces and nanoparticles.Case studies highlighting the design principles with specific applications such as bioimmobilization, protein recognition and activity modulation to cellular targeting for imaging and delivery will be discussed.

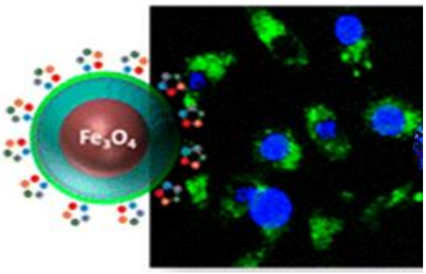

Figure 1. Polymeric coatings interfacing material and biological

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CPSA-IL-12

Biocompatible Graphene-rubber nanocomposites and poly(glycerol sebacate) based semi interpenetrated network assemblies: Structure and properties towards next generation elastomers

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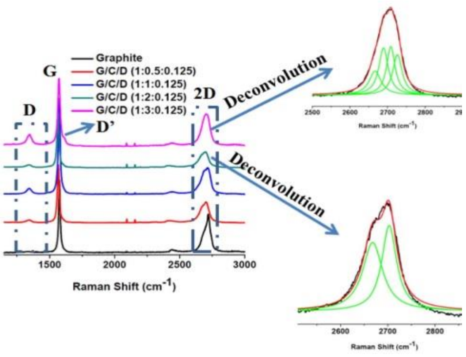
Abstract

Next generation elastomeric materials/devicesdemand a number of functional properties *viz.* (a) enhanced thermal/electrical conductivity (b) inferior mechanical properties (c) biocompatiblity and (c) use of sustainable raw materials. In this talk, our efforts to achieve these properties through preparing;(a) graphene-rubber nanocomposite and (b) poly(glycerol sebacage) (PGS) based semi interpenetrated networks, will bepresented. In this context, defect free few layers graphene is successfully prepared using a simple, scalable and safe method, wherein,melamineand naturally available phenolics(curcumin/tetrahydrocurcumin/quercetin, Figure 1) are employed asthe solid and liquid-phase exfoliating agents. The yielded graphene was mixed with the natural rubber to produce thin film nanocomposites, which show enhanced thermal conductivity and tensile strength as well as biocompatible. PGS, produced from renewable monomers such as sebacic acid and glycerol, has been explored as sustainable materials in order to enhance the tensile properties, which suit to the applications such as elastomers and rigid plastics.



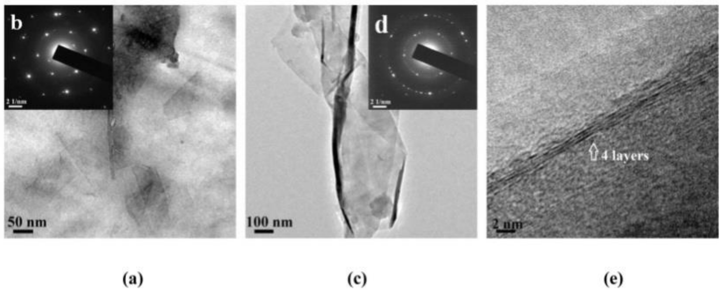


Figure 1: Produced few layers pristine graphene characterized by Raman and TEM analysis.

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CPSA-SL-01

Synthesis of tertiary amine containing hyperbranched polyesters via melt-transesterification

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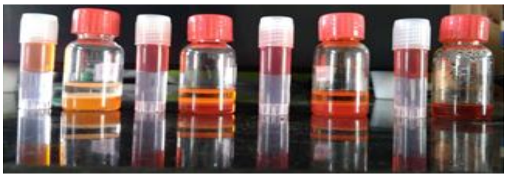
Abstract



Dye uptake studies: Dye in Water and chloroform (right)

Dye in Water and polymer in chloroform (left)

Branched polymers that contain tertiary amines in the core find wide applications from as catalytic centers, gene delivery vehicles, nano careers, etc.[1-2] The globular structure adopted by hyperbranched polymers with tertiary amines in the core could show unique property as a function of pH, ability to encapsulate guest molecule that match core environment, entrap metal ions, etc. We have synthesized two sets amine containing of hyperbranched polymer by transesterification via $A_3 + B_2 + B'$ and $A_4 + B_2 + B'$ to obtain core-shell hyperbranched polymer.[3-5]

The presence of more number of tertiary amines in the hyperbranched polymer prepared from A_4 type monomer allowed us to explore the uptake of transition metal ions as it mimics the chelating sites of ligand. Among the metal ions tested for uptake, the A_4 type polymer showed preference to chromium. The limit of chromium (VI) removal by polymer assessed spectroscopically under ambient conditions at 30ºC was found to be 6 mg of dichromate per mg of polymer. The uptake of metal ion as well as dye is instantaneous which allows to design a cross-linked network of hyperbranched polymer placed in straw as on site water purifier.

Increasing concentration of chromium solution in the presence of DPC (Ligand). Water before treating with polymer (left); water after treatment with polymer

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CPSA-SL-02

Anionic polymerization of vinyl monomer in water- is it really possible?

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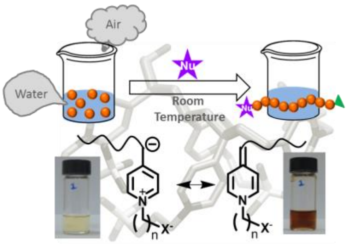
Abstract

Living anionic polymerization of vinyl monomers, after it was first reported by Michael Szwarc[1], revolutionized the field of polymer science and led to birth of a number of controlled polymerization techniques in last sixty years. All these controlled/ living polymerization techniques have enabled us to produce polymers with precise control in structures, functionalities and architectures for numerous applications. However, anionic polymerization[2-3], in general, is well known to be sensitive to polar functional groups and polar reaction media. This presentation will focus on a very exceptional example of nucleophile-initiated anionic polymerization[4-5] system for vinylpyridine (VP) based zwitterionic monomers that occurs in water under ambient aerobic conditions. Zwitterionic polymers of different chain end functionality including radically polymerizable vinyl groups were synthesized by utilizing different nucleophiles as initiator. Density functional theory (DFT) calculations of monomer and propagating species were used to validate anionic mechanism of polymerization and active-dormant resonance hybrid structure of the propagating carbanion. This is particularly a unique polymerization system where an active-dormant transition, an essential component of living/controlled polymerizations, persists in the absence of any control agent, metal catalyst or additives unlike many other living polymerization systems. This methodology of polymerization, although at the moment limited to certain type of monomers, opens up a new and a very facile way of synthesizing functional zwitterionic polymeric materials especially towards biomedical and marine anti-biofouling[6-7]surfaces.



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CPSA-SL-03

Synthesis of Responsive Chiral Poly(ionic liquids) and their applications in Catalysis

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Abstract

Polymers have shown greater promise as chiral ligands in a wide range of catalytic tranformations. These chiral polymers provide many advantages within the context of organic reactions. The poly(ionic liquids) (PILs) which are a class of polyelectrolytes are considered as special type of polymers with unique properties combining those of ILs and specific properties of polymers. The tuneable nature of PILs provides greater novelty towards their applications. We have prepared a series of imidazolium based chiral and achiral homo and cross linked PILs through controlled radical polymerization (RAFT technique). We have prepared chiral poly(ionic liquids) by introducing the chirality at the anionic site by simple anionic metathesis. It is very interesting to note that introduction of chirality at the anionic site triggered helicity in the polymer back bone.[1]These achiral and chiral homo and cross linked PILs were utilized as recyclable catalysts in different organocatalysis reactions such as Diels Alder reactions, asymmetric Baylis Hillman reaction, Michael Addition reaction.[1-5] Chemo-selective TH reduction of α,β-unsaturated carbonyl compounds under base free conditions were achieved using PIL stabilized Ni NPs.[6]We have also used these imidazolium based PILs for DNA stabilization.[7] During the presentation, synthesis of these homo and cross linked PILs and their applications will be discussed.

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CPSA-SL-04

Novel Nano sized Atom transfer radical polymerization Initiator viz., Bromo-Terminated Thiol Functionalized Au and Ag Nanoparticles for Polymerization of N-Isopropylacrylamide

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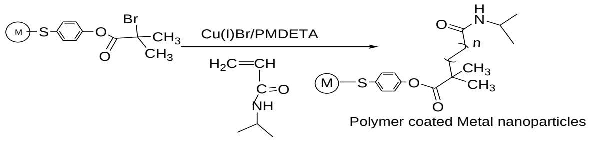
Abstract

Synthesis of new polymeric materials with increasing control over the macromolecular architectures could be achieved through atom transfer radical polymerization (ATRP) route. ATRP is a versatile and robust polymerization method to develop well defined polymers finding applications in diversified areas. It is also important to mention that the nanometer sized metal-polymer composite containing AuNPs and AgNPs, produced through ATRP method has found wide variety of applications[1,2]. In the recent past, the metal containing robust polymer specifically produced from ATRP has been extensively exploited in the fabrication of optical, electronic and photonic devices. Considering the significance of the polymer produced from ATRP, in this study, we synthesised novel nano sized ATRP initiator viz., bromo functionalized thiolates on to the silver nanoparticles (BTFAgNps) and Bromo functionalized thiolates on to the gold nanoparticles (BTFAuNps) via two step procedure: stabilization of Au and Ag nano particles with 4-mercapto phenol individually, and treatment of each with ethyl 2-bromoisobutryl bromide(2-BIB)[3] to form nano sized ATRP initiators namely BTFAuNps and BTFAgNps. These two initiators were characterized with FT-IR, Uv-Vis and TEM techniques. The initiating efficiency of these two initiators were demonstrated through surface-confined atom transfer living radical polymerisation at moderate temperature using CuBr/PMDETA(Pentamethyl diethylene triamine) as a catalyst for polymerization of N-Isopropyl acrylamide (N-IPA) as a reference reaction**.** The resulting poly-NIPAs obtained through these two initiators were characterized individually with GPC, DLS and TGA techniques, and ascertained their efficiency and structural properties. Further, the kinetics of nano poly-NIPAs was studied to evaluate the molecular weight and polydispersity index through GPC. The linear kinetic plot of $\ln([M_0]/[M])$ versus time, and the linear increase of number average molecular weight with the monomer conversion confirm that this polymerization proceeds through controlled/living in nature.



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CPSA-SL-05

Multi-Stimuli Responsive Materials: Design, Synthesis and Applications

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Abstract

3D-printed anatomical models for surgical planning and clinical training have wide applications in the hospital inpatient setting.[1,2] This leads to better outcomes, both clinically and economically, for patients, care-providers/doctors and payers. Metals have been the materials of choice, since they combine all the required properties such as durability, chemical inertness, temperature resistance or wear resistance. However, a big disadvantage of using metal is the weight. Use of a lighter material instead of metal can save a lot of fuel, which will result in reduced CO_2 emission. High performance polymers containing fluorinated backbone can be a better alternative to the metal.[3] Apart from satisfying all the criteria such as chemical resistance to acids, bases, and organic solvents, excellent weathering, and durability, polymers are lighter than the metal. Stimuli-responsive materials undergo changes in response to external stimuli such as change of temperature, pH, light, etc. Multi-stimuli responsive polymer materials exhibit improved diversity compared to single- or dual-stimuli responsive polymers.[4] However, the ability of the current multi-stimuli responsive polymers to provide the required specificity and tunability is still in its infancy. This is due to the complexity in balancing the material parameters of functionality, reaction feasibility, degradability, hydrophilicity etc. Furthermore, challenging synthesis protocols for these multi-responsive polymers has resulted in lack of fundamental understanding of the detailed structure-activity relationship. We have developed multi-stimuli responsive multi-arm-star polymers as a tunable platform to fabricate nanoengineered 3D-printed anatomical models for surgical planning and clinical training.[5] Novel functional polymers with multiple tunable responses exhibiting large changes in swelling and wettability properties in response to external stimuli (e.g. pH, temperature and light) has been designed, synthesized and characterized. The utility and impact of these multi-stimuli responsive polymer-based materials are demonstrated by the construction of adaptive and intelligent models.

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CPSA-OL-01

L-Amino acid Based Biodegradable Polyester Nano-carriers for Drug Delivery and Bio-imaging in Cancer Cells

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Abstract

L-Amino acids are biological monomers that play crucial role on the size, function and secondary structure of proteins. Synthetic polymers based on L-amino acids attracted significant interest in chemistry-biology interface due to their potential application in therapeutics and biocompatible thermoplastics. The development of new synthetic strategies for L-amino acid based polymer nano-carriers has tremendous research opportunities in the area of biomaterials. The thesis work is emphasized to develop new classes of linear polyesters from L-aspartic acid resources via solvent free melt poly-condensation method approach. These amphiphilic polyesters were self-assembled as 200 ±10 nm nanoparticles and they exhibited excellent encapsulation capabilities for delivering multiple anticancer drugs such as doxorubicin, topotecan, and curcumin etc. These polymers were in-built with pH, and enzyme responsiveness; thus, they were stable at extracellular conditions and underwent enzymatic-biodegradation exclusively at the intracellular level to release the drugs.[1] The drug administration was studied in breast cancer, cervical cancer and non-cancerous WT-MEFs cell-lines. These studies revealed that the nascent L-Aspartic acid based nanoparticles were non-toxic whereas the drug loaded polymer nanoparticles exhibited excellent cell killing in cancer cells. Fluorescent-tagged biodegradable polymer nanoparticle probes were also accomplished to track drug polymer dissociation kinetics in the cytoplasm of the cancer cells via FRET mechanism. Three FRET probes were constructed based on OPV- Nile red; TPE-Nile red and curcumin-Nile red diads and their bio-imaging capabilities were tested *in vitro* live cell imaging.[2] New classes of hydroxyl functionalized polyester nano-carriers were established as multi-purpose nano-scaffolds for drug conjugation and water dispersible FRET probe through aggregation induced emission (AIE) process. The presentation will be focused on the synthetic design strategies and the importance of L-amino acid polymer for bio-imaging application in cancer cells.

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CPSA-OL-02

Ring Opening Polymerization of L-lactide : Thermodynamic Study

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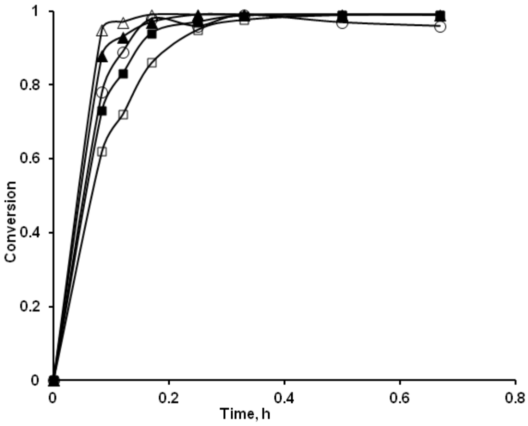
Abstract

The ring opening polymerization (ROP) of L-lactide (M) was carried out in bulk using stannous octoate as catalyst (C) and 1-pyrene butanol as co-catalyst (ROH) at M/C = 5620 and ROH/C = 17. The effect of polymerization temperature and time was studied on the kinetics of L-lactide ROP at 150 to 190°C. The ^{1}H NMR spectroscopy and Ostwald viscometer were used to measure the conversion and viscosity average molecular weight (M_v) respectively. The monomer conversion (Fig.1) and M_v increases linearly with polymerization time[1]. The depolymerization reactions are dominating at high polymerization temperature and time. Therefore, the decrease in M_v was observed at the monomer conversion of > 95%. The rates of propagation were calculated by following the method described in the literature[2].

The entropy, activation energy and the pre-exponential factor were calculated for the reversible ring opening polymerization of L-lactide. The obtained values of activation energy is E = 31.3 kJ.mol^{-1} and pre-exponential constant is lnA = 18.3[3, 4] (Fig.2).



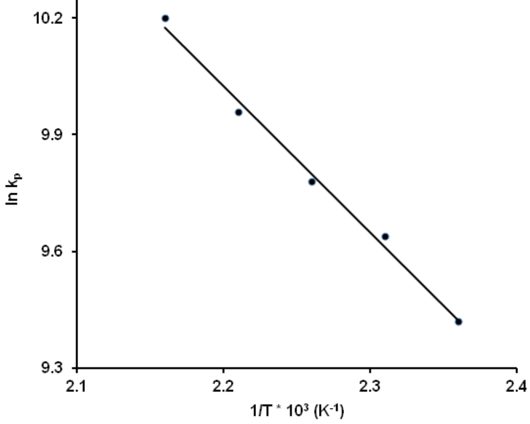


Figure 1: Plot of conversion *vs.* time. **Figure 2**: Plot of lnk_p *vs.* temperature

Experimental data: □, 150; ■, 160; ○, 170;
▲, 180; ∆, 190°

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CPSA-OL-03

H-Bonding Assisted Self-Assembly of Anionic and Neutral Ligand on Metal: A Comprehensive Strategy to Mimic Ditopic Ligands in Olefin Polymerization

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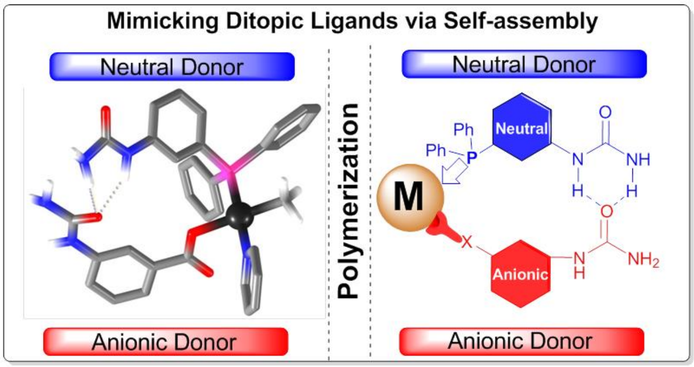
Abstract

Self-assembly of two neutral ligands on a metal to mimic bidentate ligand coordination has been frequently encountered in the recent past,[1-4] but self-assembly of an anionic ligand on a metal template alongside a neutral ligand remains an elusive target. Presented here is the self-association of anionic ligand 3-(3-phenylureido)benzoic acid (**2b**) and 1-(3-(diphenylphosphanyl)phenyl)-3-phenylurea (**1b**) on a metal template to produce palladium complex $[\{COOC_6H_4NH(CO)NHPh\}\{Ph_2PC_6H_4NH(CO)NHPh\}PdMePy]$ (**3c**). The existence of **3c** was confirmed by Job plot, 1-2D NMR spectroscopy, deuterium labeling, IR spectroscopy, UV-Vis spectroscopy, model complex synthesis and DFT calculations. These solution and gas phase investigation authenticated the presence of intramolecular hydrogen bonding between hydrogen's of **1b** and carbonyl oxygen of **2b**. The generality of the supramolecular approach was validated by preparing 6 complexes from 4 monodentate ligands and their synthetic utility was demonstrated in ethylene polymerization.[5]



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[6]

CPSA-OL-04

Synthesis and Chemical Modification of High Performance Polymers containing Clickable functional Groups

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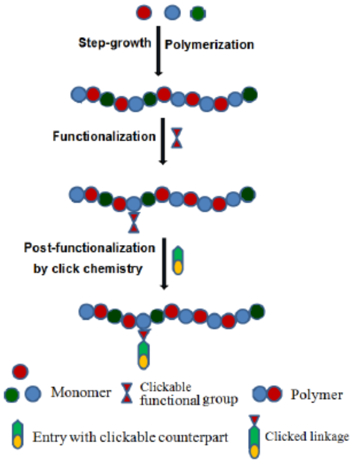
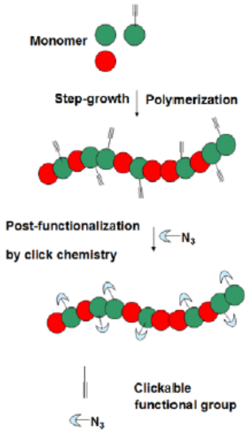
Functional polymers show improved properties relatives to their non-functional counterparts. The polymer can be modified either by chemical modification or by changing the physical nature of the polymers. Currently, two strategies have been widely used for the chemical modification (i) post-modification approach and (ii) functional monomer approach Post-modification approach encounters problems such as insufficient efficiency of the reaction in installing functional groups and undesirable side reactions because of harsh reaction conditions. In Clickable monomer approach, functional monomers with clickable moiety, clickable polymers can be achieved to construct various functional polymers clicking post to the polymerization. This approach relies on the design of monomers whose functional groups are orthogonal to polymerization reactions. Monomers containing propargyl, allyl or azido functional groups are the prominent examples of monomers used for synthesis of clickable polymers. These clickable groups can withstand certain polymerization conditions and can be conveniently transformed afterwards.

We synthesized difunctional monomers containing pendent propargyloxy, allyloxy or azido group viz,. 1,1-Bis(4-hydoxyphenyl)-1-(4'-propargyloxyphenyl)ethane, 5-(Propargyloxy)isophthalic acid, 5-(Propargyloxy)isophthaloyl chloride, 5-(Propargyloxy)-1,3-diisocyanatobenzene, 5-(Allyloxy)isophthalic acid, 5-(Allyloxy)isophthaloyl chloride, 5-(Allyloxy)-1,3 diisocyanatobenzene, 4,4'–(5-Azidopentane-2,2-diyl)diphenol starting from1,1,1-tris(4-hydroxyphenyl)ethane, 5-hydroxyisophthalic acid and 4,4'-bis(4-hydroxyphenyl) pentanoic acid. Using these difunctional monomers clickable aromatic polyester and polyamides containing pendent propargyloxy , allyloxy or azido functional groups were synthesized by interfacial polycondensation. Further the copolyesters and copolyamides were Post-functionalized by alkyne-azide or thiol-ene click reactions using representative azides or thiols.



(i) Post-modification approach



(ii) Functional monomer approach

CPSA-OL-05

Fine-tuning the Lamellar SizeinSub-10 nm Regimeusing Periodically Grafted Amphiphilic Copolymers

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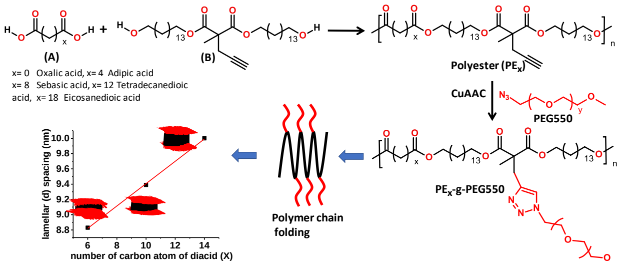
Abstract

Block copolymers (BCP) carrying immiscible segments undergo microphase separation and thereby generate a library of well-orderednanostructures, wherein the domain sizes are controlled by the block lengths.[1]BCP nanostructures have been extensively studied owing to their diverse applications, ranging from photonics, lithography, energy storage and membrane technology.[2]Thekey parameters, among several others, that regulate morphologyevolution in BCPs are relative volume ratio of the blocks and the segregation strength(χN); obtaining nanostructures with small length scales (< 20 nm) has been a longstanding challenge.



Scheme - Synthesis and structure of clickable parent polyesters and PEG clicked derivatives; and a plot showing the variation of lamellar spacing with the diacid length

Recently, we demonstrated that sub-10 nm microphase separated domains can be created using periodically grafted amphiphilic copolymers (PGACs);[3,4] crystallization of the pendant and/or backbone segments further stabilize the nanophase morphologies. Further, we demonstrated that the lamellar size can be fine-tuned by varying the length of the "clicked" pendant PEG chains.[4] In the present study, the backbone segment length (i.e., the periodicity of grafting) has been varied using a simple strategy of condensing different α,ω-alkane dicarboxylic acid chlorides (**A**) with a suitably designed "clickable" diol (**B**), as shown in the scheme; using azide-yne click reaction, MEPEG550 is subsequently grafted to enable immiscibility-driven folding and generation of lamellar morphology. Based on detailed investigations using DSC, WAXS, SAXS, and variable temperature FT-IR studies, the evolution of the lamellar morphology and the variation of the inter-lamellar spacing has been rationalized; further studies to understand the effect of replacing the linking ester units along the polymer backbone to H-bonding moieties, like amide, carbamate and urea, are currently underway.

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Abstracts for Invited, Short and Oral Lectures Under the Theme Supramolecular Polymers and Nano-assemblies (SPNA)

SPNA-IL-01

Supramolecular Machines for Life-inspired Systems.

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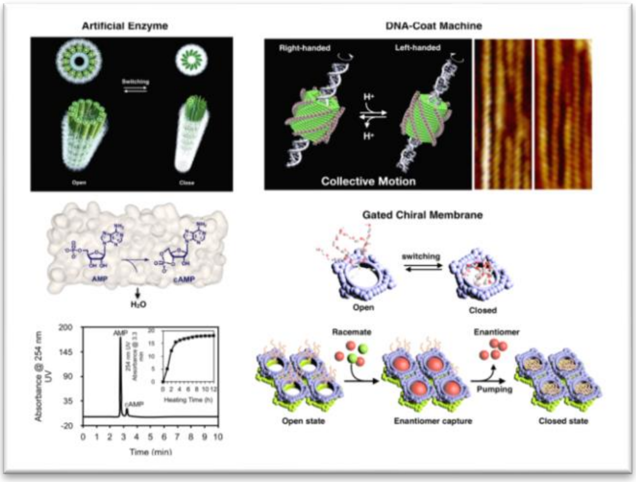
Abstract

In this symposium, I will introduce our recent results how to construct dynamic self-assembled nanostructures exhibiting switchable functions, inspired by life systems. For example, synthetic tubular pores are able to undergo open-closed switching driven by an external signal. The pore-switching mediates a water pumping action for the dehydrative cyclization of AMP nucleotide. When self-assembled tubules embed DNA inside the hollow cavities, the DNA-coat assembly undergoes collective motion in helicity switching in physiological conditions. In the case of toroid assembly, the static toroids are able to undergo spontaneous helical growth when they switch into out-of-equilibrium state, similar to microtubules. Moving from 1-D to 2-D structures, the internal pores are able to form chiral interior which selectively capture only one enantiomer in racemic solution with perfect pore performance. I will discuss recently discovered these results with their biological implications.



Several Examples of Supramolecular Machines.

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SPNA-IL-02

Controlled/Living Supramolecular Polymerization and Precision Assembly

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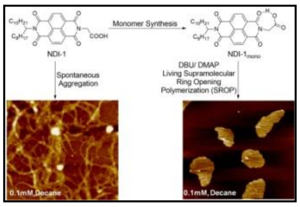
Abstract

Spontaneously assembled supramolecular polymers, albeit having an internal order, lack structural accuracy in mesoscopic scale unlike controlled/living covalent polymerization by chain growth mechanism. “Living supramolecular polymerizations” (LSP) can be realized by kinetically trapping the active monomer in a dormant state and initiating the polymerization by an externally added seed resulting in well-defined structure with controllable length and dispersity. We have recently developed a widely applicable new strategy for LSP. The monomer (NDI-1) contains a naphthalene-diimide (NDI) chromophore-appended carboxylic acid functionality which is well known for its multiple H-bonding motifs. In a hydrocarbon solvent decane, it showed spontaneous aggregation (NDI-1_{agg}) producing irregular fibrillar network by inter-molecular H-bonding among the carboxylic acid groups. However, by fine tuning the solution preparation protocol, NDI-1 could be trapped (same solvent and concentration) in a meta-stable dormant monomeric state (NDI-1_{mono}) in which the COOH group was arrested by intra-molecular H-bonding with the adjacent carbonyl group of the imide functionality. NDI-1_{mono} was quite stable under ambient condition and did not show any signature of aggregation even after 2-3 days. However, in presence of a seed (prepared by sonication of the aggregate) LSP was realized. We also have shown recently remarkable impact of solvent geometry in pathay diversity of NDI-derived building blocks and utility in LSP. More recently we have shown, instead of seed, even in presence of catalytic amount of DBU or DMAP (Molecular entity instead of seed), supramolecular polymerization of NDI-1_{mono} could be realized leading to the formation of ultra-thin (2.0 nm) 2D nano-sheet in sharp contrast to the irregular fibrillar network produced by the same species under spontaneous aggregation. Preliminary mechanistic investigation revealed that DMAP/DBU helped in ring opening of the intra-molecularly H-bonded monomer breeding *in situ* the free acid, which, beyond a critical concentration, initiated living supramolecular ring opening polymerization (SROP). Furthermore, the initially formed 2D polymer could be used as a macro-initiator which enabled chain extension up to subsequent two cycles producing much extended nano-sheet (without compromising the structural regularity) and thus unambiguously established living nature of the present SROP. The presentation will highlight our recent results in this area.



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SPNA-IL-03

Responsive assemblies in aqueous media: from controlled rheology of polymer solutions to mechanical reinforcement of covalent hydrogels.

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Abstract

By working at the molecular level with physical interactions taking place in polymer solutions, it is possible to drive and to finely tune macromolecular assemblies in order to improve the performance of soft formulations under specified environments. This strategy, which has been successfully applied in the development of complex fluids with important applications in oil, cosmetics and biomedical industries, finds actually new potentialities in the design of tough hydrogels. Indeed, the combination of both covalent and physical cross-links within the same architecture is actually one of the most promising strategies in this field.At the border between these two domains (liquids and solids), we will present in this lecture different functionalities that can be used to control macromolecular assemblies in aqueous formulations and describe how these functionalities can be used to design covalent hydrogels with improved mechanical properties (**Figure 1**).Based on a simple toolbox including a macromolecular backbone and polymer side-chains, with or without added covalent cross-links, we will demonstrate the versatility of this approach for the design of responsive and reversible assemblies with a special emphasis on the structure/properties relationships [1-4].

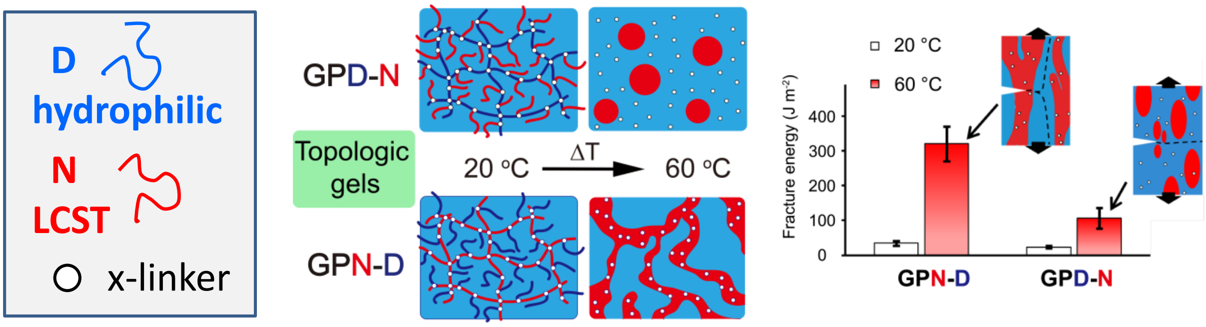

Figure 1. Thermo-toughening of hydrogels under isochoric conditions.

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SPNA-IL-04

Spin Dewetting: A Novel Generic Meso Fabrication Technique

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Abstract

It is well known that spin coating is widely used for creating ultra thin films spanning over large areas. However, the film may rupture during coating itself, particularly on a non wettable substrate. Such a sample is generally considered as a waste, as it fails to produce a good film. We utilize the physics associated with rupture of a film during spin coating and create variety of ordered meso scale structures with different materials such as homopolymers,1 polymer blends,2 and liquid crystal.3 We show that unlike dewetting of a thin polymer film, which is dominated by the amplification of thermally excited capillary waves, spin dewetting is dominated by Marangoni Instability in the rapidly evaporating solvent. We finally show some of our recent result on spin coating mediated formation of colloidal arrays and a novel, all purpose colloidal transfer printing that works irrespective of the nature of the colloidal particles and the target substrate.4

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SPNA-IL-05

Unravelling Competing Pathways in Metallosupramolecular Polymers

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Abstract

Self-assemblies of metal complexes have gained considerable attention not only because of the inherent properties of the metal ions but also due to the versatility of non-covalent interactions when a metal fragment is part of the molecular design.[1] Our group has investigated the supramolecular polymerization of dichlo(bis)pyridyl Pd(II) and Pt(II) metal complexes featuring a □-conjugated surface derived from oligophenyleneethynylene (OPE).[1] The introduction of polar triethylene glycol (TEG) chains induces a slipped stacking of the monomer units within the self-assembled structure.[2] In contrast, remarkably different packing modes (slipped *vs*. parallel for Pd(II)[3a] and Pd(II),[3b] respectively) are observed if alkyl chains are attached. This distinct self-assembly behavior prompted us to exploit hydrogen bonding synthons to explore the possibility of competing packing modes. To this end, we investigated a new Pt(II) complex with S-chiral chains and amide groups (Figure 1).[4] Detailed spectroscopic, microscopic and theoretical studies allowed us to identify two coexisting stable assemblies in solution with different molecular packing (slipped *vs*. pseudo-parallel) that do not interconvert over time. These findings in supramolecular polymers bear close resemblance to the phenomenon of *concomitant packing polymorphism* that has been observed in crystals.

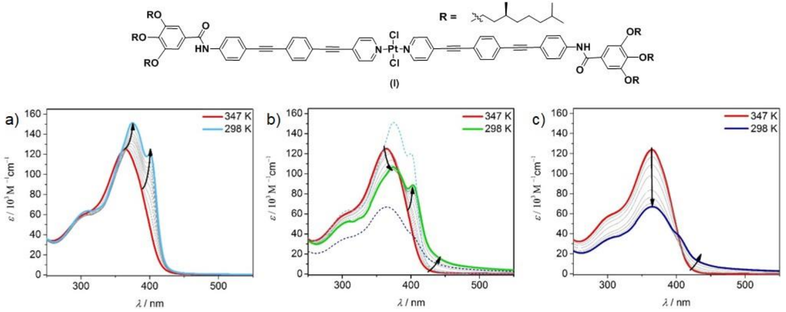

Figure 1. Chemical structure of Pt(II) complex (I) and variable temperature UV-Vis (100 □M) in methylcyclohexane with a cooling rate of a) 2K min^{-1} , b) 0.5 K min^{-1} and c) 0.1 K min^{-1}.

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SPNA-IL-06

Regulated Assembly of Multicomponent Supramolecular Polymers

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Abstract

Aqueous self-assembly of molecular building blocks into ordered architectures, polymers and materials opens exciting avenues for fundamental developments in nanoscience and applications in biomedical technologies, optoelectronics and catalysis (*Chem. Rev.* **2016**). I will present my group's recent efforts in controlling peptide and glycopeptide supramolecular polymerisations in solution and off surfaces (*Angew. Chem.* **2016**, *Angew. Chem.* **2018**), as well as recent efforts on self-assembled Au(I)-metallopeptides (*Chem. Commun.* **2015**, *Chem. Commun.* **2018**, *J. Am. Chem. Soc.* **2018**).Inspired by protein functionality in their biological setting, we have produced electrostatic- and redox-regulated supramolecular polymerisations in water *(Angew. Chem.* **2013***, Chem. Eur. J.* **2015***, Polym. Chem.* **2015***).* The synthons are based on β-sheet encoded anionic and cationic peptides that form anisotropic supramolecular copolymers with a nanorod-like morphology. The materials are designed for on-off polymerization in response to pH-, as well as redox-triggers. The pH-triggered monomer-polymer transition is simply tuned via thermodynamically controlled comonomer affinities, whereas kinetically controlled assemblies are achieved only by coupling multiple equilibria through enzyme catalysed redox-processes, leading to temporal resolution in aqueous supramolecular polymerisations (Fig. 1, *Angew. Chem.* **2017**).Balancing out positive non-covalent interactions with repulsive forces produces well-defined peptidic nanorods (*Chem. Eur. J.* **2015**, *Macromolecules* **2017**). In view of recent reports that anisotropic shapes in the design of biomedical carrier materials outperform conventional isotropic structures, we are particularly interested in the development of supramolecular multifunctional glycopeptide materials and their biomedical applications.

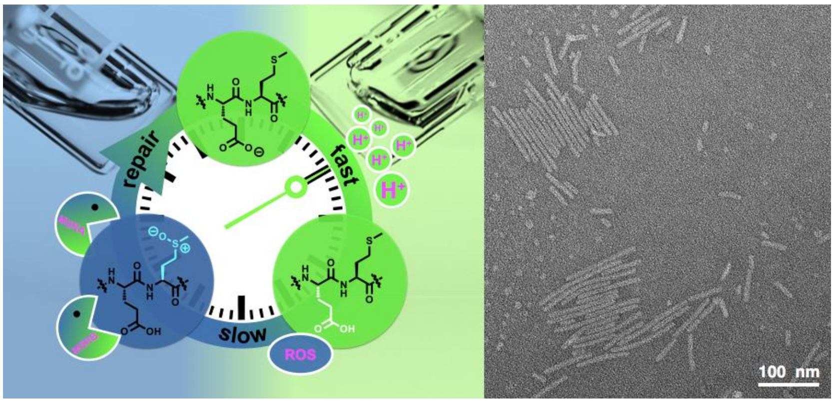

Figure 1. Transient Hydrogels Mediated by Redox-Responsive Supramolecular Polymerisation

SPNA-IL-07

Responsive soft materials self-assembled from cyclodextrins

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Abstract

Self-assembly is emerging as a superior method to prepare adaptive and responsive nanomaterials. The structure and function of these materials is entirely determined by the dynamic and weak interactions of the constituent molecular “building blocks” of the material. Since the inherent interactions are weak, these versatile materials readily respond to even small changes and stimuli in their environment. Moreover, these materials are biomimetic and contain large amounts of water, so that application in biomedical technology can be foreseen. This lecture will highlight self-assembled nanocontainers based on cyclodextrins that respond to various external stimuli. Amphiphilic cyclodextrins form bilayer vesicles in aqueous solution and the surface of these vesicles can be functionalized using host-guest chemistry. Shear-thinning hydrogels result if the cyclodextrin vesicles are mixed with adamantane-functionalized polymers, which act as supramolecular cross-linkers. Photo-triggered payload release from supramolecular hydrogels is enabled by incorporation of azo-modified peptides. Polymer-shelled vesicles and polymer nanocontainers are obtained if the cyclodextrin vesicles are decorated with adamantane-terminated poly(acrylic acid), which can be cross-linked with diamines. Recently, we have also shown that this polymer shell is redox-responsive if the cross-linker contains a disulfide. The resulting nanocontainers can deliver cargo into cells. Magnetoresponsive soft materials are obtained by supramolecular incorporation of magnetite nanoparticles into vesicles and gels. Finally, vesicles can be decorated with luminescent Ir-complexes and used as contrast agents.

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SPNA-IL-08

Design of gyroid-structured polymer films based on polymerizable bicontinuous cubic liquid crystals

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Abstract

Infinite periodic minimal surface (IPMS) is a unique surface with three-dimensional periodicity and continuity (Fig. 1). We expect that construction of IPMS with proton conduction ability will be a potential approach for creating ideal electrolytes for fuel cells.

Recently, we have focused on the development of molecular technology for creating IPMSs with a nano-sized cubic lattice, that is to use the self-organization of "*liquid crystals*". Nanostructured liquid crystals are a class of liquid crystals forming well-ordered molecular assemblies through nano-segregation of incompatible molecular segments. A variety of nanostructures with one-, two- or tree-dimensional periodicity can be obtained depending on the molecular design of amphiphilic liquid crystals.[1] These liquid crystals have been used for new functional materials. Recently, we have strongly interested in bicontinuous cubic liquid crystals forming an IPMS. Although these bicontinuous cubic liquid crystals are known to be a class of liquid crystals that are difficult to design, we have succeeded in designing liquid-crystalline materials exhibiting bicontinuous cubic phases by using various ionic liquids.[2-5] In this presentation, I will talk about our molecular design for liquid-crystalline molecules forming IPMSs. In addition, our strategy to convert these fluidic liquid-crystalline materials to polymer materials with keeping the original nanostructures will be shown.

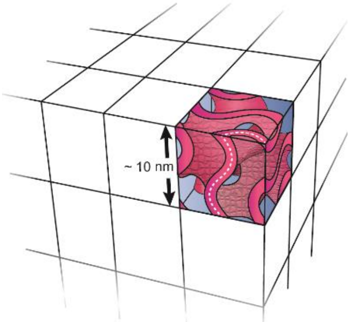

Fig1. An illustrated image of gyroid minimal surface

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SPNA-IL-09

Self-Assembled Ion Channels for Transmembrane Cl^- Transport

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Abstract

Transport of ions across biological membranes is facilitated by ion channel proteins. Chloride channels are involved in processes such as transepithelial salt transport, acidification of cellular compartments, cell volume regulation, etc.[1] Recent studies showed that artificial chloride transport into cells leads to apoptosis. Thus, it is of prime importance to develop biomimetic systems to facilitate transport of the ion. In this lecture, I will present our recent research approaches to design self-assembled transmembrane chloride channels. Recently, we have designed bis-alkyl substituted fumaramides and realized that the self-assembly of fumaramides largely depend on the nature of the end-groups. The bis-cyclohexyl substituted fumaramides give intermolecular hydrogen bonded barrel-rosette self-assembly in the lipid bilayer membrane and allow selective chloride transport.[2] On the other hand, the bis-cholate substituted fumaramides give intermolecular hydrogen bonded barrel-stave self-assembly to facilitate the transport of chloride ions.[3] We have also studied the hydrogen bonding of 1,2-dihydroxy compounds for ion channel formation. A bis(ketal)-protected mannitol derivatives form trimeric rosettes with the help of anions and these rosettes further self-assemble into ion channels.[4] Chloride transport through this channel occurs through a relay-based anion hopping process. A bis(1,2-dihydroxyl) based system on the other hand form dimeric rosettes which then form chloride channels in the membrane.[5] These hydrogen bonded supramolecular channels showed apoptotic cell death by perturbing the chloride homeostasis of cells. We are now working to apply synthetic chloride transport systems to target cancer.

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SPNA-IL-10

Nano-Patterned Polyelectrolyte Multilayers

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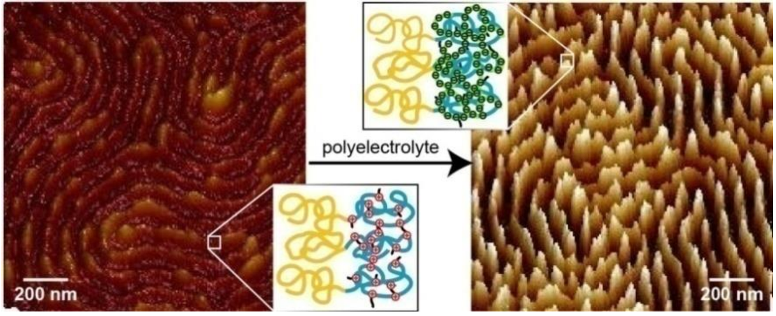
Abstract

Nano-patterned materials exhibit unique properties, such as increased surface area and morphology-dependent response. However, obtaining nanoscale patterns usually requires the involvement of electron beam lithography, which is limiting when device-scale patterns (typically spanning square centimeter areas) are sought. The presentation will describe a modular approach for the construction of *nano-patterned* polyelectrolyte multilayers. This approach utilizes the surface patterns that are formed spontaneously in thin films of block copolymers as templates, which guide the assembly of polyelectrolytes using electrostatic layer-by-layer deposition. The presentation will discuss the fundamentals of selective polyelectrolyte adsorption on confined nano-domains and will delineate potential applications.



AFM images showing a block copolymer pattern before and after selective deposition of a polyelectrolyte (height scales: left image: 5 nm; right image: 15 nm).

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SPNA-IL-11

Sequence Controlled Supramolecular Block Co-Polymerization

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Abstract

Study of supramolecular polymers has entered an era that demands assemblies with more structural and dynamic control. Living supramolecular polymerization has emerged as a synthetic strategy to construct supramolecular assemblies with well-defined structure and dispersity. On the other hand temporal control over dynamic materials is now being extended to non-equilibrium regime. While both of these controls are desirable, strategies to achieve them have been mostly chemically distinct. The synergy between structural and temporal control is important for the advent of supramolecular polymers to be employed as functional adaptive materials. To gain this symbiosis it is imperative that common strategy is sought. Looking into the biological realm can provide a necessary inspiration for the conundrum. We, in our laboratory, are driven by this philosophy and are currently trying to develop and study a chemical-fuel controlled supramolecular system that not only follows living supramolecular aggregating regime but also can be regulated temporally through various molecular cues. We have attempted to create thermodynamically stable dormant states for the monomers, which can be triggered by various chemical/bio-fuels to achieve a temporally modulated supramolecular polymerization. This talk describes our efforts in designing multi-component supramolecular block co-polymers (Linear organic heterostructures) via kinetically and thermodynamically controlled Supramolecular Polymerization (unpublished results). These unique structures made from semi-conducting monomers would be interesting materials to control exciton migration, axial p-n junctions and many other new functional properties.

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SPNA-IL-12

Functionalized Nucleosides as Supramolecular Synthons and Probes

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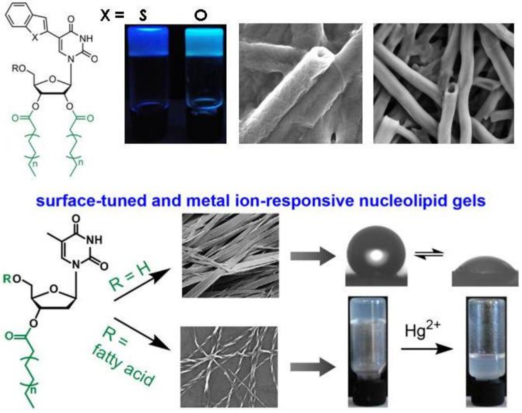
Abstract

Remarkable recognition and precise folding properties have rendered nucleic acids as useful supramolecular synthons for constructing programed architectures for applications in nanotechnology. However, scalability and fabrication of nucleic acid nanostructures still remain a major challenge. In this context, the basic components of nucleic acids, nucleosides and nucleotides, when appropriately modified can serve as useful supramolecular synthons and probes. In this presentation, a simple design strategy to construct a new family of supramolecular nucleolipid synthons will be presented. The nucleolipids are made of a heterobicycle-conjugated nucleobase, which serves as the head group and environment-sensitive fluorophore, and classical fatty acid acyl chains attached to the sugar residue as the amphiphile tail. Depending on the type of modification on the base and sugar residues the nucleolipids self-organize into supramolecular gels, which show aggregation-induced enhanced fluorescence, self-sorting behaviour and surface-switchable properties.[1,2] In the second part of the talk, development of a nucleotide toolbox for labeling nucleic acids by using bioorthogonal reactions like azide-alkyne cycloaddition, Staudinger ligation and metal-catalyzed reactions will be presented. This post-polymerization labeling method provides access to nucleic acids labeled with variety biophysical probes suitable for imaging nucleic acids in cells.[4,5]



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SPNA-IL-13

Supramolecular polymeric materials functionalized by host-guest interactions and its mechanical properties

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Abstract

Molecular recognition chemistry and supramolecular chemistryhave received much attention, owing to their effects on catalytic activity, molecular switches, and materials. Stimuli-responsive supramolecular polymers is relevant not only for biological functions but also for a range of other applications. Our research group has employed cyclodextrins (CDs) as host molecules. In this presentation, I would like to introduce our studies to realize sol-gel switching, self-healing, adhesion control, and contraction-expansion properties through the formation of inclusion complexes with CDs.**Adhesion and self-healing material:**First, adhesion between the host hydrogel with βCD and the guest hydrogel with an adamantyl (Ad) group was investigated. The βCD hydrogel selectively adheres to the Ad guest hydrogel. Next, we prepared effective self-healing materials based on βCD and Ad units. When two cut surfaces were brought into contact, the two pieces adhered. The adhered materials showed almost complete recovery of the initial material strength. The recovery ratio of the rupture strength increased with adhesive time. Interestingly, only cut surfaces showed a self-healing property, whereas uncut surfaces did not. **Photoresponsive materials**: Two structural approaches may realize supramolecular actuators through host–guest interactions: a method with a linear main chain and one with a side chain in the polymer structure. We have prepared photo responsive supramolecular actuators by integrating host–guest interactions on the polymer side chains. Another supramolecular hydrogels containing CD-based [c2]daisy chains as crosslinkers contract and expand through photoresponsive sliding motions of the [c2]daisy chain.

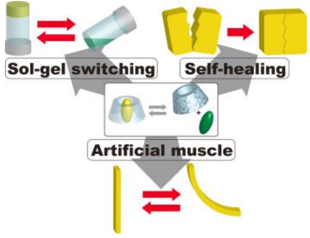

Figure 1. Supramolecular materials based on host-guest interactions with cyclodextrins (CDs).

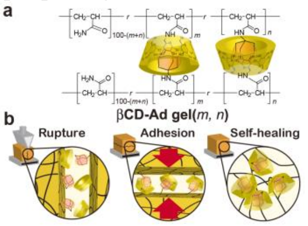

Figure 2. Self-healing materials based on host-guest interactions.

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SPSI-IL-14

A water harvesting polymer via unconventional solid-state synthesis

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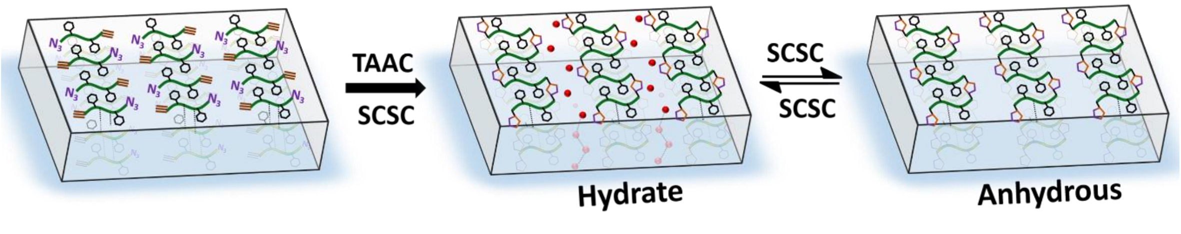
Abstract

Many natural proteins or polypeptides (e.g. silk, wool, keratin, collagen, soy protein *etc*.) are useful materials. However, they are prone to chemical or enzymatic degradation due to the lability of peptide linkages and hence there is a lot of interest in polypeptide mimics having robust non-natural linkages as peptide surrogates.[1] 1,2,3-Triazole motif has been established as a stable bio-isostere of peptide linkage.[2] Topochemical Azide-Alkyne Cycloaddition (TAAC) reaction, thermal 1,3-dipolar cycloaddition of proximally placed azide and alkyne motifs in the crystal to form triazole, has proven to be an efficient method for the synthesis of various triazole-linked biopolymer mimics.[3] Small peptides modified with azide and alkyne that form β-sheet like alignment in their crystals could be employed as precursors for TAAC reaction to form pseudoproteins.[4] We have designed the diphenylalanine derivative, N_3-Phe-Phe-$NHCH_2CCH$ for its topochemical azide-alkyne cycloaddition (TAAC) polymerization. This dipeptide adopted β-sheet arrangement as designed, in its crystals, but the azide and alkyne were not fitly aligned for their topochemical reaction. However, the voids present around these groups allowed them to attain a reactive geometry upon heating and their consequent TAAC polymerization to a pseudoprotein in a single-crystal-to-single-crystal (SCSC) fashion. This motion led to the creation of channels in the product-crystal and it absorbed water from the surroundings to fill these channels as H-bonded water wire. The pseudoprotein undergo reversible hydration/dehydration in SCSC fashion many times under mild conditions; hydration at low relative humidity and dehydration at low temperature. Vapor sorption analyses suggest that this fully-organic polymer might be useful as energy-efficient desiccant material for controlling indoor humidity and for water harvesting from atmosphere.[5]



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SPNA-IL-15

Rational Design of Stimuli-Responsive Protein Complexes

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Abstract

Self-assembly of proteins into higher order super-structures is ubiquitous in biological systems. Genetic methods comprising both computational and rational design strategies are emerging as powerful methods for design of synthetic protein complexes with high accuracy and fidelity. Although useful, most of the reported protein complexes lack dynamic behavior that may limit their potential applications. On the contrary, protein engineering using chemical strategies offers excellent possibilities for the design of protein complexes with stimuli-responsive functions and adaptive behavior. However, designs based on chemical strategies are not accurate and therefore yield polydisperse samples that are difficult to characterize. In this seminar, I will talk about our lab efforts to construct protein complexes through bottom-up approach using a supramolecular chemical strategy. Micelle-assisted activity-based protein labeling technology has been developed to synthesize library of facially amphiphilic synthetic proteins, which self-assemble to make protein complexes through hydrophobic interaction. The methodology is amenable for the synthesis of protein complex libraries with molecular weights and dimensions comparable to naturally occurring protein cages. The designed protein complexes display very rich structural diversity, oligomeric states, sizes and surface charges that can be engineered through macromolecular design. The broad utility of this method is demonstrated by design of most sophisticated stimuli-responsive systems that can be programmed to assemble/disassemble in a reversible/irreversible fashion using pH or light as a trigger.

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[1] Britto S Sandanaraj, M. Mohan Reddy, Pavankumar Bhandari, Sugam Kumar, Vinod K Aswal*Chem. Eur. J.* 10.1002/chem.201802824

SPNA-SL-01

Programming Macromolecular Assembly by Orthogonal Non-covalent Interactions

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Abstract

Precise organization of synthetic macromolecules into well-defined nanostructures is relevant in various applications including biomedicine, organic electronics or catalysis. Nature displays examples of biopolymers such as proteins that utilize directional interactions such as H-bonding as the primary tool for adopting well-defined conformation, which is essential for their incredible complex functions. To emulate the structural elegance and functional diversity of biological system, self-assembly of foldamers, amphiphilic block copolymers and various other exciting hybrid materials such as polymer-peptide conjugates have been studied with great interest. However, introduction of specific directional supramolecular interactions into polymeric scaffolds and thereby investigating their impact in programming macromolecular assembly is still at its infancy. In the recent past, halogen(X)-bonding interactions have gained renewed interest particularly in the field of crystal engineering, while little is known about their influence in solution states. It is envisaged that orthogonal self-assembly (systems where more than one type of molecular interaction operates independently) of H- and X-bonding motifs can be an interesting combination for introducing structural complexity in simple polymeric systems. With this idea, we have studied the co-assembly of a polymeric halogen bond (XB) donor with an XB accepting aromatic discotic molecule, which can grow into a 1D supramolecular polymer (SP) on its own by 3-fold H-bonding and pi-stacking. Concomitantly, orthogonal X-bonding plays a decorative role by organizing the macromolecules or other functional molecules into the periphery of the SP. Such unique hybridization of a covalent polymer with its supramolecular analogue by orthogonal non-covalent interactions creates higher order structures in solution phase with unprecedented stability. This concept of orthogonal self-assembly and its generalized implications in macromolecular organization will be the topic of the oral presentation.

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SPNA-SL-02

Glucose Base Materials Synthesis and Their Applications

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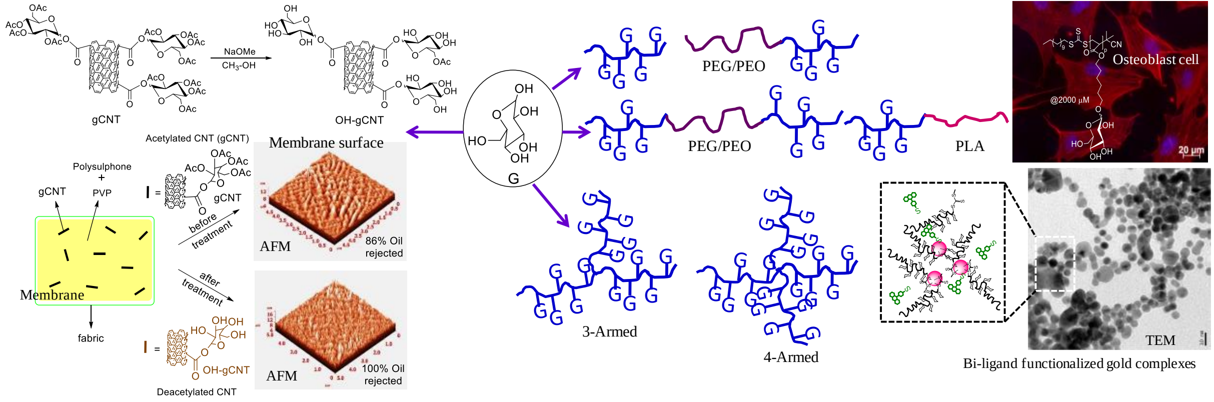
Abstract

Design and synthesis of various glucose based material/polymer architectures have attained a significant interest in current chemical technology, biology and medicine due to their multi ligand nature, hydrophilic character, possibility of further chemical modification, better biocompatibility and ability to mimic glycoproteins in the biological systems. We have synthesized glucose based carbon nanotubes (gCNTs) and having different pendant chain length (meth)acrylate glucose, galactose and manose monomers by using protection and selective deprotection chemistry. Using these monomers, we prepared well-defined glycopolymers such as linear, 3- and 4-armed polymers and di- and tri-block copolymers with different pendent alkyl chain lengths by using living radical polymerization processes. We have employed these gCNTs in fabrication of UF membranes for oil separation from industrial oil-water emulsions and deacetylated water soluble macromolecular archetectures were prepared to understand glucose moieties response on mice and human osteoblast cells in terms of cell adhesion, viability and proliferation. Further, these polymer architectures were used to achieve bi-ligand functionalized multivalent glycopolymer-gold nanoparticle complexes. Details of the synthetic protocols, characteristics and achievements of these novel glucose based materials/polymers will be discussed in our presentation.



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SPNA-SL-03

Design, Synthesis and Folding of Sequence-Controlled Polymer Chain

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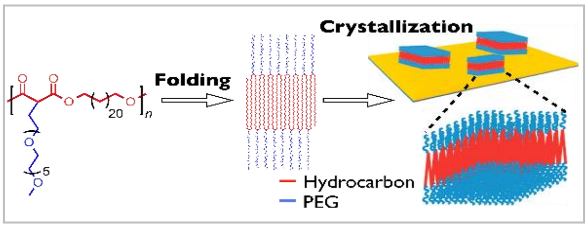
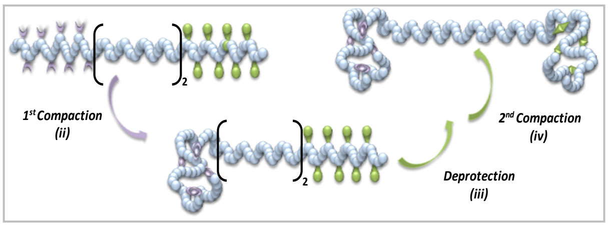
Abstract

The synthetic polymers have revolutionized our modern life in such a way that we can´t imagine spent a day without using it. The successful story of polymers is mainly due to its light weight, durability, design-flexibility and cheap price. For the applications purposes, apart from replacing the metals, woods or stones, quite often the inspiration for the design of manmade polymers comes from the Nature. In this regard, the sources of bio-inspiration are very diverse and occur at different scale i.e. macroscopic, microscopic and molecular level. We already have remarkable progress on mimicking strategies at the macroscopic level, for example many researchers have mimicked the superior mechanical, optical, self-repair, stimulus-responsive, or surface properties of biomaterials using synthetic polymers and to some extent at nanoscale as well by self-assembly of block copolymers.[1] However, such mimicry at molecular level is most challenging mainly due to the gap between structurally-defined biopolymers (sequence-defined primary structure) such as nucleic acids, proteins, and polysaccharides and polydisperse synthetic polymers prepared by classical polymerization techniques such as chain-growth or step-growth polymerizations. Quite recently, there has been a surge interest in developing sequence-controlled polymers that are inspired by Nature, but that are chemically different from proteins and nucleic acids.[2] In my presentation, I will discuss our approaches for this emerging field of sequence-controlled polymerizations.[3a,b] Apart from the synthesis, I will also discuss the microscopic and molecular level folding of such sequence-controlled polymers by using either non-covalent interaction or covalent linkages. In a slightly different context, I will also demonstrate the potential applications of sequence-defined polymer for information storage purposes.[4]





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SPNA-SL-04

Anti Amyloidogenic Activity of Novel Tryptophan-Cardanol Conjugates

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Abstract

Amyloids are considered as remarkable biopolymers and they are formed from proteins with very different amino acid sequences; the individual proteins constituting the amyloid fold predominantly into a β-sheet structure. The formation of the amyloid fibrils occurs through non-covalent interactions between primarily the β-sheets, causing the monomers to stack into fibrils. The aggregation of α-synuclein is believed to play an important role in Parkinson's and other neurodegenerative diseases. A-synuclein is an abundant brain protein of 140 aminoacids and is naturally present in a natively unfolded state due to the very high net (negative) charge at neutral pH and low intrinsic hydrophobicity of the molecule. In this study, our aim is to investigate the effect of an indole based molecule that could act as inhibitors for synuclein fibrillation. The tryptophan introduces indole moiety in the molecule (Trp-PDP-Trp). The study will exploit the effect of this newly developed molecule on the anti-fibrillation and the disaggregation behaviour of α-syn/α-syn fibrils. The amine groups along the termini of the tryptophan could offer hydrogen bonding interactions to the amino acids of synuclein. The indole N-H also could offer N-H---π hydrogen bonding with aromatic aminoacids of the protein. The PDP offers a vibrant three dimensional conformation for effective binding to the protein. The hydrophobic central PDP could reinforce hydrophobic interactions with amyloid peptides as well. All these factors together could influence the normal fibrillation process in α-synuclein. The tryptophan-hexyl-tryptophan (Trp-hexyl-Trp) has also been synthesized as control to understand the role of pentadecyl phenol spacer as compared to a linear spacer.

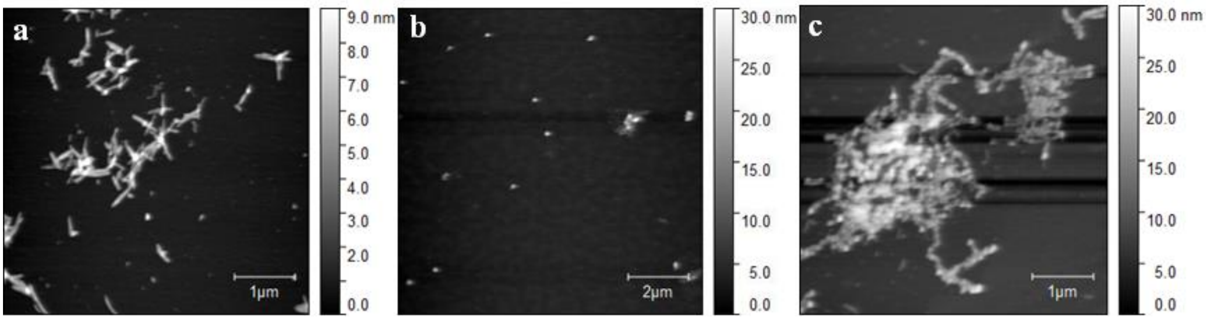

Figure : Morphology of (a) α-synuclein fibrils formed at a concentration of 50 μM at pH 7.4 in tris buffer incubated for 7 days with seeding(b) α-synuclein fibrils inhibition in presence of Trp-PDP-Trp (molar ratio 1:1), (c) α-synuclein fibrillation in presence of Trp-Hexyl-Trp (molar ratio 1:1)

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SPNA-SL-05

Self-assembled Cellulosic Microvesicles and Tubes for Drug Delivery

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Abstract

Polysaccharide based nanostructures are finding increased interest in chemotherapy and controlled delivery of drugs owing to the biocompatibility and non-toxic nature. Cellulose and hemicelluloses modified with natural molecules showed self-assembly in solvents into vesicular or tubular micro/nano morphologies. Nano-fibrillated cellulose modified by controlled regio-selective amidation with oleylamine (OA) showed self-assembly into unilamellar vesicles of 5-6 μm diameters with a wall thickness of 200-400 nm in tetrahydrofuran (THF) at 2.5 mg mL^{-1} attributed to the folding into bilayers driven by long *cis*-unsaturated aliphatic chains in polar aprotic solvents stabilized by hydrogen bonded interactions whereas the modified xyloglucan system showed tubular assembly owing to the branched structure. These results indicated a novel strategy to tailor the micro morphologies formed by self-assembly of polysaccharides by fine tuning the structure of the polymer architecture for possible applications in biomedical field.

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SPNA-SL-06

Supramolecular self-assemblies of AIE active organic small molecules

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Abstract

Machinery of life was developed biologically in long-term evolutionary processes, and there is no protocol about the experiments, which finally succeeded. Chemists have been successful with synthesis, isolation and analysis but not with the reproduction of the working molecular apparatus. The introduction of yoctowells as a surface-engineered phenomenon allowed us to address one of the great challenges on nanoscale level – the separation, containment and manipulation of individual molecules and allow studying molecular interactions. The primary motivation to work with such membrane yoctowell cavities instead of proteins was strain after simplicity, which would make it possible to answer some simple biological questions experimentally on nanoscale level, which are difficult to approach in complex biological modules.

We recently became interested in the design and synthesis of novel TPE luminogens and their supramolecular self-assembly to produce variety of nanostructures such as star shaped, controlled helical, highly efficient near-IR solid emitter, metal organic framework, and use in various applications such as sensing of organic volatiles, pH sensor, bioimaging, and donor-acceptor system for solar cells.[1-5] We have shown for the first time that achiral TPE molecule bearing alkyl chains can induces chirality in supramolecular helical structures, and helicity shown to be controlled use of odd and even carbon chains. We have also shown that use of dumbbell shape TPE having long alkyl chain produced flower-like morphologies. This talk will focus on discussion of innovative and cutting-edge research program on smart functional material on the nanoscale level and their applications such as molecular recognition, environmental (purification, separation), energy (solar cells), and drug delivery.

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SPNA-OL-01

Anti-solvent inducedspacio-temporal evolutionof cellulose spherulites in cellulose/AmimCl solution

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Abstract

The self-assembly of polymer molecules into spherulites is commonly observed duringpolymer crystallization. Recently there have been reports on the formation of spherulites from concentrated cellulose/ionic liquid solutions in the presence of an anti-solvent.[1,2] This study involves investigation of cellulose spherulites in concentrated microcrystalline cellulose (MCC)/1-Allyl-3-methyl imidazolium chloride (AmimCl) solutions due tocontrolleddiffusion of water. A film of 20 wt% MCC/AmimCl solution confinedbetween two coverslips,is exposed to water such that the diffusion of water occurs only through the edges. All experiments are conducted at specific temperature and humidity. The greater affinity of AmimCl to water leads to local rearrangement of cellulose moleculescausing the self-assembly of cellulose molecules to form spherulites. The effect of film thickness on themorphology and kinetics of cellulose spherulites growthisstudied by means of polarization optical microscopy (POM). Irrespective of the film thickness, the diameter of the spherulites is observed to grow linearly during the early stages of crystallization, followed by a plateau.While positive spherulites of ~500 μm average diameter formed in thinner films(~100 μm),relatively smaller spherulites of average diameter ~300 μm are formed when the film thickness increased to ~500 μm.In the latter, secondary growth of *shish-kebab*-like morphologies and elongated spherulites, extending from the edges of the film to the inner regions, are observed at different planes, probably due to the relatively faster diffusion of moisture. The temperature induced melting behavior of cellulose spherulites is also studied.

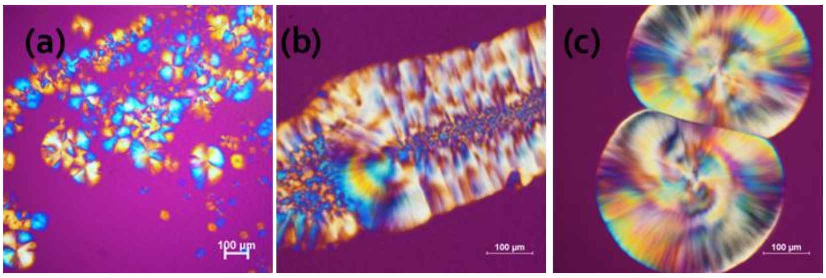

Figure 1(a) secondary growth and (b) shish-kebab like morphologies found in thicker film and (c) shows large spherulites found in thinner film.

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SPNA-OL-02

Chiral Amino acid Functionalized PolyfluorenesSupported on Mesoporous Anodic Aluminium Oxide (AAO) Membranes for Enantioselective Separation

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Abstract

Functionalization of conjugated polymers with chiral moieties like the amino acids are known to confer homochirality to the parent conjugated polymer. Homochiral materials have the ability to perform chiral sensing as well as enantioselective separation. Although asymmetric synthesis is one of the most common methods reported for obtaining chiral materials (1), they have the limitation that high enantiomeric purity can be acheived only for exceptionally enantioselective reactions. In this regard, protected L-glutamic acid appended polyfluorene was shown to achieve efficient heterogeneousenantioselective separation and chiral sensing of a widevariety of substrates from their aqueous racemic mixture (2).

In this work we present optically active polyfluorenes bearing protected chiral amino acids (D & L Aspartic acid) as pendant groups. Mesoporousanodic aluminium oxide (AAO) membraneswith 200 nm pore size were used as support for the immobilization of these chiral amino acid appended polyfluorenes.D or L Aspartic acid appended polyfluorene dissolved in tetrahydrofuran (THF) as solvent was passed through the alumina membrane under suctionto generate enantioselective chiral porous membranes. The chiral polymer immobilized alumina membranes demonstrated selective uptake and high enantiomeric separation of D and L phenyl alanine as a representative chiral molecule from their equimolar racemic mixture.Circular dichroism (CD) spectroscopy was used to demonstrate the enantioselective separation.

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SPNA-OL-03

Fluorescent Biodegradable Block Copolymer Nano-assemblies for Bioimaging and Delivery

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Abstract

Biodegradable block copolymer nano-scaffolds are emerging as important area of research for various applications in drug and gene delivery, bio-imaging and tissue engineering in cancer treatment. The thesis work is emphasized to engineer new p-conjugated fluorescent polycarprolactone (PCL) block copolymer nano-assemblies as efficient intracellular enzyme-responsive nano-carriers for both drug delivery and bio-imaging in cancer cells. New carboxylic substituted caprolactone monomer was synthesized through tailor-made approaches and employed in controlled ring opening polymerization to yield narrow molecular weight carboxylic functional polycaprolactone block copolymers. Hydroxyl functionalized p-conjugated oligo-phenylenevinylene (OPV) chromophore was designed and it was incorporated in the substituted polycaprolactone block copolymer via ring opening polymerization. These unique triple block nanoparticles showed excellent stability and selective rupturing in the presence of lysosomal esterase enzyme. *In vitro* studies indicate that these blue fluorescent block copolymers self-assembled into PCL nano-particles for delivery of doxorubicin.[1] New fluorophore-tagged biodegradable polycaprolactone (PCL) block copolymer FRET-probe was also developed for intracellular imaging in cancer cells.This blue-luminescent OPV-PCL triblock self-assembled as < 200 nm spherical nanoparticles (FRET donor) and it encapsulated water insoluble Nile red (NR, FRET acceptor) to yield OPV-NR FRET probe. Selective photo excitation of OPV chromophore in block copolymer nano-assemblies enabled the excitation energy transfer from the OPV to NR and facilitated the efficient FRET process in aqueous medium.[2] This approach was expanded to make new classes of red-luminescent PCL block copolymers using perylenebisimide as chromophore. These red-luminescent biodegradable nano-assemblies were employed for cellular imaging in cancer cells. Additionally, the carboxylic PCL block copolymer provided unique opportunity to address the problem of Pt-drug resistance in breast and ovarian cancers. These perylene based tri-block PCL-copolymers were complexed with cisplatin aquo complex to produce PCL-cisplatin produgs. The triple block nanoparticles are stable under physiological condition and selectively degrade in the presence of lysosomal esterase enzyme to deliver drug.

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SPNA-OL-04

Fuel-Driven Kinetically Controlled 1D and 2D Living Supramolecular Polymerization

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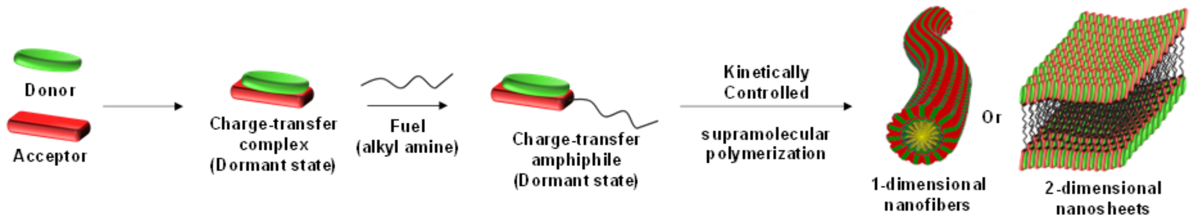
Temporally controlled growth[1] has aroused interest in the scientific community as a tool to control the structural properties[2] of supramolecular polymers such as dispersity and size and functions via programmable transient lifetime.[3-4] Research so far has tended to focus on systems showing such a kinetic control rather than building novel design strategies as a generic approach. The current challenge involves the creation of novel dormant states that can be actuated via a fuel for a kinetically governed supramolecular polymerization for a wider range of molecular designs.[1] Recently, our group has ventured to create novel thermodynamic dormant state[5] that is activated by chemical fuel, similar to natural systems, to attain controlled dispersity and size in 1 and 2-dimensions. In our approach, we designed a coronene tetrapotassium salt (CS) or pyranine (PN) donor and methyl viologen benzaldehyde (MVCHO) acceptor to form a non-assembling CT complex. The aldehyde group act as the reactive center for the nucleophilic reaction of amine to form imine bond that converts a non-assembling dormant CT complex to an activated amphiphilic structure that can spontaneously undergo supramolecular polymerization.. Interestingly, the nature of amine added renders the specific property to the supramolecular motif thus formed. The imine bond is dynamic covalent bond and responsive to pH, hence by exploiting its pH dependency, the kinetics of imine bond formation and therefore self-assembly was controlled for a 1- or 2-dimensional supramolecular polymerization. The retarded nucleation-elongation growth also renders a control over dispersity and size via a living supramolecular polymerization.



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5) Unpublished results

SPNA-OL-05

Influence of Metal Coordination and Light Irradiation in Hierarchical Self-Assembly Processes

Kalathil K. Kartha,[1] Naveen Kumar Allampally,[2] Antiope T. Politi,[3] Deepak D. Prabhu,[4] Rodrigo Q. Albuquerque,[3] Shiki Yagai[4] and Gustavo Fernández[1*]

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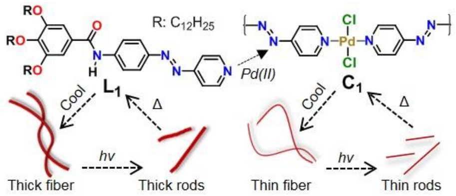
Abstract

Hierarchical organization of light-responsive π-systems are widely explored because it enables the modulation of the functional properties associated with the self-assembly pathwayupon photoisomerization. However, light responsive metallosupramolecular assembly is rare because the introduction of metal result in a rigid system thereby making it dormant to light. Herein, self-assembly and photo responsive behavior of a π- ($\mathbf{L_1}$) and corresponding metal (Pd)-π system ($\mathbf{C_1}$) has been elucidated with a detailed mechanistic insight. Target ligand $\mathbf{L_1}$ undergoes complex time-, temperature- and concentration-dependent self-assembly pathways driven by amide H-bonding leading to fiber-like associates via various intermediate structures. Irradiation with UV light leads to a reversible transition from long to short fibers, leading to a reversible sol-to-gel transition. On contrary, Pdcomplex $\mathbf{C_1}$with amide functionality (N-H) and Cl(-Pd) directs a novel N-H…Cl driven assembly[1]leading to the attenuation of the supramolecular growth into short thin fibers. More interestingly, we monitored a reversible transition of long thin fibers to short thin fiber upon irradiation of $\mathbf{C_1}$ with UV light. Thus, a reversible long to short thin fiber transformation leading to a sol-gel transition of a metallosupramolecular assembly by UV light is demonstrated. The mechanism of self-assembly and photo responsive behavior of a π- and corresponding metal (Pd)-π system (Scheme 1) has been elucidated with UV-Vis, 1D and 2D NMR,AFM investigations and comprehensive semi-empirical calculations.[2]In conclusion, these results shed light on the effect of light and metal incorporation on the self-assembly pathway of a discrete photoresponsive π-system.



Scheme 1. Self-assembly and photoresponsive behavior of $\mathbf{L_1}$ and $\mathbf{C_1}$.

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Abstracts for Invited, Short and Oral Lectures
Under the Theme
Bio-Inspired and Bio-derived Polymers (BIBDP)

BIBDP-IL-01

Non-isocyanate routes to biobased polyurethanes: some recent advances

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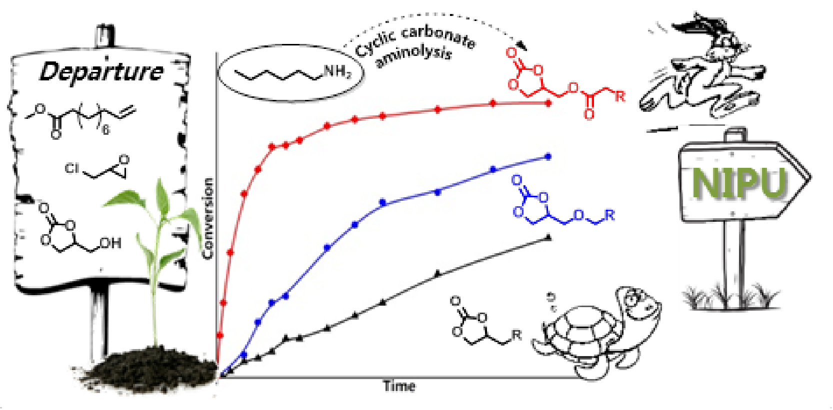
Abstract

Polyurethanes (PUs) are specialty polymers found in many markets, such as coatings, paints, elastomers, adhesives and, of course, foams. Nonetheless, the current industrial pathway for the synthesis of conventional polyurethanes involves the use of toxic isocyanates to react with polyols. The combination of fossil resources price variations together with environmental and health concerns pushes scientists to develop green chemistry strategies in the course of polymer synthesis. To that purpose, the development of bio-based monomers and the use of safe chemicals and processes are two main challenges that we address in this study. Indeed, among the routes to non-isocyanate PUs, the polyaddition between a bis-cyclic carbonate (bisCC) and a polyamine, leading to poly(hydroxyurethane)s, PHUs, bearing pendant hydroxyl groups linked to the polymer skeleton, is quite promising. Nevertheless, this pathway still presents some limitations such as rather low reaction kinetics and the low PHUs' molecular weight generally obtained.[1]Strategies investigated at the Laboratory to overcome such limitations, that include the design of 'activated' cyclic carbonates[2] and the use of reactive extrusion process[3] will be discussed in this presentation.



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BIBDP-IL-02

Sustainable Methods for Separating Chitin from Seafood (Crustacean Shell) Waste

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Abstract

Two kinds of polysaccharides are common in nature: cellulose, characteristic of the plant kingdom, and chitin, found in members of the animal kingdom. Together they are the most abundant organic materials in nature. About 10^{10} to 10^{12} tons of chitin is synthesized per year by arthropods (insects & crustaceans), molluscs and fungi. The main biological function of chitin is structural. Chitin as well as oxygen (50 to 85 % of what is available in the globe) is produced by phytoplankton's using sunlight, water and other mineral resources available in water. One species of plankton alone produces 100 billion tons of chitin per year.Chitin is essentially □-1,4- linked polymer of 2-acetamino-2-deoxyglucopyranose and constitutes significant part of crustacean (shrimp, prawn, crab, lobster, etc.) shells.More significantly, chitin contains a nitrogen atom per repeat unit and can be an excellent source for the production of a series of nitrogen-containing organic chemicals in a sustainable manner.[1,2] Few important chemicals such as N-acetyl glucosamine[3], N-containing amino sugar alcohol and acetyl monoethanolamine have already been synthesized from chitin.[2,4,5] Every year, some 6 million to 8 million tonnes of waste crab, shrimp and lobster shells are discarded. For example, about 40 % of the shrimp is edible and remaining 60 % account for the processing discards, causing diverse environmental problems. In some countries, waste shells are often just dumped in landfill or the sea.Crustacean shells are 20–40 % protein, 20–50 % calcium carbonate and 15–40 % chitin.[6]In recent years, chitin and its derivatives, being biodegradable and non-toxic, have generated interest in various fields such as biomedical, pharmaceutical, food and environmental industries.[7] Similarly, calcium carbonate, the other component present in the shell, has extensive applications in the pharmaceutical, agricultural, construction and paper industries. It currently comes mainly from geological sources such as marble and limestone. These sources are plentiful but might contain heavy metals that are difficult to remove. Currently, large-scale production of chitin from the shell waste is done by the chemical method, independent of the composition of crustacean shells. This method consists of two harsh chemical treatments in sequence: demineralization and deproteinization using a mineral acid and concentrated sodium hydroxide, respectively.[8] This process enables the separation of chitin alone while eliminating calcium carbonate as calcium salt, an effluent. For example, to separate 100 g of chitin from crab shell waste, ~ 1 L (972 mL) of 35% by weight of hydrochloric acid is required. In addition, it releases 220 g (112 L at STP) of carbon dioxide into the atmosphere[9] which was trapped by crustaceans during the mineralization process.[10] In fact, mineralization is sequestration of carbon dioxide by aquatic animals carried out for the formation of a reinforced exoskeleton.[10]The chemical process of separation of chitin is destructive, wasteful, expensive and hazardous to the environment and is known to produce a very large quantity of contaminated water.There have been several alternative reports on deproteinization of chitin. Biotechnological method is thought to be a green alternative method for

chitin extraction, which may enable the recovery of protein as amino acids.[11,12] But the lack of efficiency in deproteinization required subsequent chemical treatments.[13] Effective elimination of protein is important for biomedical application as the fraction of people allergic to crustacean proteins is large.The limit of residual protein content for pharmaceutical grade chitin/chitosan is 0.3 %. Recently, treatments using ionic liquids,[14-16] deep eutectic solvents,[17] subcritical water[18]were reported for isolation of chitin. However, the protein present in the shells, which are important source of carbon and nitrogen, has been given less consideration in these methods.

In so far as mineral recovery from the crustacean shells is considered calcium carbonate is separated by burning organic matter present in shells of the chicken egg, cockle and oyster, at high temperature, since they possess less organic content (~5 %).[19]Although crab shell can be considered as a source for mining calcium carbonate in addition to chitin, the burning of ~30 % organic matter present and recovering calcium carbonate (70 %) would be energy intensive and could produce undesirable air pollutants. On the other hand, if the proportion of the organic content in crab shells can be reduced then recovery of calcium carbonate could be carried out as in the case of oyster shells.

The facile and sustainable separation of chitin, protein and calcium carbonate from the shells of shellfish is a challenging task. The best method known to date for commercial production of chitin is the chemical method and it is not sustainable due to the reasons stated earlier. A simpler method of deproteinization and demineralization or one of the two along with effective use of the organic content present in the shells is the need of the hour. We have been working on developing sustainable methods to separate chitin from the crustacean shells. Thus we have developed three independent methods, namely, treatment with hot glycerol,[20] hydrothermal treatment with 2 weight % urea[21] and treatment with the crude extract from pineapple fruit waste[22]. We have also developed a novel and simple method of separating calcium carbonate (without converting it to calcium chloride) from crab shell waste involving mechanical grinding followed by separation by density and thermal treatment. The method, for the first time, enables the recovery of calcium carbonate present in the shell refinery under milder conditions. In this talk*, the details of the methods developed by us for sustainable separation of chitin from crustacean shells shall be presented in detail.

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BIBDP-IL-03

Nanocellulose- High Value Nanomaterial from Waste Biomass

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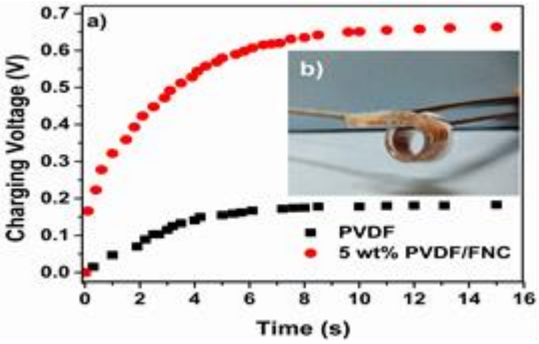
Abstract

Cellulose is a biodegradable, low cost, most abundant renewable agro-polymerthat has gained tremendous attention for manufacturing advanced materials. The ability to convert cellulose from waste biomass into ultrafine dimensions has further expanded the property portfolio and scope of application for this biopolymer. Nanocellulose refers to two different types of nanomaterials: short, low aspect ratio cellulose nanocrystals or cellulose nanowhiskers (CNC or CNW) and long, high aspect ratio cellulose nanofibrils(CNF).CNCs and CNFs are attractive as mechanical reinforcements and rheology modifiers.In this talk, we will report our recent work on nanocellulose (CNC and CNF) based composite materials with emphasis on tailoring the morphology and surface of nanocellulose and leveraging its properties in applications such as ferroelectric energy harvesters, polymer electrolyte membranes, pickering emulsions and microencapsulation.



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BIBDP-IL-04

Biodegradable Plastics for Commodity, Engineering and Biomedical Applications

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Abstract

This presentation highlights the challenges and opportunities towards replacing conventional fossil based plastics with biobased and biodegradable plastics in Engineering, Commodity and Biomedical Applications. Biopolymers extracted from renewable feedstock such as plants, marine animals, insectsetc. have limited applications in large scale plastic production. Among various bio-based synthetic plastics, poly(lactic acid) (PLA) has made its own place due to its biodegradability and potential to replace conventional fossil based plastics. The properties such as melting point, heat deflection temperature and gas barrier propertieshave limitedtheiruseinhigh temperature commodity and engineering applications. However, these limitations can be overcome by developing a new class of high molecular weight stereocomplex PLA (sc-PLA). In this context, we have synthesized sc-PLA and its sc-PLA-bionanocompositesby using different biobased nanofillers which includes cellulose nanocrystals, silk nanocrystals, modified chitosan, etc. The GPC analysis reveals that the synthesized stereo-complex based bionanocomposites hasnumber average molecular weight higher than 100 kDa. The formation of stereocomplex crystallites is confirmed by the XRD analysis. Melting point of the composite is increased to >225°C which suggests the formation of stereocomplex crystallites. Further, thehead distortion temperature is enhanced upto ~155°C atnanofillerloading of 5 wt%. Due to the presence of various bionanofillers, ultimate tensile strength is enhanced significantly. Based on the studies, it can be concluded that bionanofillersare good candidates for enhancing the stereocomplexation in the PLA.Further, fabrication strategies for synthesis of stereocomplex-PLA-bionanocomposites and evaluation of their properties along with possible applications will be discussed.This talk also introduce other bionano-fillers, their use in the development of bionanocomposites, caste films, trays for food packaging, injection molded products for biomadical and in hydrogen storage and supercapacitors for energy applications.

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BIBDP-IL-05

Development and applications of biopolymeric hydrogels towards controlled release of model drugs

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Abstract

Recently, in authors' laboratory, novel functionalized biopolymeric hydrogels have been synthesized via free radical polymerization.[1-7] β-Cyclodextrin, dextrin, glycogen have been used for further functionalization to develop the hydrogels. The synthesized gels are biodegradable, non-cytotoxic. They demonstrates excellent gel strength, show shear thinning behavior and are stimuli-responsive. The fabricated gels are capable to load different drugs substantially, released them in the targeted area in sustained manner, which make them efficient drugs carrier.

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BIBDP-SL-01

Renewable Resources for Binder Synthesis in Coating Applications

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Abstract

With continuous depletion of petrochemical feedstock and their rising prices, the chemical industry is now looking for alternative renewable and sustainable materials. Till date a number of researchers have reported various possible chemistries to produce high performance functional materials from renewable resources. These materials have been proved to be suitable replacements for their petroleum counterparts in resin synthesis, adhesives, paints, coatings, composites, constructions, pharmaceuticals, food applications etc. In view of this, we have explored few of the renewable resources including vegetable oils and fatty acids, Tartaric acid, Citric acid, Cashew nut shell liquid (CNSL), vanillin etc. for their various modifications and suitable applications in coatings. In addition, this research also focuses on development of polyols, polyamines, epoxies and hybrid materials based on renewable resources to be used as coating components. Major applications of these modified chemistries include anticorrosive, flame retardant and radiation curable coatings. The work also explains modification of vegetable oils, fatty acids as well as hydroxy acids for various curing chemistries for development of solvent borne and waterborne coatings. As a contribution to greener concepts in polymer synthesis, development of isocyanate free polyurethanes derived from natural resources and their applications in coatings are also discussed.

Keywords: Renewable resources, Coatings, CNSL, vanillin, Binders

BIBDP-SL-01

Renewable-origin Polybenzoxazines:Conventional to Unconventional Applications

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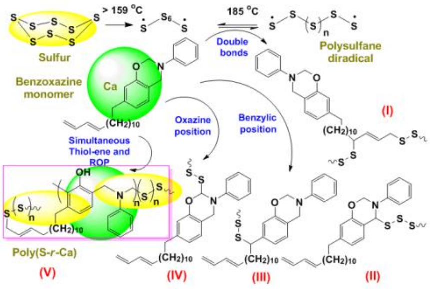
Abstract

To meet the ever-growing needs of polymer industry, over dependence on petroleum industryfor feedstock is an issue. The rising costs of feed-stock, non-renewability, non-biodegradability, non-sustainability and raising environmental concerns demands exploration of sustainable alternatives.Besides providing feedstock for polymers, petroleum refining industries are too involvedin generating waste mainly, elemental sulfur (S) in irrepressible quantities, and demands effective measures to tackletheir abundance. Phenols and their derivatives are omnipresent in polymers.In current work, potential of renewable phenols in a new class of phenolic thermoset polymers, polybenzoxazine, PBz will be discussed. PBzs emerged as superior class of resins due to their attractive thermo-mechanical and flame resistant properties.The materials revealed good adhesive properties. Further such benzoxazine monomers effectively demonstrates their capability to chemically link to elemental sulfur to form copolymers, with new scope of applications as cathode materials in battery applications. Current work illustrates waste utilisation and fixation to form polymers enhancing their scope of applications towards sustainable future.



Fixation of elemental sulfur (petro-waste) in cardanol (agro-waste) benzoxazine monomer

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BIBDP-SL-02

Synthesis, characterization and applications of plant oil derived polyurethane, bioepoxy resin

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Abstract

The utilization of renewable feedstock for the development of polymeric material is attracting attentions due to concerns about the sustainability development necessity to develop more ecofriendly material. World production of major oilseeds has increased from 331 million tonnes to 529 million tonnes in the last decade. Vegetable oils are used for cooking, various industrial uses (personal care, cosmetics, soap, perfume, candle, wood treatment, coating, biofuel, hydrolyic fluid, insulator fluid, lubricant, additive chemicals and polymers). Vegetable oils are one of the cheapest and most abundant, annually renewable natural resources, sustainable and biodegradable. Triglycerides in vegetable oil contains fatty acid chains, with unsaturation, hydroxyl, epoxy and carbonyl groups which are reactive sites for further functionalization. Epoxy resins are an important class of materials which are used extensively in electrical, automobile and other applications because of their excellent properties. Biobased polyols are used in major polyurethane applications to provide an alternative to petroleum based polyols.
In the present study effectiveness of vegetable oils (i.e. karanja, cotton seed, algae, tung, mahua, soyabean oil) as renewable alternative feed stock for synthesis of polyurethane (foam and coatings) and bioepoxy resin were examined (fig. 1). Various properties were compared with their petroleum analogues and various applications were tested.

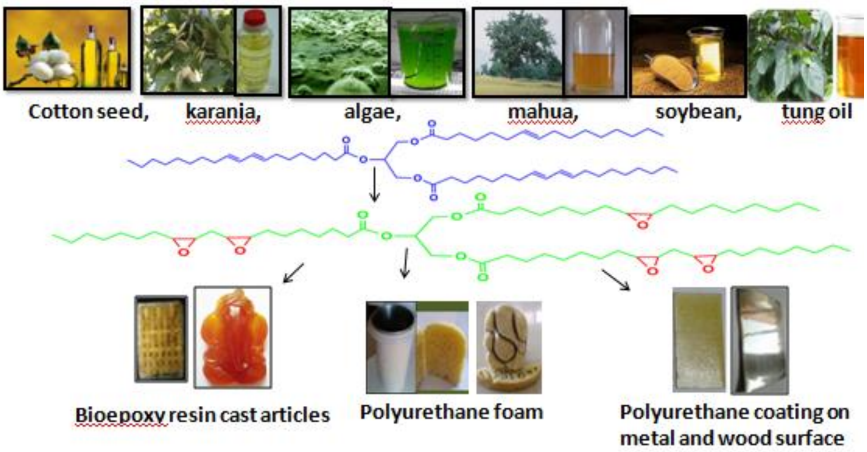

Fig. 1: Schematic scheme showing vegetable oil to bioepoxy resin and polyurethane

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4.

BIBDP-OL-01

Polysaccharide Nanovesicle Platform for Combination and Targeted Drug Delivery in Cancer Cells

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Abstract

Design and development of polymer based controlled drug delivery systems are emerging as important areas of research to target specific organ or host location in cancer therapy. Among the various challenges, delivering multiple anticancer drugs from single polymer nano-carrier is a unique concept to address the tumour resistance to the individual drug molecules through combination therapy. In this work, new class of enzyme responsive polysaccharide (dextran) nano-vesicles were designed and developed to address several challenges in drug delivery. Renewable resource amphiphile was utilized as structure directing agent to bring appropriate vesicular self-assembly in dextran backbone. Carboxylic functionalized dextran was tailor-made for the chemical conjugation of cisplatin drug. DNA-intercalating drug doxorubicin.HCl (DOX) and topoisomerase type I inhibitor drug camptothecin (CPT) were used in combination with cisplatin to produce dual or triple drug loaded vesicular nano-carrier. These dextran vesicles exhibited unique shielding effect for Pt-polymer drug conjugate against glutathione (GSH) detoxification under physiological conditions.[1] In vitro cytotoxicity studies revealed that free cisplatin was highly detoxified by the GSH in breast cancer cells whereas the enhanced stability of Pt-stitched dextran vesicle against GSH facilitated ~ 99 % killing in breast cancer cells. Biotin tagged multi-responsive dextran derivatives were also made and employed for targeted drug delivery of DOX in cervical cancer cell line.[2] Fluorescent dextran vesicles were custom designed by conjugating tetraphenylethene (TPE) in the polymer backbone and the resultant vesicles were found to be luminescent via aggregation induced emission (AIE) process. These fluorescent TPE-dextran vesicles were encapsulated with different anticancer drugs or fluorescent dyes to construct Turn-On bio-probes as well as FRET bio-probes for theranostic applications. Further, the dextran vesicles were used for delivering MLN 8237, Aurora kinase A inhibitor, to study the anchorage independent growth in breast cancer cells.[3] Attempt was also made to deliver the cisplatin and MLN 8237 together to achieve better therapeutic efficacy in 3D cell model. The presentation will be focussed on the design parameters of polysaccharide vesicles and demonstrates the potent application of these vesicles in bioimaging and drug delivery to cancer cells.

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BIBDP-OL-02

Chemoenzymatic Polymerization of Natural and Unnatural Amino Acids having Poor Affinity to Papain

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Abstract

Chemoenzymatic polymerization using proteases is an environmental friendly and atom economical method of polypeptide synthesis. This method uses reverse reaction of proteases under mild aqueous conditions. By this method, we have successfully synthesized many of the novel polypeptides including mimicking some of the natural structural proteins like, spider silk and elastin. Recently, we successfully polymerized proline, valine which has low affinity for proteases. Using tripeptide strategy, we sandwiched proline between glycine units resulting in the polymerization of tripeptide GlyProGly. We also synthesized ValProGly tripeptide and ValGly dipeptide ester and copolymerized them using chemoenzymatic polymerization. The poly(ValProGly-co-ValGly) showed temperature dependent structural transition similar to elastin, resembling most repeated sequence of elastin, namely, ValProGlyValGly. The post-polycondensation of this repeated sequence showed specific secondary structure and thermal behavior similar to elastin. Using the same tripeptide strategy, we have incorporated unnatural amino acids into the peptide backbone. By introducing unnatural units, we can tune the properties of the peptides. We have sandwiched ω-aminoalkanoic acid units (nylon monomer unit) between glycine (Gly) or alanine (Ala) units. The resultingtripeptideesterswerechemoenzymaticallypolymerizedusingpapain. The polypeptides containing approximately 33 mol% nylon units showed a melting point above 200°C. The nylonunitincorporationintothepolypeptidebackbone, which in turn reducedtheintermolecular hydrogen bondingamongthepeptidechaininducingmeltingbehavior. This results in themeltingofpolypeptidebeforedegradation. Hence, thenylonunit in thepolypeptidebackboneinducedthemeltingbehavior.

BIBDP-OL-03

Selective Modification of Ultrafiltration Membranes by Antifouling Hybrid Nanogels Bearing CuO-Polyphosphoester for Controlled Antibacterial Performance

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Abstract

Rational design of polymeric architectures with well-defined structural features is required for controlled delivery of potential antibacterial agents in water filtration system. Here, surface selective crosslinking of ultrafiltration polyvinylidene fluoride–styrene maleic anhydride (PVDF-SMA) membranes by copper oxide–polyphosphoester (CuO-PPE) hybrid nanogels with antifouling and antibacterial characteristics was developed. Based on the solubilization of lipid bilayers of bacterial membrane by SMA copolymer as immiscible blend in PVDF and interaction with phospholipids, these polyphosphoesters are degraded by the active enzymes secreted by bacteria and resulted in accelerated CuO nanoparticles (NPs) release. The CuO NPs composed into the hydrophilic shell of PEG-PPE and subsequently grafted to PVDF-SMA by alkyne-addition reaction. The distinctive antibacterial and antibiofouling performances of the crosslinked PVDF-SMA membranes could be imparted from the unique structure and the controlled delivery of copper ions. Moreover, these modified PVDF-SMA membranes are durable and possess long-term stability due to the strong covalent interaction between CuO-PPE and PVDF-SMA. Flux, porosity and protein adsorption studies were performed for the pristine and modified PVDF-SMA membranes and found an enhanced flux and better recovery ratio for the modified one due to the pendant PPE groups (from CuO-PPE) and prohibiting irreversible protein adsorption on the PVDF surfaces. The cytotoxicity of CuO-PPE is greatly reduced because effective coverage of CuO NPs by biocompatible PPEs. This study opens up the fabrication of "smart" inorganic nanoparticles can be confined into soft hybrid polymeric gel network and control the release of ions for preventing from ubiquitous bacterial treatment in water filtration system.

BIBDP-OL-04

Cellulosic Materials for Sustainable Circular Economy

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Concept of circular economy is gaining traction and today industries have started taking steps to align themselves with the future industrial trends [1]. In this context, cellulose and its derivatives perfectly suits the purpose due to its abundance, biodegradability and renewable origin. There are several potential markets for cellulose based materials for both low and high end markets. These include pulp and paper, food additives, organic cosmetics, personal care products [2], structural materials, and for high end applications such as printed electronics and batteries [3]. Chemically modified cellulose was synthesized and chemically cross-linked to improve the water absorption capacities of unmodified cellulose. The cross-linked cellulose showed marked enhancement in water retention capacity, therebyuseful for utilization in varied applications and contributing to sustainable circular economy.

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BIBDP-OL-05

Dendritic Polyglycerol based Polyanionic Hydro-and Nanogels for Biomedical Applications

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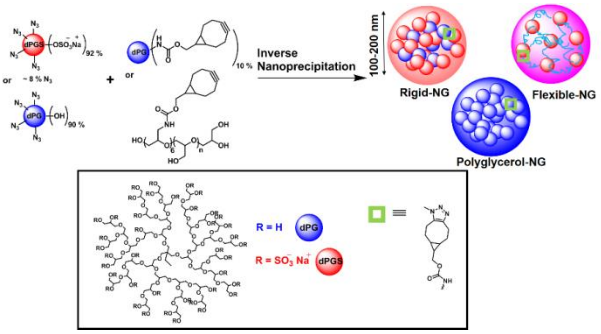
Abstract

The structural environment, cell-biomaterial interaction, and biological signals incorporated in the scaffold played an important role in tissue development. Naturally-derived materials have desired biological properties but limited mechanical strength or fast degradation profiles make them unsuitable for clinical applications. We discuss an approach for the design of a dendritic polyglycerolsulfate (dPGS) – polyethylene glycol (PEG) hydrogels by strain promoted azide-alkyne cycloaddition reaction with an overview over the results obtained from chondrocyte encapsulation studies.[1]dPGS is a highly branched polysulfated heparin analogues with high anti-inflammatory activity.Degradability was introduced in the dPGS hydrogels by preparing a strained cyclooctyne terminated PEG-polycaprolactone linker.[2]



Heparan sulfate (HS) moieties are cell surface molecules which is involved in the infection of manyviruses, including herpesviruses, and arteriviruses, through facilitating their internalization. Cellular HS mimicking sulphated nanogels (NGs) based on dPGSwith different flexibility are prepared by the inverse nanoprecipitation techniquevarying two different spacers,dendritic and linear polyglycerols.[3]In addition, the effect of flexibility of these NGs towards the inhibition of herpesviruses will be discussed. Cellular uptake of these sulphated and hydroxylated NGs were tested *in vitro* in HUVEC, macrophage, and HeLa cells.The sulphated NGs have higher propensity to be uptaken by HUVEC and macrophages compared to hydroxylated NGs. Furthermore, these observations were confirmed by injecting these NGs intravenously in a zebrafish embryo.[4]Hydroxylated NGs were long circulating whereas sulphated NGs were accumulated in the endothelial walls of claudal vein.[4] The hydroxylated NGs were mainly accumulated in the granuloma areas significantlywhen they were injected intravenously in a tuberculosis model in a zebrafish embryo.[5]

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BIBDP-OL-06

Clickable Polyamides Starting from Lignin Derived Aromatic Diacid Bearing Pendant Alkyne Groups: Synthesis, Characterization and Post-Modification

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Abstract

A new aromatic diacid monomer, *viz*., 5, 5’-dimethoxy-6, 6’-bis (prop-2-yn-1-yloxy)-[1, 1’-biphenyl]-3, 3’-dicarboxylic acid was synthesized starting from bio-based vanillic acid. A series of new aromatic (co)polyamides containing pendent alkyne groups were synthesized by Yamazaki polycondensation reaction of 5, 5’-dimethoxy-6,6'-bis(prop-2-yn-1-yloxy)-[1,1'-biphenyl]-3,3'-dicarboxylic acid or different molar ratios of 5, 5’-dimethoxy-6,6'-bis(prop-2-yn-1-yloxy)-[1,1'-biphenyl]-3,3'-dicarboxylic acid and isophthalic acid with 4,4-oxydianiline. Inherent viscosities of polyamides were in the range of 0.46 to 0.79 dL/g indicating formation of reasonably high molecular weight polymers. The effect of incorporation of pendent alkyne groups on polymer properties was examined by TGA, DSC and XRD analysis. The synthesized polyamides containing alkyne groups were post modified by copper catalyzed azide –alkyne click reaction.

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BIBDP-OL-07

Biodegradable-compatible Polyurethanes synthesized from Amino acids

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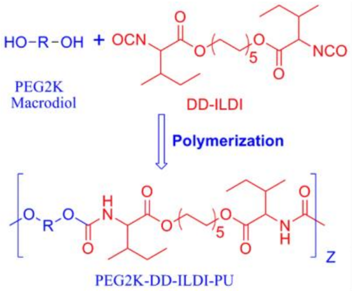
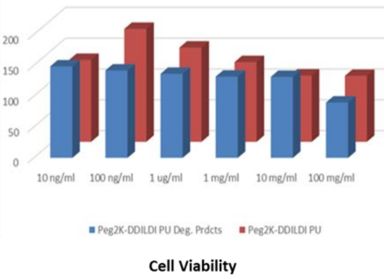
Abstract





There is a serious toxicity issue with the amine by products of polyurethanes (PUs) made from commercial diisocyanates which cause several serious health hazards. To address this toxicity, series of *N*-BOC protected diesters, diamines and diisocyanates were synthesized from renewable resources like amino acids and diols. The polyurethanes made from these diisocyanates can address the toxicity problem of amine by products of commercial PUs. The diamines and *N*-BOC diesters are useful for the synthesis of non-isocyanate based polyurethanes/hydroxyurethanes. All these monomers (diester, diamine and diisocyanates) are thermally stable up to ~230° C. The synthesized polyurethane from 1, 10-decane diol and isoleucine based diisocyanate (DD-ILDI) and polyethylene glycol (PEG-2K) is readily degradable in phosphate buffer saline pH 7.4 at 37° C up to 15% in 30 days, whereas it is completely degraded with 1N NaOH in just 4 hrs. Amino acids are the degradation products of these polyurethanes and are biocompatible when studied *in-vitro*. Both the PU and its degradation products has shown excellent cell viability with HEK 293T cells from Nanogram to milligram concentrations. The studies proved that these polyurethanes/hydroxyurethanes made from these new degradable monomers are promising for the development of bio implants, medical devices and bioplastics with superior properties.

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Abstracts for Invited, Short and Oral Lectures
Under the Theme
Polymers in Health Care and Medical Diagnostics (PHCMD)

PHCMD-IL-01

Detection and Treatment of Fungal Disease using Smart Polymers

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Abstract

Fungal diseases are a growing problem in the tropics and can be fatal for patients with supressed immune systems. Treatment often requires the use of relatively toxic drugs such as amphotericin B. Therefore, increasing the efficacy of this and similar drugs addresses a significant need. On the otherhand detection of fungal infections and differentiation from bacteria is a key goal in the fight against antimicrobial resistance. Here we describe a branched polymer with amphotericin end groups. We show how the polymer binds to its usual target, ergosterol, and retains antifungal activity. The polymer responds to the binding of the target by desolvation of polymer chain segments and we report early indications of increased activity against some strains of fungi. The MIC against two strains of *Candid albicans* were 1.23 (SC5314) and 1.0 (ATCC90028) µmol of amphotericin mL^{-1} compared to MICs against the same strains of 0.48 amd 4.76 µmol of amphotericin mL^{-1} for amphotericin B not attached to the polymer. The action of the polymer against fungi is in contrast to our previously reported work on similar polymers, which respond to bacteria (by desolvation) but did not kill the organisms. We tentatively propose that the maintenance of the efficacy is associated with increasing local concentration of the amphotercin ligands and the potential for the desolvated globule to disrupt the cell membrane. Importantly the polymer showed no toxic effects to corneal epithelial cells even at concentrations as high as 5 mg ml^{-1}. In contrast amphotericin B was toxic at and above 10 μg ml^{-1}. Improved and faster diagnosis can inform treatment and negate strategies such as polypharmacy.

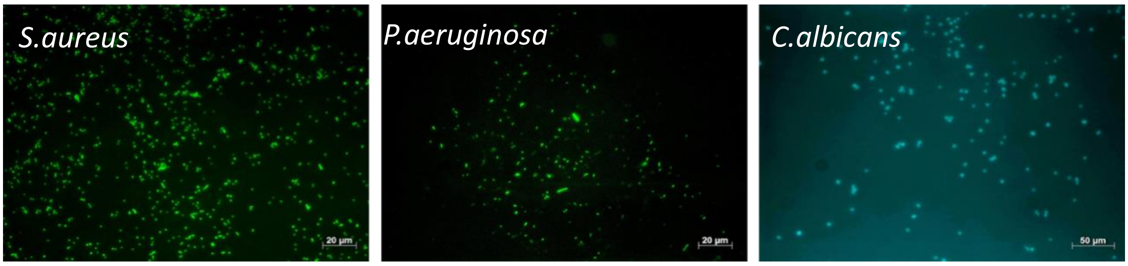

Figure 1 Bacteria and fungi attached to hydrogel functionalzed with H-PNIPAM carrying ligands each

We have, therefore, developed a diagnostic device that carries three HB-PNIPAM polymers functionalized with ligands for Gram-negative, Gram-positive or fungal infections. Each of these polymers is attached to a methacrylic hydrogel membrane. These three classes of organism can then be attached the membrane as shown in Figure 1. Importantly in this immobilized format the amphotericin HB-PNIPAM does not kill fungi. The device has been sown to be effective for sampling infections in *in vivo.*

PHCMD-IL-02

Engineering Polymeric Biomaterials in the Era of Antimicrobial Resistance

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Abstract

As arsenal of antibiotics dwindle, increasingly more effort is being focussed on the development of novel strategies to tackle drug resistant bacteria. This talk focusses on our efforts in engineering new polymeric materials to tackle antimicrobial resistance and infection.[1] Recently we have developed various biocompatible/biodegradable water-insoluble and organo-soluble antimicrobial paints from synthetic and natural polymers to prevent infections.[2] We have also developed a variety of water-soluble macromolecules as potent antimicrobial peptide mimics that are selectively active against microbes and re-sensitize obsolete antibiotics.[3] In another set of studies, injectable hydrogels were developed which are inherently bioadhesive and antimicrobial, and shown to possess wound-healing properties thus suitable to combat surgical site infections.[4] Further, both injectable and preformed antimicrobial hydrogels were developed to deliver antibiotics/antimicrobial agents locally to combat topical/deep tissue infections.[5]

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PHCMD-IL-03

Antibiofilm Coatings for the Prevention of Implant Associated Infection

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Abstract

Synthetic polymers have played critical roles in the success of many clinical applications and are widely used for drug delivery, drug conjugation and as implants. Focus of our laboratory at the Centre for Blood Research, University of British Columbia (www.cbr.ubc.ca) is tailoring the molecular level interactions of synthetic polymers with biological systems to design novel biomaterials in a translational setting to address unmet clinical needs. Bacterial attachment and growth on the surface pose major challenges to the optimal performance of indwelling catheters and devices. For example, catheter-associated urinary tract infections (CAUTIs) represent one of the most common hospital acquired infections with significant economic consequences and increased patient morbidity. Antimicrobial and antifouling coatings on implant or device surface offer an important solution to address this important clinical problem. In this talk, I will discuss various strategies we developed based on anti-adhesive polymer coating towards antifouling surfaces. Further, the development of antibiofilm coatings with broad spectrum activity and long-term durability based on tethered polymers and antimicrobial peptides will be discussed. Finally, translation of the developed technology onto a clinically relevant biomedical plastics, polyureathane (PU), and the demonstration of the antibiofilm activity in mouse infection models will be presented.

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PHCMD-IL-04

Functional Nanogels in the world of Bioengineering

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Abstract

Polymeric biomaterials have become increasingly interesting in medical science over the past few years. With the increasing demand for a biomaterial with better acceptability and functionality to the biosystem, stress has been focused on the development of newer materials. The major requirements for biomedical applications are nontoxicity, the ability to be sterilized, mechanical properties and the most important one is the biocompatibility of the material with the biological systems. The development of polymers with bioactive coating is an important area of research focused on solving the problem of contamination by infection in wound care systems. We have observed that a bioactive component may be incorporated within the hydrogel matrix to make it infection resistant. Herbal drugs and essential oils have been incorporated into either natural hydrogels like chitosan, pectin and dextran by blending approach. A wide range of natural bioactive agents such as aloe vera, curcumin, sandal wood oil, clove oil and honey are available to develop excellent materials for wound care. These dressings have been evaluated in wound healing using mouse as the animal model. Excellent healing with minimum scar by hydrogel dressings has been observed.The innovation of present work is to reconstruct the surface of polymers at nano level in such a way that it acquires antimicrobial nature without much altering its bulk properties which are quite appropriate for suture application. The nanoconstruction can be carried out so that surface chemistry of the material is selectively altered. For this we have followed plasma processing as the mean for the surface modification. The most attractive feature of the plasma processing is that by exerting proper control over the exposure conditions such as exposure time, plasma power and gas flow, a tailored surface with desired chemical functionality and morphology may be produced.

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PHCMD-IL-05

Functional Polymer Based Smart Nano-vehicles for Site-specific Theranostics Application

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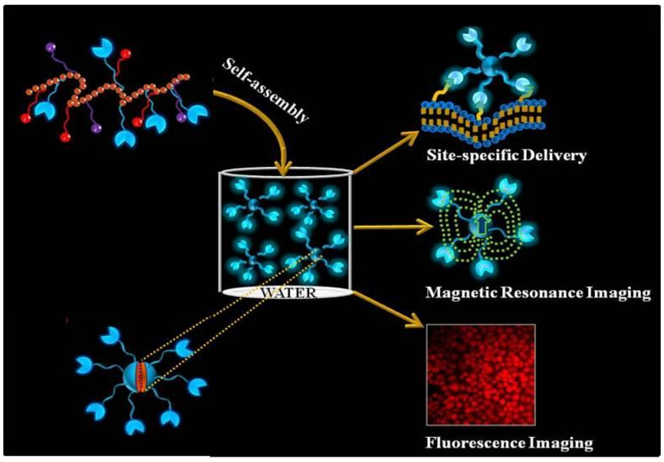
Abstract

Theranostic based nanomedicine plays a crucial role in the field of cancer therapy. This is due to having the capability to combine both therapy and diagnosis together in single system. Herein a new class of metal-ligand based nanocarrier in a polymer backbone has been designed as a theranostic system. To prove the MRI capabilities of copolymer nano-aggregates, NMR experiment is performed at room temperature. Cell viability studies suggest the biocompatibility nature of the copolymer. Flow cytometry as well as epi-fluroscence microscope experiments clearly demonstrate the dual-imaging ability of the newly designed copolymer. The much higher relaxivity ratio (r_2/r_1) of the present method clearly establishes the superiority of our system as one of the best contrast agent known to the practitioners of magnetic resonance imaging.



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PHCMD-IL-06

Ceramic-Polymer Core-Shell Nanoparticles as Bone Substitute Materials in Drug Delivery

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Abstract

Delivery of therapeutic agents to treat diseases such as tumors, osteoarthritis and tuberculosis need systems that deliver the drugs in a controlled manner for prolonged periods of time. Nanotechnology-based controlled drug delivery systems possesses unique advantages over conventional treatment such as increased bioavailability by enhanced permeation and retention effect (EPR), increased retention time and controlled release over a period of time. Various kinds of ceramic-based nanoparticles (NPs) were reported as bone graft substituents and drug delivery vehicles. Development of new bone-filling materials using hydroxyapatite (HA)-polymer composites are of much interest due to their similarity with bone minerals, as well as their osteoconductive and mechanical properties. In this study, model NPs with HA core were grafted with poly(vinyl alcohol) (PVA) shell to deliver methotrexate (MTX) in a sustained manner. The NPs were characterized using various techniques. Grafting efficiency on HA NPs was in the range of 44-52 wt%. MTX was conjugated to the grafted PVA resulting in a drug payload of 20 wt%. MTX as well as gemcitabine and a model protein such as bovine serum albumin were also loaded onto the NPs by physical absorption. *In vitro* release data showed that combinational delivery of two drugs or one drug and a protein was possible for several days from the NPs. Biocompatibility studies of these NPs performed in osteosarcoma MG-63 (OMG-63) cell line showed dose-dependent cytotoxicity of the NPs.

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PHCMD-IL-07

Nature-Inspired Elastic Capsules, Tubes and Hairy Surfaces

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Abstract

Natural structures such as eggs, embryos, plant seeds, vegetables like the onion, and body parts like the spinal disc, all have multiple concentric layers surrounding a central core. Each layer typically has a unique compositions and thereby a distinct function. The synthesis (morphogenesis) of these structures in nature typically proceeds in an “inside-out” fashion, where a core is formed initially, followed by a first shell and then additional shells. Taking inspiration from the above, we have developed an inside-out technique to synthesize a range of soft materials. First, we have created “onion-like” polymeric capsules with multiple concentric shells surrounding a gelled core [1]. Each polymer shell is formed by free-radical polymerization. A given shell grows outward from the surface of the previous shell; thus, the shell thickness steadily increases with time and can be controlled. Using this technique, we can juxtapose widely different polymers next to each other in a capsule, as shown, for example, in Figure 1. The resulting capsules exhibit a range of unusual properties. One specific property to highlight is the ability of capsules to rapidly swell due to gas evolved from a reaction in the core; such swelling can be violent enough to eject the core. Multilayered structures in nature also exist in other geometries. Our blood vessels are examples of multilayered tubes, while many tissues in our body have outer layers of hairs called villi and microvilli. We have extended our inside-out technique to cylindrical and planar geometries to create polymeric multilayered tubes and hairy surfaces. The multilayered tubes exhibit spontaneous changes in tube diameter in response to the properties of the flowing liquid, which is reminiscent of blood vessels. The hairy surfaces absorb solutes much more efficiently than a bare surface, akin to the villi-covered surfaces of the gastrointestinal tract.

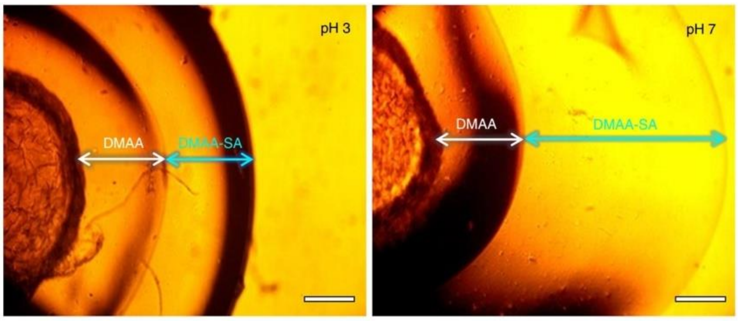

Figure 1. Multilayer capsule with one layer responsive to pH

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PHCMD-IL-08

Instantly formative hydrogels for artificial vitreous body

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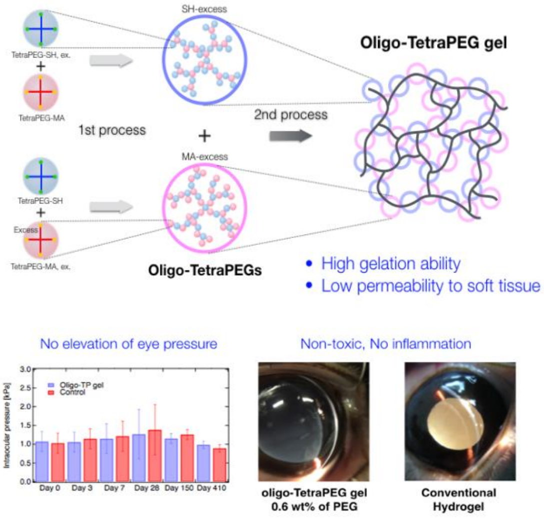
Abstract

If a material can be introduced without a surgical procedure, treats the disease, and does not harm surrounding tissues throughout its full lifecycle *in vivo*, this represents a significant advance as a biomaterial. Such minimally invasive installation can be achieved using hydrogels by simply injecting a polymer solution into a target space, followed by crosslinking. The solution eventually becomes a hydrogel and fills the space inside the body. However, with regard to the final destination, conventional hydrogels have undesirable properties (i.e. swelling) that compromise their morphological and mechanical compatibility *in vivo*. Indeed, the swelling pressure exerted by conventional hydrogels is sufficiently large to cause severe adverse reactions to surrounding tissues. In this respect, we report here a new class of *in situ* forming hydrogels that guarantee safety throughout the full life cycle. The oligo-TetraPEG hydrogel has an extremely high water content and a polymer content of only 4.0 g/L, resulting in an exceptionally low swelling pressure.

The oligo-TetraPEG hydrogel was successfully injected and gelled inside a living body within a clinically relevant manipulation time and little cytotoxicity. The oligo-TetraPEG hydrogel exhibited an appropriate stiffness, similar to that of soft tissue, with extremely low swelling pressure thus being compatible with living tissues. The oligo-TetraPEG hydrogel functioned as an artificial vitreous body for over a year without any adverse effects, and was effective for treating retinal detachment as an intravitreous tamponade material.



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PHCMD-IL-09

Antimicrobial Polymers from Nature-derived Precursors

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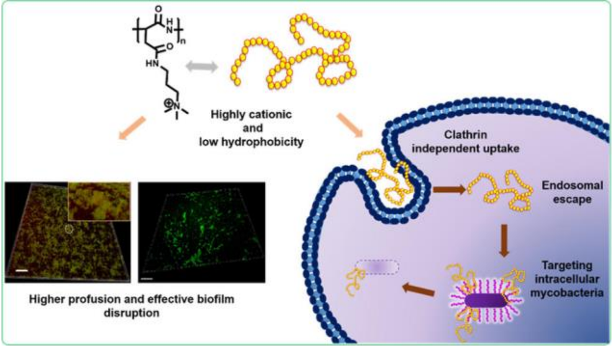
Abstract

Microbes are ubiquitous in our world and are continuously interacting with us. Along with beneficial ones such as *Lactobacillus*, we are also exposed to pathogenic microbes such as *Salmonella*, *Escherichia* and *Mycobacteria*. Due to uncontrolled use of antibiotics in recent times, these pathogenic microbes are progressively becoming resistant to them. These drug resistant microbes have emerged as a significant health challenge of this century. Polymers with antimicrobial activity have shown immense promise in tackling this emergent health crisis. Synthetic antimicrobial polymers derived from natural precursors are expected to discriminate between the microbe and the mammalian host cells better than the current regimens. We have been engaged in the design, synthesis and characterization of antimicrobial potency of chemical polymers derived from natural precursors. We employ polyaspartamides as the modular, biocompatible and biodegradable precursors that are amenable to chemical functionalization towards antimicrobial applications. In this talk, I will cover our efforts in the direction of creating polymers that show potent and selective killing of *Mycobacteria*,both in planktonic as well in biofilm form.[1,2]We also demonstrate the ability of these polymers to target *Mycobacteria* residing within the confines of host macrophages that act as safety refuge for these microbes.[2]In addition to these promising results, I will also discuss our recent efforts in the direction of templated polymerization of dopamine to obtain antifouling coatings on biomedical surfaces such as latex catheters.[3]



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PHCMD-IL-10

Cellular uptake of mannose-6-phosphate modified glycopolypeptides and their self-assembled nanostructures

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The ubiquitous expression of mannose-6-phosphate receptor on majority of human cells makes it a valid target in the quest to deliver therapeutics selectively to the lysosome. These receptors, which include the ~300 kDa insulin-like growth factor-II (IGF-II)/cation-independent (CI) multifunc-tional transmembrane glycoprotein mannose 6-phosphate (M6P) receptor (CI-MPR), bind lysosomal enzymes containing phosphomannosyl residues in the trans-golgi network (TGN) and transport them to an acidified compartment of lysosomes. Synthesis of high molecular weight M6P-glycopolypeptide having pendant M6P moieties in side chain as a natural mimic of proteins bearing M6P moieties can help us understand the complexity and individuality of CI-MPR trafficking for lysosomal targeting. In addition, amphiphilic glycopolypeptides bearing mannose-6-phosphate can be self-assembled into vesicles, micelles and nanorods. This lecture will discuss the cellular uptake of mannose-6-phosphate gly-copolypeptides and soft nanostructures made from these glycopolypeptides. An end functionalized polyvalent (M6P-GPs) with high molecular weights (Up to 22 KDa) have been synthesized via NCA polymerization. These synthetic M6P-GPs were found to display minimal toxicity to cells in vitro and show exceptional selectivity for trafficking into lysosomes in various cell lines. Comparison of cellular uptake behavior of M6P-GP and the corresponding Mannose-GP polymer reveals that incorporation of phosphate moiety at the 6-position of mannose completely alters its trafficking behavior and becomes exclusively lysosome specific. We also demonstrate that trafficking of M6P-GPs in mammalian cells is likely associated with the CI-MPR receptor pathway.

PHCMD-IL-11

Controlled Drug Delivery for Better Healthcare

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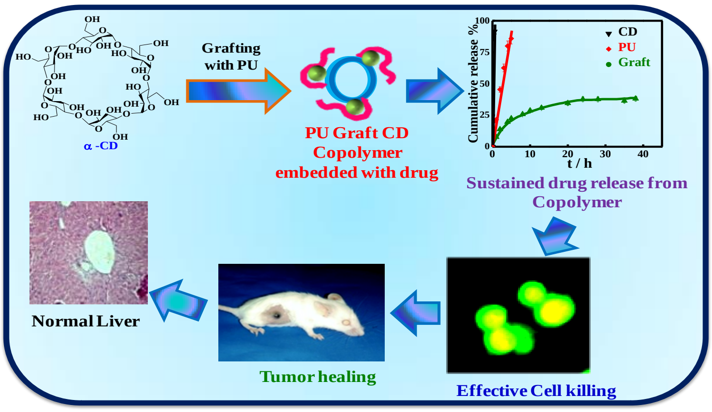
Abstract

Controlled drug delivery technology is one of the most rapidly growing areas of science in which chemists, pharmaceutics and chemical engineers are contributing to human healthcare. Controlled drug delivery systems provide several advantages as compared to conventional dosages in terms of improved efficacy, reduced toxicity, improved patient compliance and convenience. A variety of synthetic and natural polymers are extensively used for designing the control drug delivery systems but precise control of drug requires modification of polymer either to regulate the release rate or to target delivery of drugs. In this report, we emphasize on the chemical and physical modifications of synthetic and polymers from renewable resources to realize the regulated delivery of drug. Various forms of vehicles like hydrogel, scaffold, patches are developed for improved healthcare. Cellular studies and animal models are explored to understand the mechanism of action and efficacy of the delivery vehicles.



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PHCMD-IL-12

Supramolecular Nanoparticle for Impairing Endoplasmic Reticulum in Cancer Cells

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Abstract

The endoplasmic reticulum (ER) is one of the most important organelles controlling myriads of cellular functions including protein folding/misfolding/unfolding, calcium ion homeostasis and lipid biosynthesis. Subsequently, due to its functional dysregulation in cancer cells, it has emerged as interesting target for anti-cancer therapy. However, specific targeting of ER in cancer cells remains a major challenge due to the lack of ER-selective chemical tools. Furthermore, for performing multiple cellular functions ER is dependent on nucleus through complicated cross-talk. To address this, we have engineered a supramolecular self-assembled hexameric rosette structure from two small molecules: tri-substituted triazine and 5-fluorouracil (5FU). This rosette structure consists of ER-targeting moiety with fluorescence tag, ER-stress inducer and nuclear DNA damaging drug simultaneously, which further self-assembled into ER-targeting spherical nano-scale particle (ER-NP). These ER-NPs internalized into HeLa cervical cancer cells by macropinocytosis and specifically localized into ER to induce ER stress and DNA damage leading to cell death through apoptosis. Interestingly, ER-NPs initiated autophagy, inhibited by a combination of ER-NP and chloroquine (CQ) to augment cancer cell death. This work has potential to exploit the concept of supramolecular self-assembly into developing novel nano-scale material for specific sub-cellular targeting of multiple organelles for future anti-cancer therapy.

PHCMD-IL-13

Bio-polymers in Clinical Translation : OncoDiscover Liquid Biopsy Technology for Early Metastasis Detection

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Abstract

Polymeric multi-component conjugation mediated by targeting biomarkers and nanoparticles has immense clinical implications. The talk will highlight, '*seed and soil theory*' of cancer metastasis progression, the detection, and enumeration of circulating tumour cells (CTC) from cancer patients blood[1-2]. CTC analysis is implicated for early-stage metastasis detection as a prognostics value, for monitoring cancer relapse, and in personalized cancer therapy.[3-5] CTC measure is associated as a non-invasive '*real-time liquid biopsy*'. However, capturing CTCs endure high challenge due to their very low abundance in blood (1 CTC per million other blood cells)[3]. The CTC capturing technology was approved by USFDA (CellSearch) and remain unmet need in India. The technology is prohibitively expensive. The detection and enumeration of CTCs offers the utility with respect to prognosis in epithelial origin cancers, example, breast, colorectal, head and neck, and prostate cancers etc. The OncoDiscover platform consist of magneto-polymeric nanosystem which is synthesized through series of chemical reactions. The talk will feature - CTC targeting, rapid isolation, and imaging of cancer cells using clinical blood samples in monitoring disease progression. OncoDiscover, technology has been clinically evaluated with regulatory permissions and guidelines (FDA-India/ Drug Controller General, India). Finally, the talk will disclose clinical validation outcome using cancer patients blood samples. OncoDiscover 'Liquid Biopsy Technology' offer availability and affordability with immense clinical benefit to cancer patients in India.

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PHCMD-IL-14

Modular Targeted Drug Delivery Systems using Dendron-Polymer Conjugates

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Abstract

In recent years polymeric micellar systems have emerged as an important class of nano-pharmaceuticals due to their capability to improve pharmacokinetics and bio-distribution of chemotherapy drugs, along with reduction of systemic toxicities. While micellar delivery systems inherently benefit from passive targeting through the enhanced permeation and retention effect leading to increased accumulation in the tumor, additional active targeting through surface modification of micelles with targeting groups specific for over-expressed receptors of tumor cells can further increase their efficacy. In this presentation, fabrication of non-toxic, biodegradable, and modularly tunable micellar delivery systems using dendron-polymer conjugates will be disclosed (Figure 1).[1,2] AB and ABA type dendron-polymer constructs poly(ethylene glycol) based hydrophilic component and hydrophobic polyester dendrons as hydrophobic constructs are used as primary constructs to fabricate micelles. These micelles can be doped with an AB type dendron-polymer containing a cRGDfK targeting group as secondary constructs to actively target cancer cells over-expressing $\alpha_u\beta_3/\alpha_u\beta_5$ integrins. Increased drug release from these constructs was observed under acidic conditions, compared to that in neutral environment. Enhanced cellular internalization of Nile red doped micelles by MDA-MB-231 human breast cancer cells was observed for targeting group bearing micelles. *In vitro* cytotoxicity experiments on MDA-MB-231 breast cancer and A549 lung carcinoma cells exhibited improved toxicity for the targeted micelles. Overall, it is established that targeting group containing micellar constructs fabricated with dendron-polymer conjugates provides a promisingdrug delivery platform due to their facile synthesis, excellent stability in biological media and their preferential targeting of cancer cells.

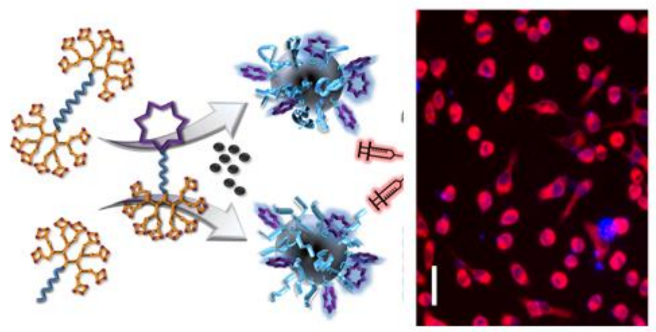

Figure 1. Fabrication and Targeting of Modular Micellar Systems.

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PHCMD-IL-15

Co-ordination assisted self-assembled nanostructure: a Futuristic Engineered nano-formulation for advanced therapeutic application

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Abstract

Co-ordination assisted self-assembly of the macromolecules is one of the unique approaches to achieve a stimuli-responsive monodispersed nano-formulation (NF) applicable in biomedicines. The stimuli-responsive structural reorganization property of these NF's draws an enormous attention in the field of NF based biotherapy. Herein we came up with two different types of smart-formulation showing stimuli-responsive structural deformation followed by their therapeutic performance towards the specific biological environment. Firstly, the macromolecule, pentaerythritol poly(caprolactone)-b-poly(acrylic acid) form Fe^{+3} ion induced light-responsive NF with the unique structural arrangement as like spherically shaped human brain. The DOX-loaded NF undergoes structural deformation in the presence of light and shows a release of DOX molecule (85.2% at 120 min). Administration of the DOX-loaded NF to C6 glioma rat model (*in vivo*) offered tremendous inhibition (~91%) of tumor growth without any toxic side effects. Secondly, mannose conjugated antimicrobial polypeptide, poly(arginine-r-valine)-mannose undergoes Zn^{2+} ion induced self-assembly into a NF with a unique structural appearance as like Taxus baccata fruits. The NF uptake by the bacterial membrane led structural deformation followed by exposing of free polypeptide molecules. These molecules are enforced to lysis the bacterial membrane followed by diffusion of cytoplasmic component out of the membrane that culminates final death of bacteria (MIC values varies from 0.67 to 2.55 μM). Indeed, NF's remain non-toxic against both the mammalian as well as red blood cell as reflected from their higher order of cell viability (> 80%) and very insignificant hemolytic effect (<13%). Hence, metal ion assisted self-assembly approach brings about a new therapeutic window, where the fully exposed macromolecule can be formulated into compact NF with enhanced therapeutic performance.

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*Speaker

Reference:

"Metal Ion Ornamented Ultrafast Light-Sensitive Nanogel for Potential in Vivo Cancer Therapy" by Sudipta Panja, Goutam Dey, Rashmi Bharti, Pijush Mandal, Mahitosh Mandal and Santanu Chattopadhyay*, ***Chem. Mater.*** 2016, 28, 8598−8610.

PHCMD-IL-16

Fabrication of electrospun curcumin loaded thiocarbohydrazide modified gelatin nanofibers for effective wound healing

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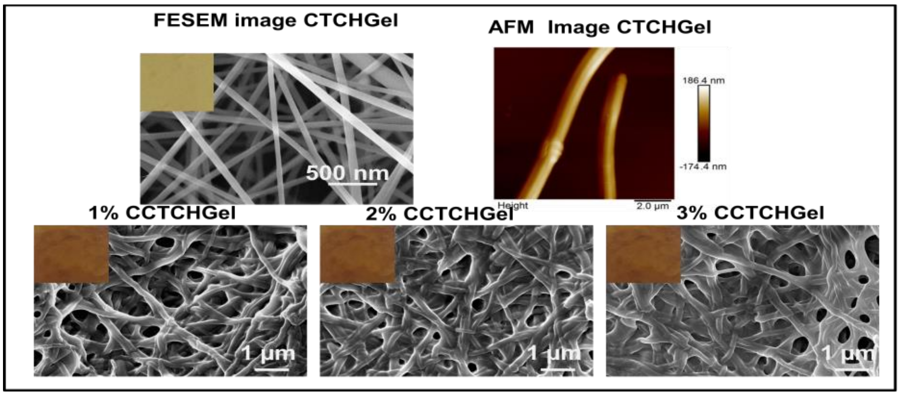
Abstract

Electrospun nanofibers have been extensively utilized in clinical applications such as antimicrobial patches, wound dressings, drug delivery systems owing to their tunable morphological properties. Our proposed hypothesis of enhanced antibacterial activity using thiocarbohydrazide modification of gelatin was evaluated. Curcumin was blended along with modified gelatin into nanofibrous mats by electrospinning using 50% acetic acid solution to enhance the bioavailability of the hydrophobic curcumin for wound treatment. Further, crosslinking of nanofibres was performed in order to determine the efficiency for drug release application. The electrospun curcumin loaded thiocarbohydrazide gelatin nanofibrous mats were studied for curcumin release at different pH for wound healing application. This demonstration improved antibacterial activity against *E.coli* and enhanced *in vitro* wound healing results. The results provide a different material using functionalized gelatin nanofibers prepared via electrospinning technique at clinical level.



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PHCMD-IL-17

Design of Multifunctional Nanomaterials for Cancer Gene Therapy

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Abstract

Primary objectives of gene therapy are to correct the genetic defects that underlie a disease process and to provide supplemental therapeutic modality through genetic engineering. Over 75% of current gene therapy is performed using viruses as gene delivery vehicles. However, with viruses, there are serious concerns over the issues of toxicity, immunogenicity, payload gene size limitations, and difficulty in scale up for industrial production. Non-viral vectors therefore have attracted attention from academic and industrial point of view. Among the non-viral vectors, polymeric systems offer several important advantages. Since two decades, much progress has been made towards designing polymeric gene carriers with high transfection efficiency and low cytotoxicity and in elucidating the relationship between their structure and gene delivery performance. However, effective delivery of nucleic acids such as DNA, siRNA, transcription factors for successful treatment of various fatal diseases possess unique challenges that have not yet been fully addressed. **First**, polymers are tremendously versatile and can provide physical, chemical, and biological properties that are necessary for gene delivery applications. **Second**, polymers can be synthesized in parallel synthesis pathways for high-throughput screening of biocompatibility and transfection efficiency. **Third**, various formulations, designs, and geometrics can be made from polymeric materials for specific types of gene delivery applications. Moreover, the surface chemistry of polymers can be easily modified with biological ligands for site specific targeting in the body. The need for a safety and biocompatibility approach extends to in vitro investigations, as modifications intended for in vivo applicability can significantly affect both in vitro and in vivo performance.

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PHCMD-IL-18

Stimuli-responsive Polymer-hybrid Materials for Targeted Anti-cancer Drug Delivery and Imaging

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Abstract

Cancer is the life-threatening disease even in the present day. The heterogeneous nature of cancer microenvironment is the greatest obstacle to cure the patient to lead a healthy life. Despite the clinical success of several small molecular chemotherapeutics against tumor; it is an unprecedented challenge to get desire pharmacokinetics of a particular drug with minimum adverse side effect as small molecular drugs nonspecifically distribute throughout the body.[1] Additionally, many medications such as peptide and protein, antibody, vaccine and gene-based drugs, in general, may not be delivered using common route because they might be susceptible to enzymatic degradation or cannot be absorbed efficiently due to molecular size and charge issues. Thus functionalized natural /synthetic polymers are intensively used encapsulation of therapeutic agents and deliver to the target place. Typical sub-microscopic particle size (10-200 nm) and stealthy surface nature of polymers, allow them as an efficient- vehicle for targeted drug delivery. Recently, “theranostic” a combination of chemotherapeutic and diagnostic tools become an attractive strategy in clinical medicine. It can improve the biodistribution and systematic administration of therapeutic in the target place; additionally, the diagnostic tool in the nano-formulation can collect the information on state and status of disease before and after specific treatment.[2] In this context, we have developed endogenous stimuli-responsive theranostic in a combination of the optical modulator and chemotherapeutic agents; which released chemotherapeutic agent to the target cancer cells upon encountering with overexpressed enzymes/co-enzymes and various reactive oxygen species (ROS) in cancer cells.[3-4] The extent of active chemo-release to the target cells was estimated by fluorescence modality. The polymer-supported theranostic have shown receptor-mediated endocytosis with chemoselective activation of chemotherapeutic agents in cancer cells.

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PHCMD-SL-01

Carbon Dots for Drug Delivery and Cellular Microenvironment Sensing

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Abstract

The growing need for new, functional, biologically active materials has arisen from our inability to detect and treat many diseases with traditional therapies or procedures. Nanomaterials are showing great potential in the fields of biomedicine and biology not only due to their unique size-dependent properties but also since their size is on a similar scale as that of proteins and other biomolecules. This presentation will focus on strategies for making carbon dots customized to have desirable properties for various bio-applications in drug delivery and bio-imaging. For instance, despite the promising photo-physical properties of fluorescent graphene quantum dots (GQDs), their cellular toxicity needs to be addressed before their full potential could be completely realized in biomedicine. A simple method for mitigating the toxicity of GQDs by embedding them in PEG matrix will be discussed. These more biocompatible p-GQDs have enhanced loading and efficient intracellular delivery of therapeutics. In yet another example, the talk will highlight the development of a fluorescence carbon dot based platform, which can detect changes in pH in the cell microenvironment. pH values in living system plays important role in deciding rate of chemical reactions, health of organ, tissue or body. Variation in pH can be used to detect and monitor a disease. Organic pH sensitive fluorescent dyes have been developed which show pH sensitive change in fluorescence output. These dyes suffer from problems of photo bleaching or toxicity or both. The developed carbon dot based pH nanosensor can be encapsulated with live cells in transparent spherical PEG microgel using droplet based microfluidics and UV photo-polymerization. The fluorescent carbon dots have excitation dependent emission, which was found sensitive to changes in pH in the range of 10 to 4. The intensity of emission increases as the pH is lowered and becomes more acidic. Since, the nanosensors can sense pH changes in the physiologically relevant range of 7.6 to 5.8, the developed system can be used to study biological process or disease progression in 3D. As an example of the application of these pH nanosensors, development of a platform for sensing bacterial growth will be discussed.The platform can differentiate between resistant and non-resistant strains of E.coli in ~ 6 hours, which is better than currently used clinical methods.

PHCMD-SL-02

Bioactive Liquid Crystal Droplets

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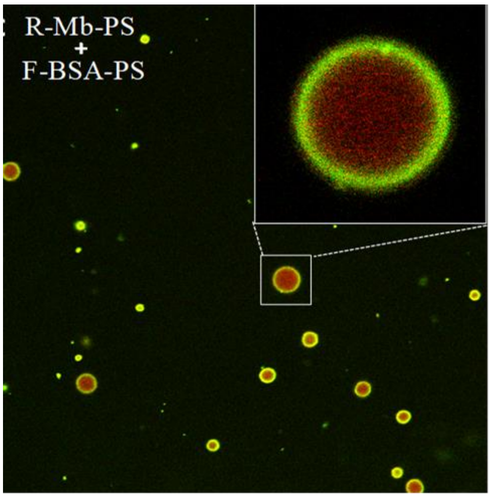
Abstract

A facile method for fabricating protein-sequestered liquid crystal microemulsion droplets based on the uptake of surface-engineered protein-polymer surfactant (PS) core-shell nanobioconjugates will be described in the talk. Uptake of myoglobin (Mb-PS), bovine serum albumin (BSA-PS), Zn-porphyrin myoglobin (ZnIX-Pr-Mb-PS), horseradish peroxidase (HRP-PS) and glucose oxidase (GOx-PS) occurs without structural or functional degradation, and gives rise to sequestration within the interior or at the surface of 4-cyano-4$^{/}$-pentyl biphenyl (5CB) nematic droplets depending on the net surface charge of the protein-PS conjugate. We use differences in uptake behaviour to achieve the spontaneous positional assembly of multiple proteins in the LC droplets, and demonstrate the use of spatially separated GOx and HRP enzymes to produce LC droplets capable of housing an enzyme cascade reaction. Our method opens a pathway for the development of bioactive liquid crystal droplets and could have potential applications in the optical sensing of biomolecular substrates.



PHCMD-SL-03

Functional biocompatible crack-resistant coatings of silk fibroin for breast implant

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Abstract

Surface coatings for biomedical implants have been used to prevent premature failure of implant due to bacterial biofilm formation and foreign body reaction. Delamination, cracking, crazing, etc. are frequent problems associated with coatings when implants are subjected to mechanical deformation either during surgical handling or during use. We demonstrate here, a novel process that results in the formation of a coating that is stable under mechanical stresses in tensile, torsion and bending modes. The coating process involves a combination of two conventional coating processes – namely dip coating and electro-spinning. Polydimethylsiloxane was selected as the substrate owing to its wide use in biomedical implants. Silk fibroin, a natural biocompatible protein polymer obtained from *Bombyx mori* silkworm, was used for demonstrating the process of coating. The coating was also further functionalized using a green biomolecule - glycomonoterpene prepared using citronellal and glucose. These functional compounds are being touted as the next generation antibiofilm molecules on account of quorum sensing inhibitory activity.We have demonstrated that the quorum quenching activity of the biomolecule is retained during the processing steps and the coatings exhibited excellent antibiofilm activity against common infection causing bacterium *P. aeruginosa* and *S. epidermidis*. These silk fibroin-glycomonoterpene coatingscan be used for implants in biomedical applications such as breast implants and catheter tubings.

PHCMD-SL-04

Polymer Antibodies: An Approach Towards Bacterial Affinity Ligands

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Abstract

The rapid and efficient detection, identification and quantification of microorganisms such as bacteria remain a well known challenge in applied medicine, fermentation technology, forensic sciences and environmental monitoring. THE INTERACTIONS BETWEEN SYNTHETIC POLYMER-BASED MATERIALS AND BACTERIAL SURFACE IS OF SIGNIFICANT INTEREST IN THE CONTEXT OF BIOANALYTICAL AND BIOMEDICAL APPLICATIONS. IN THE PRESENT WORK WE developed a concept that an array of synthetic organic polymers incorporating a range of charged, hydrophobic and hydrogen bonding functional groups can give a unique pattern of affinity for a specific bacterial species. For the present library the charge was incorporated into the nanoparticles (NPs) using acrylic acid for negatively charged monomer NPs and either of (3-acrylamidopropyl) ammonium chloride (APM), (3-methacrylamidopropyl) guanidinium chloride (Gua) or (3-acrylamidopropyl) trimethylammonium chloride (ATC) for positively charged NPs. The hydrophobicity was varied using the varied mole fraction (0 or 40%) of *t*-butylacrylamide monomer. With this small library we could get the unique signatures for six out seven bacteria that were investigated. Expanding this library by changing the percent hydrophobicity in the nanoaprticles preparation and by incorporating new positively charged monomers can produce different signature patterns for a wider range of bacterial species.

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PHCMD-SL-05

Prolonging food shelf-life by controlled released antibacterial and antioxidant actives from multi-layered polymer particles

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Abstract

The aim of this talk is to demonstrate a set of novel dual active (antioxidant and antibacterial) loaded multilayered microparticles and to release the actives at rates suitable for long-term inhibition of bacteria as well as lipid oxidation in food. For example, antibacterial active can be released initially at a faster rate to provide immediate protection, after that the release will be controlled and continuous to provide long-term inhibition of bacterial growth. However, the other active eg. antioxidant can be released at a slower rate to provide intermediate/long-term protection of lipid oxidation. In order to achieve this goal, multilayered polymer particles with different hydrophilicity at each layers have been designed. The outermost layer consists of more hydrophilic polymer (PLGA: Poly(*dl*-lactic-co-glycolic acid, 50:50) with antibacterial (benzoic acid) encapsulated in it and the inner core contains hydrophobic polymer (PLLA: Poly(*l*-lactic acid) with antioxidant (tocopherol) localized in it. Selective encapsulation of antibacterial and antioxidant in shell and core layers respectively are feasible by one step emulsion solvent evaporation method. Long-term antibacterial and antioxidant studies demonstrate that controlled co-delivery of benzoic acid and tocopherol from multilayered microparticles produces a greater reduction in bacterial growth and inhibition of lipid oxidation over a period of 60 days compared with single-active-loaded particles. This study provides how multilayered microparticles can be utilized to tune the release profiles of multiple actives simultaneously without having active-active interactions and how co-delivery can potentially prolong the food shelf-life.

PHCMD-SL-06

Highly Bactericidal Macroporous Antimicrobial Polymeric Gel for Point-of-Use Water Disinfection

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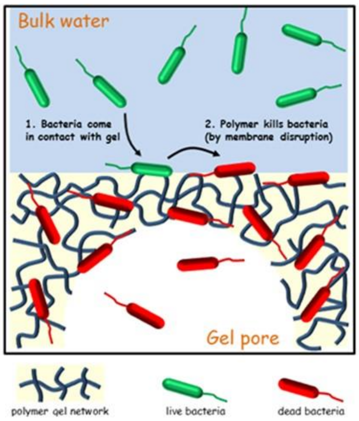
Abstract

Access to clean and safe water supply remains inadequate in many developing countries.[1] One of the key challenges is to remove pathogenic bacteria from the water supply via effective water disinfection technologies to prevent the spread of diseases and to ensure the safety of consumers. Herein, a highly effective point-of-use (on-demand) water disinfection technology, in the form of a polymeric scaffold called macroporous antimicrobial polymeric gel (MAPG), is demonstrated. MAPG is easy to fabricate, completely organic and possess inherent antimicrobial property which makes it non-reliant on inorganic compounds[2] such as silver where the long-term toxicity remains unknown. MAPG is highly bactericidal and can disinfect bacteria-contaminated water (ca. 10^8 CFU mL^{-1}) at a capacity of about > 50 times the mass of the organic material used, inactivating > 99% of both Gram-negative and Gram-positive bacteria including Escherichia coli, Vibrio cholerae and Staphylococcus aureus within 20 minutes of treatment. When fabricated in a syringe, MAPG eliminates E. coli from contaminated water source by > 8.0 $\log_{10}$ reduction in bacteria counts (i.e., no viable bacteria were detected after treatment), and the syringe can be reused multiple times without losing potency. The MAPG technology is not only restricted to water disinfection but may also be applicable in other bacteria inactivation applications.



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PHCMD-SL-07

Shear-Thinning, Shape-Forming and Self-Healing Polymeric Hydrogels in Healthcare

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Abstract

Different properties of hydrogels such as shear-thinning, shape-forming and self-healing has been explored in tissue engineering and regenerative medicine area. We have developed chitin/PLGA hydrogel with $CaSO_4$ and FGF-18 for regenerating irregular bone defects. This developed chitin/PLGA hydrogel is injectable and has shear-thinning property. Chitin/PLGA hydrogel with $CaSO_4$ and FGF-18 showed an enhance bone formation in mouse cranial bone defect. In an another work, we developed injectable in-situ shape forming oxidized alginate-gelatin hydrogel with whitlockite nanoparticles and simvastatin drug. The in-situ gel formation was due to the Schiff base reaction between aldehyde group of oxidized alginate and amine group of gelatin. The gelation time was significantly reduced due to the presence of whitlockite nanoparticles which helps shape formation in short duration (<30s). This shape forming hydrogel showed a sustained release of simvastatin drug. The prepared shape forming hydrogel showed an enhanced bone formation in mouse cranial bone defect. This shear-thinning and shape-forming hydrogel has potential application in regenerating irregular bone defects. We also prepared *N, O*-carboxymethyl chitosan based hydrogel using EDTA and $FeCl_3$. This developed hydrogel showed good self-healing and adhesive property. The presence of Fe^{3+} driving the gelation through coordination chemistry and as well as self-healing property, which could be used as glue for closing wounds.

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PHCMD-SL-08

Carbon dot-Hydrogel Nanocomposites for Controlled Drug Delivery

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Abstract

Hydrogel nanocomposites are hydrated polymeric network incorporated with nanomaterials and are potential candidates in myriad applications in the area of biomedical research.In this work, we are focussed on the synthesis of carbon dotsincorporated agarosebased hydrogel nanocomposites for the controlled delivery of drug.Carbon dots are carbon nanoparticles of size less than 10 nm which exhibitunique optical properties, good biocompatibility, low toxicity, great aqueous stability andwavelength-dependent fluorescence upon excitation.A one pot green synthesis was adopted for the preparation of carbon dots from naturally available materials. The hydrogel nanocomposite of carbon dots incorporated modified agarose hydrogels were fabricated and characterised. The nanocomposite hydrogels exhibited an intense blue emission at 440 nm with high stability.The composite showed excellent swelling and drug loading properties.Drug release, cytotoxicity and biodegradation of the hydrogel composites were carried out.Synergistic combination of properties of polymer and nanomaterial is made use in this work for an efficient and controlled drug delivery.

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PHCMD-SL-09

Polymer Based Nanomedicine for Trans-Epithelial Oral Delivery of Ivermectin for Zika

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Target specific delivery vehicles have emerged as important technologies to treat illness and develop preventive measures for various cancers and viral diseases. Polymer based nanomedicine can be used for the treatment of lethal viruses, such as the Zika virus, by facilitating oral drug delivery across the epithelial barrier. We have proposed that nanotechnology in combination with chemical biology can combat the catastrophic neurological complications caused by the Zika virus(ZIKV). ZIKV is known to be transmitted by an infected Aedes species mosquito [1]. The ZIKV outbreak in Florida and its association to microcephaly and other neurological conditions such as Guillain-Barre syndrome, myelitis, and meningoencephalitis pose a universal health emergency[2]. To understand and tackle this problem, we have developed Fc-Ivermectin-NPs, an oral formulation composed of neonatal Fc receptor (FcRn) with decorated nanoparticles (NPs), that mediate the transport of Ivermectin across the epithelial barrier and release the drug in a controlled fashion to the Zika virus infected blood.

Acknowledgment: This work is supported by Florida Department of Health

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PHCMD-OL-01

Polymer Topology Driven Drug Delivery for Cancer Therapy

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Abstract

Conventional chemotherapeutic drugs available in the market are all small molecules that are rendered ineffective due to their poor biodistribution, target specificity, short half-life and consequential side effects like cardiotoxicity, nephrotoxicity and neurotoxicity. This obstacle in cancer treatment led to the development of "Polymer therapeutics" wherein polymers served as the nano-carriers for efficient delivery of drug molecules to the target site with reduced side effects and prolonged half-life. Star-shaped polymer architectures have been shown to have prolonged blood circulation as compared to their linear counterparts having the same molecular weight. They exhibit better pharmacokinetics, high molecular weight leads to increased $t_{1/2}$ and relatively small sizes prevent RES uptake. The present investigation is aimed at understanding the role of polymer topology on the biodistribution, renal clearance, RES uptake and tumor accumulation wherein the molecular weight is maintained the same for the star-shaped polymer and the linear diblock counterpart[1]. For this, the ideal candidates were biodegradable Polycaprolactone (PCL) based block copolymers synthesized via ring opening polymerization of caprolactone and carboxylic substituted caprolactone monomers based on our expertise[2]. Further, PEG-*b*-PCL-*b*-CPCL triblock copolymers were also synthesized and they were able to deliver anticancer drugs cisplatin and doxorubicin in a single polymer dose achieving synergistic combination therapy[3]. Hence, moving up on the same ideology, fully biodegradable star-shaped PCL block copolymers were synthesized. The star-shaped polymers self-assembled into unimolecular micelles of sizes in the range of 30-50 nm as determined using DLS, SAXS and microscopy techniques such as FESEM, AFM and HR-TEM. Their unimolecular nature was reinstated from the pyrene experiment wherein there was no change in the I_1/I_3 value. The *in vitro* studies carried out in cervical cancer cell lines (HeLa) exhibited enhanced cellular uptake of the unimolecular micelles compared to the free drug and the linear diblock micelle. Thus, our aim is to validate the same in wild type mice by investigating the half-life of these carriers in blood, study their bio-distribution in kidney, liver, spleen and brain.

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PHCMD-OL-02

Biodegradable Thermoresponsive Polyesters for Drug and Protein Delivery

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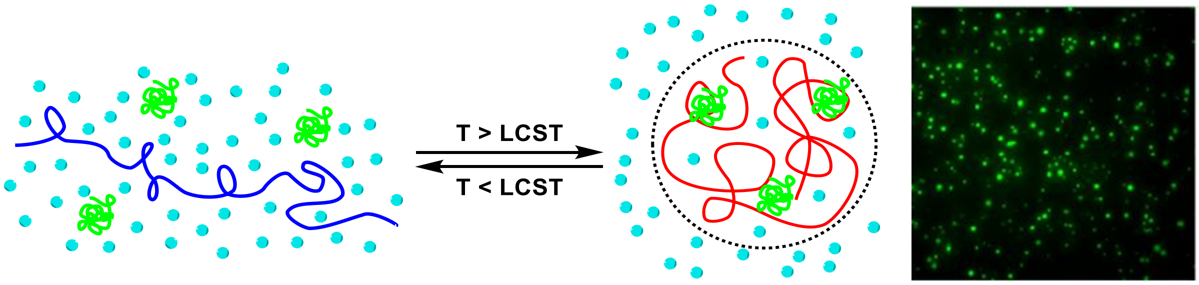
Abstract

Thermoresponsive polymers can undergo reversible temperature-dependent phase separation which changes its structure and solubility. Above a lower critical solution temperature (LCST), the extended polymer structure collapses to an insoluble globule conformation which makes them attractive for therapeutic molecular delivery cargo. However, clinical applications are limited due to the nondegradable backbone of many well-studied thermoresponsive polymers, such as poly(acrylamides) (PAs).Our lab has developed a new class of thermoresponsive polyesters (TR-PEs) with a range of LCSTs (0 to 100°C) inspired by biodegradable elastin-like peptides and PAs. Interestingly, these TR-PEs do not exhibit complete dehydration above LCST which makes them a suitable candidate for therapeutic encapsulation and controlled delivery in addition to their hydrolytically degradation property. Moreover, the interaction between TR-PEs and target molecules can be tailored by non-covalent forces depending on different pendant groups of copolymers. Our recent studydemonstrated the successful encapsulation and release of Fluorescein isothiocyanate tagged bovine serum albumin as a model protein.



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PHCMD-OL-03

Vitamin C conjugated polymeric nanoparticle for biomedical applications

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Abstract

Vitamin Cis a natural antioxidant. It is known to reduce the adverse effect of cancer at high dose[1] (> 4 mM). Howeveroral or dietary delivery of vitamin C for treatment is not effective due to its poor chemicalstability andspontaneous oxidation (half-life <70 mins) to dehydroascorbic acid at physiological condition.[2]Hencse current research is directed towards the development of biocompatible, targeted delivery with increased bioavailability of vitamin C at specific site. In this context we have developed polymeric nanocarrier of vitamin C.Our designed nano-vitamin C iscomposed ofa biocompatible poly-amino acid based polymeric backbonethat is conjugated with folateand vitamin C.[3]We have synthesised poly-L-aspartimide biodegradable, non-toxic polymer micelle as carrier of vitamin C. The chemical functionalization approach restricts the conversion of vitamin C to dehydroascorbic acid (half-life > 2 days) in physiological conditions and high concentration. Our nano-carrier shows glucose-responsive delivery of vitamin C to specific cancer cell.At moderately higher concentration nano-vitamin C produces reactive oxygen species (ROS) and kill cancer cells. On the other hand atlower concentrationnano-vitamin C induces autophagosome formation[4] that can be used as a therapeutic tool for autophagy mediated clearance of intracellular protein aggregates.So our nano-vitamin C has broad potential applications in cancer treatmentas well as can be used as therapeutic tool in neurodegenerative diseases.

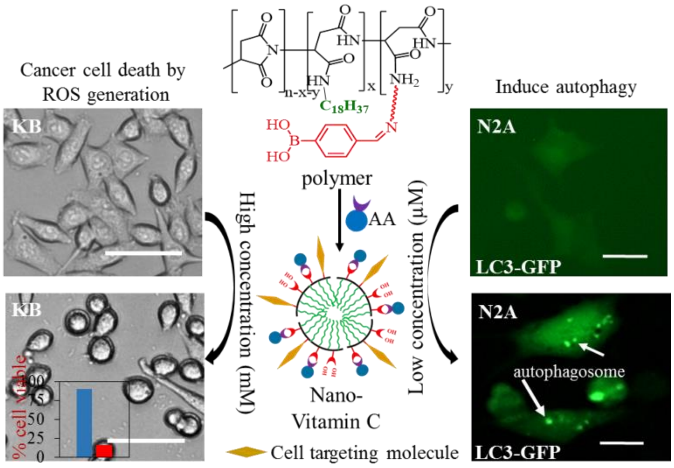

Figure: Nano-vitamin C induced cancer cell death at higher dose and autophagosome formulation at lower dose.

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PHCMD-OL-04

A Novel Biodegradable Hydrogel from Agarose and Polyethylene Glycol for Norfloxacin Delivery

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Abstract

Nowadays, conventional drug administration generally leads to a fluctuation of drug concentration in the blood stream, which further causes undesirable side effects such as toxicity and reduced efficiency. The main advantage of controlled delivery systems is that, it is target specific, provide constant drug delivery and better control of drug levels in blood. The main aim of this study is to maintain the drug concentration at a predetermined rate, in the body (blood plasma) within the therapeutic limits for extended periods of time. A novel biodegradable and pH sensitive composite hydrogels, based on agarose (AG) and polyl ethylene glycol (PEG) copolymer, was successfully prepared by using glutaraldehyde (1% GA) as a cross-linker. Norfloxacin (NFX) was used as model drug to investigate the in vitro release behaviour, when NFX alone and NFX is in the complex form. Structural changes of AG-g-PEG hydrogels have been characterized using FTIR and TGA/DSC analysis. The surface morphology of AG-g-PEG hydrogel shows highly porous surface. The in vitro results of cytotoxicity assay confirmed that the cross linked hydrogel is non-toxic. The swelling and in vitro drug release study of the hydrogel was carried out at 37 ^{0}C temperature. The in vitro release study demonstrates that AG-g-PEG hydrogel releases NFX in a sustained way when NFX is in the form of complex.

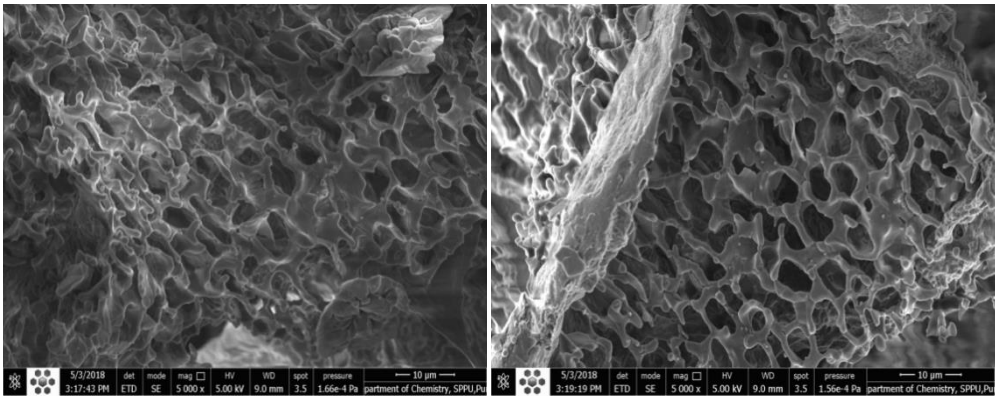

Figure 1: Surface morphology of AG-g-PEG hydrogel

Abstracts for Invited, Short and Oral Lectures Under the Theme

Polymers in Renewable Energy Applications (PREA)

PREA-IL-01

Polymer Semiconductor Electronics and Optoelectronics: Enabling new Energy and Information Technologies

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Abstract

Conjugated polymer semiconductors have emerged as the foundation for a range of new technologies. Advances in the molecular engineering of conjugated polymer semiconductors of diverse molecular and supramolecular structures have greatly expanded the scope of promising organic semiconductor-based electronics and optoelectronic devices and technologies, including: organic light-emitting diodes (OLEDs), organic/polymer solar cells, photodetectors, image sensors, lasers, thin film transistors for printed and flexible electronics, high density electronic memories, etc. Our work is focused on the molecular engineering of materials and devices, encompassing synthesis, processing, and investigation of solid-state structure, properties, structure-property relationships, and device applications of both *p*-type and *n*-type semiconducting polymeric materials. Some examples of our recent advances in a few of these areas will be discussed, including [1-5]: n-type polymer semiconductors for highly efficient non-fullerene organic photovoltaics (NF-OPVs) for low cost solar energy power generation; high-mobility n-type polymer semiconductors for n-channel transistors, complementary circuits, and electronic memories; and highly efficient multilayered OLEDs for displays and lighting, enabled by solution-processed electron transport materials.

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PREA-IL-02

Scaling of ionic and electronic conductivity in mixed conducting polymer PEDOT:PSS using geometrical confinement effects

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Abstract

Conformation of polymers in confined channels modifies the transport properties of the polymers when the geometrical confinement length scale is comparable to the characteristic length scale of polymer chain. Poly(3,4-ethylenedioxythiophene) doped with poly(styrene-sulfonate), PEDOT:PSS, a well-known conducting polymer studied over two decades with wide applications in energy storage, bioelectronics, robotics, and antistatic coatings have both ionic (PSS^-) and electronic ($PEDOT^+$) contributions. We explore the scaling of these mixed (electronic and ionic) as a function of confinement. Ordered and patterned alumina templates consisting of well defined confined volume[1] were used for this purpose. Systematic studies of conductance over a wide range of frequency and temperature reveal distinct trends. We propose a semi-classical model to understand these features.

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PREA-IL-03

Polymer architectures towards Solvent-free Solid Polymer Electrolytes in Batteries

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Abstract

For future battery applications, solid state polymer electrolytes (SPEs) are highly recommended due to their clear advantages in processing, lamination and lightweight in addition to high mechanical strength and ionic conductivity. We study the influence of backbones such as polynorbornene, polyethenesulfonate and polymethacrylate in bottle brush polymer architectures, in which PEO is attached to various kinds of backbones (see fig.). In order to suppress the inflammability of SPEs, we also used perfluorinated EO analogue side chains in polyethenesulfonate brushes. We also exploited the inherent microphase separation property of a brush block copolymer to design solid polymer electrolytes incorporating mechanically stable phases and efficient Li-ion conducting phases in a single component system All the polymers were mixed with different amounts of LiTFSI salts and the ionic conductivity, Li-transfer number and electrochemical stability of these solvent-free SPEs were determined using impedance spectroscopy and cyclic voltammetry. We could achieve 10^5 Pa shear modulus at 60°C for such a brush block copolymer exhibiting ionic conductivity between 10^{-3} and 10^{-4} S/cm over a temperature range of 80 to 30°C.

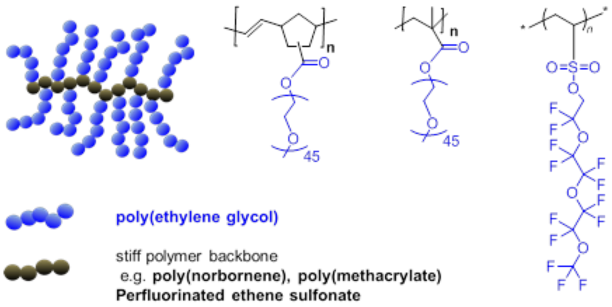

Figure 1. Sketch and chemical structures of brush copolymers of PEO in which the backbone is varied from polynorbornene to polymethacrylate to polyethenesulfonate and perfluorinated EO side chains were implemented.

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PREA-IL-04

Flexible and Compressible Energy Devices

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Abstract

Flexible and compressible energy devices are required to power wearable electronic devices. Energy conversion and energy storage devices that are compressible and flexible are required to fulfill various type of wearable devices. Towards this objective, we have developed flexible flexible dye sensitized solar cells with efficiency of 4.2%. The innovation is in the photoanode. The efficiency of the DSSC while using rigid substrate is 10.2%. The details of the device performance and fabrication will be discussed in the talk. We have developed polyphenols as reductive and protective coating to prepare metal films on flexible and compressible substrates. The gold coated substrates were coated with polymer and filled with gel electrolyte. The results of the devices will be discussed during the talk.

PREA-IL-05

Polymers for Photothermal Batteries

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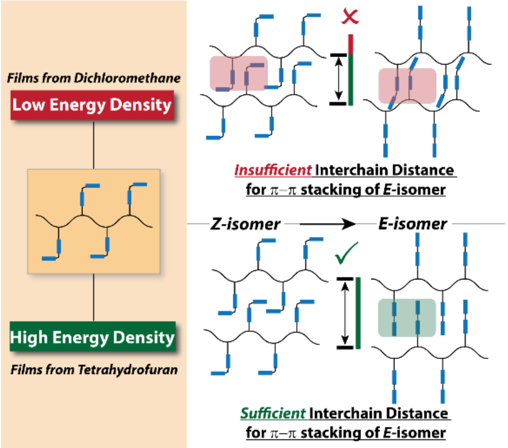
Abstract

We have studied polymer with pendant azobenzene moieties for storing energy from light in chemical bonds. We have achieved energy storage densities of ~510 J/g (max: 698 J/g) in azobenzene-based syndiotactic-rich poly(methacrylate) polymers. We found that the processing solvent and its interactions with the polymer are important to achieve morphologically optimal structures for high-energy density materials. Our work shows that morphologies of syndiotacticpolymers play an essential role in controlling the activation energy of*Z*-*E*isomerization of azo-benzenes as well as the shape of the DSC exotherm. Thus, our study shows the crucial roles of the tacticity of the polymer backbone, intra- and interchain pi-pi stacking interactions, and solvent-polymer interactions in achieving higher energy densities in polymers for photothermal batteries.



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PREA-IL-06

Conducting Polymer Nanotubes and Their Applications

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Abstract

Conducting polymer nanostructures with defined size, shape, architecture and chemical functionality have received more attention nowadays, because they are the forefront of many next-generation organic optoelectronic technologies. Among several conducting polymers, polyaniline (PANI) has been most extensively studied because it exhibits good environmental stability and its electrical properties can be modified by both the oxidation state of the main chain and protonation. However, the control of the size and morphology during the synthesis of nanostructured PANI still remains a challenge. The reported methods for the synthesis of PANI nanostructures include interfacial polymerization method, electro-spinning, seeding polymerization and template method (hard and soft). Among them, the soft-templated method utilizing the assembly of surfactants, poly-electrolytes and organic dopants to create network 1D structure is promising as it uses the bottom-up approach of supramolecular chemistry. Inspired by the easy preparation of PANI and the use of water as an environment friendly solvent, we wonder if we could directly obtain nanoscale PANI based on soft templated method by self assembly of organic acids in aqueous medium. Herein, we report a simple process of synthesis of nanostructure of PANI doped with several tetracarboxylic acids (aromatic and non-aromatic) in bulk quantity via *in-situ* polymerization. The architectures and properties of the formed PANI nanotube (Figure 1) will be presented. This lecture will discuss about the architectures and properties of the formed PANI nanotube, particularly recent applications as SERS substrate, water purifier, energy generation and storage.

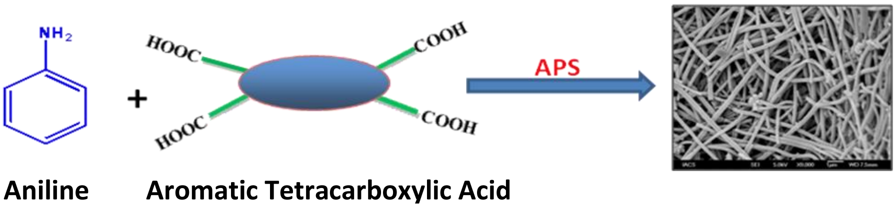

Figure1: Schematic view of formation of PANI nanotubes doped with aromatic

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PREA-IL-07

Multifunctional Porous Organic Polymers: Emerging Materials for Light Harvesting, Energy Storage and Photocatalysis

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Abstract

Porous organic materials have attracted significant attention in the last few years due to their high surface area and functionalizable pores. Considering the facts of (i) the superior chemical, thermal and hydrothermal stabilities arising fromstrong covalent bonds, (ii) structural and functional tunability, (iii) lightweight because of B, C, N, O, H-based building blocks, porous organic polymers (POPs) have emerged as an important theme in the current research.[1]The tunable pore size with the high surface area as well as excellent structural robustness triggers their extensive utilization from the gas storage and separation to heterogeneous catalysis and water purification. Amidst all the advantages, the judicious inclusion of π-electron conjugation in the network makes the conjugated porous organic polymer (CPOPs) unique from all other porous materials.Hence, CPOPs became popular for their multimodal applications like sensing, light harvesting, photocatalysis, and energy storage. In this present scenario of the field, our group took up the problem to meet various challenges like designing the task-specific building blocks, tuning the band gap and porosity[2a] and most importantly the development of POPs with solution processability.[2b,d] Along with the design strategy, we have also demonstrated the efficacy of POPs in diverse applications ranging from chemo/ biosensing, light harvesting,[2b] energy storage,[2c] photocatalysis,[2d] to metal-free CO_2 fixation. A brief appraisal of POPs and their promising future scope will be presented.

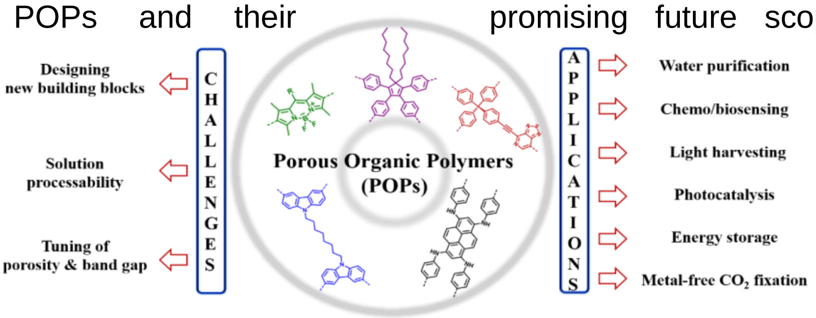

Figure 2: ***Schematic illustration depicting the challenging aspects and the versatile applications of porous organic polymers.***

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PREA-IL-08

Designing Heteroaromatic π-Conjugated Systems: Role of alkynes

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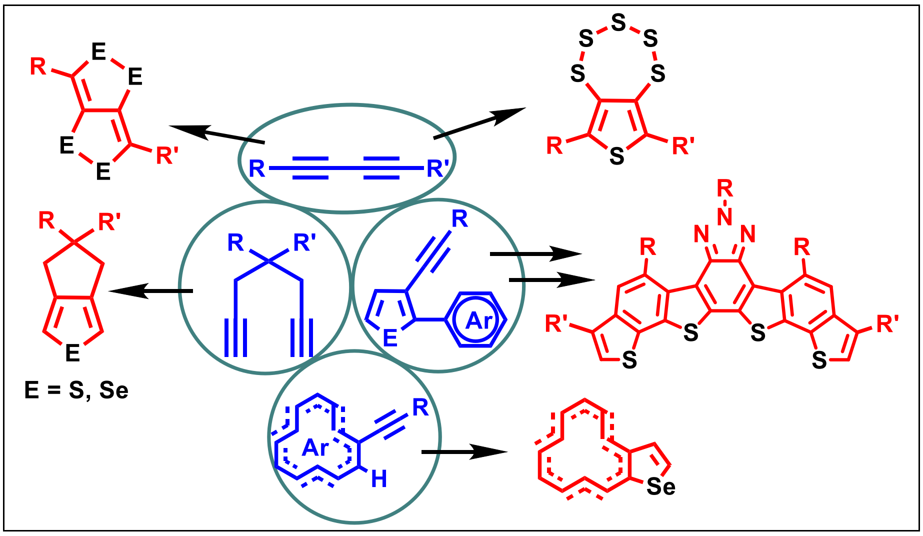
Abstract

Organic conjugated systems have attracted considerable attention for their applications in organic electronic devices such as organic solar cells (OSCs), field effect transistors (OFETs), light emitting diodes (OLEDs) and electrochromic devices (ECDs). Here we present the design and various synthetic approaches of conjugated systems based on alkyne precursors and their structure-property relationships. The main emphasis will be given to (i) 3,4-cyclic substituted thiophene and selenophene derivatives, such as cyclopenta[*c*]thiophene and –selenophene, (ii) conjugated systems with multiple heteroatoms (diselenolodiselelenols and thienopentathiophenes), and (iii) heteroacenes. Change in heteroatoms in the conjugated systems showed an interesting trend in their properties. Thus, the properties of resulting conjugated systems were tuned by using atomistic approach.



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PREA-IL-09

Squaraine Based Dyes for Dye-Sensitized Solar Cells

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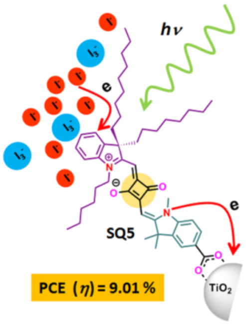
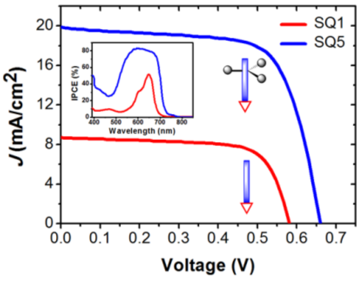
Abstract

In dye-sensitized solar cells (DSSCs), out of all the interfaces formed by various device components, TiO_2-dye/electrolyte interface plays an important role in modulating the charge injection and dye regeneration process. Further, aggregation of organic dyes on the TiO_2 surface leads to self-quenching of photo-excited states which hampers the charge injection process which in turn affects the device performace. However, aggregation of dyes helps to broaden the absorption profile of light absorbing sensitizers due to the formation of either H- or J-type aggregates. Hence controlling the aggregation or self-assembly of dyes on TiO_2 surface for both broadening the spectrum and improving the charge injection process is desired for achieving the better device performace. Though visible light harvesting donor-□-acceptor (D-□-A) have been widely designed and synthesized, there are only few NIR light absorbing chromophores have been exploited in DSSCs research. We have utilized a donor-acceptor-donor (D-A-D) configured squaraine (SQ) dyes which absorb the far red and NIR photons. To modulate the electronic properties of SQ dyes, various donors have been incorporated to the SQ dyes to shift the absorption towards the NIR region. Aggregation of dyes on the TiO_2 has been controlled by integrating both *in-plane* and *out-of-plane* branched alkyl groups to the dye structure. Results on the synthesis of various donors for the SQ dyes and DSSC device performace will be discussed.





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PREA-IL-10

Opto-electronic enhancement in nano-structured polymer thin film photovoltaic devices

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Abstract

Nano-structured platforms have been explored in the context of enhanced absorption in photovoltaic systems [1, 2]. However facile fabrication of nanostructures remains a challenge. Also identification of important device length-scales over which nano-scale effects result in enhanced and combined opto-electronic performance is a problem seldom addressed. We present our work on identification of enhancement mechanisms in both the optical and electrical domains, in a proof of concept polymer photovoltaic system shown schematically in Figure 1(a). The experiments are carried out a nano-structured platforms fabricated by facile methods involving template-based moulding.

The nanostructured device are seen to result in a significantly improved photocurrent, as seen from the external quantum efficiency curves in Figure 1(b) and the enhanced absorptance of the structured architecture in Figure 1(c). We see that the enhancement in due to simultaneous improvements in optical absorptance and charge transport.

Further we also present our findings on the effects of the length scales of the various layers in the device architecture and the consequent trade-offs between nano-structured enhancement and increased parasitic losses with nanostructures. This leadsto design rules for geometry and material selection in the general context of thin film photovoltaic devices. Further, our novel fabrication method opens up a simplified experimental method to make device quality nano-patterned substrates at an applied level, and studying nano-scale phenomena at the fundamental level.

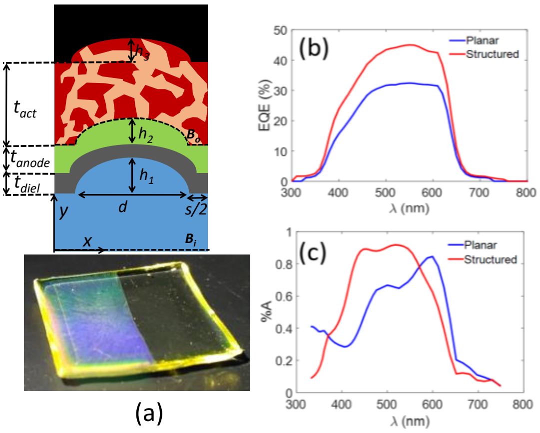

Fig. 1(a) Schematic device architecture employed (above) and structured substrate (below), (b) External quantum efficiency of planar and structured devices, (c) Computed absorptances of planar and structured devices.

Example References

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PREA-IL-11

Polymer Electrolytes: Challenges & Opportunities in Realizing Next Generation Electrochemical Devices

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Abstract

Socially and geo-politically, with the pressure on the non-perennial resources mounting, addressing environmental concerns, gaining energy security while maintaining growth are now national priorities world-wide. The global urgency for green and sustainable energy generation has pitched a major technological challenge notably in the domain of excitonic solar cells. Analogous demand for efficient portable power, have also driven research in the field of energy storage and delivery technologies. In this perspective, new nano-structured materials and polymers promise to make considerable impact on the design, efficiency and viability of the next generation devices. One of the key constituents in multi-component electrochemical systems is the '*electrolyte*'. In such systems, apart from all the other parameters related to electrodes, dyes, catalysts, etc., the device performance and life-time is dominated by the functioning and stability of the electrolytes under operational conditions. Over the years, electrolyte research has evolved to satisfy the requirement of the industry as well as consumers in both stationary and portable applications. A long-standing goal in electrolyte research is the preparation of an ideal electrolyte that combines the processing characteristics of polymers and the ionic conductivity of low molar mass liquids. *Polymer electrolytes* contrast sharply compared to the usual electrolyte materials with respect to the mode of charge transport and the value of ionic conductivity; however, for electrochemical applications the flexibility offered by the PE is important. Coupled with high volumetric power densities, the volume changes in a cell during cycling can be easily accommodated without physical degradation of the interfacial contacts, thus allowing space-efficient battery designs. Though the PEs are projected to address multiple issues related to device performance, factors such as relatively low ionic conductivity, the ability of polymer electrolytes to operate with highly reactive electrodes such as lithium over a wider temperature range without deterioration in the charge capacity and electrolyte properties, the high interfacial electrode-electrolyte impedances are still a major technological challenge and far from practical realization. The presentation would provide a brief overview on the role of electrolytes in the prospective energy generation and storage devices, the present status, bottlenecks and opportunities. Our continuing efforts towards the design and development of polymer / polymer-nanocomposite electrolytes along with the highlights of some encouraging results and future research directions would be discussed in the context of the identified gap areas.

PREA-IL-12

Fluorescent Polymers for Selective Detection of Explosives

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Abstract

Trinitrotoluene (TNT) and research department explosive (RDX) are two widely used military explosives, found in different explosive formulations posing threats to human life and environment.[1,2] Detection of these explosives is a global demand in the current era of increasing terror attacks and hence it has been a matter of great concern to scientists working in the area of explosive detection.[3,4] Detection of such compounds by cost effective and simple techniques would be a great achievement and of national/international importance. A major drawback in the established fluorescence based TNT sensors is majority of them use fluorescence quenching signals and hence lack specificity for TNT/RDX. Fluorescence based sensors exhibit same or nearly same results for structurally similar nonexplosives also. In addition, other established detection techniques are either expensive or complicated in handling. In order to address the problems associated with currently developed explosive sensors, multi-mode sensing is highly desirable and it will eventually lead to precise and selective detection of explosives. In this context, we have developed a fluorescent polymer for dual mode selective detection of TNT. Upon contact with TNT, fluorescence quenching of the polymer film along with visible color change is observed. In this method, TNT even up to pM concentration can be selectively detected in dual mode. The developed strategy enables to differentiate TNT from other nitroaromatic derivatives at very low concentration. Similarly, fluorescent molecule doped polymer films have been found effective for low level detection of RXD.

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PREA-OL-01

A new high temperature synthetic strategy for designing a metal free, redox active quinoxaline-benzimidazole based organic polymers having high energy storage capacity

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Abstract

Herein we report the new method of the successful high temperature (>100 °C) polymerization for preparation of high inherent viscosity quinoxaline based organic homopolymer (QOP) and quinoxaline-benzimidazole based organic copolymer (QOP-BOP) via the simple one-step polymerization of aromatic tetraamines with 2, 5-bis- [(4-benzoylcarbonyl) phenyl] -3-4 diphenyl thiophene (TPTPBC)for applications in electrochemical energy storage or conversion system. Presence of characteristics bands and expected elemental peaks of monomer and polymer was confirmed from FT-IR and NMR spectroscopy. QOP-BOP electrode showed high energy storage capacity with a specific capacitance of 305 F/g respectively at 2 A/g current density and good cyclic stability with 88 % retention of its initial specific capacitance after 1000 cycles. Due to the mesoporous nature of synthesized polymers, water can easily intercalate inside the pores. Thus, positive ions in aqueous electrolyte can easily intercalate or de-intercalate, i.e. ionic conductivity increases and hence the supercapacitance increases.The resulting polymers were highly thermally stable and soluble in some organic solvents. The XRD patterns showed that the QOP and QOP-BOP have amorphous nature. Thermogravimetric analysis of polymers showed 10% weight loss in the range of 433 to 779 °C indicating good thermal stability.This work establishes the first use of thiophene integrated with quinoxaline-benzimidazole unit in energy storage applications and delivers strategies for further developments in the performance of redox active and metal free conjugated polymer materials.

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PREA-OL-02

Synthesis of Isomerically pure Thienoacene and Ladder Polymer and their Electronic, Mechanical and Optical Properties

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Abstract

With their electron rich skeleton thienoacenes have traditionally been used as hole transporting materials in organic electronic devices. Also, small molecule semiconductors are now gaining attention in organic electronics and are a field of active research for material chemists as these materials are easy to purify and form crystalline films for the fabrication of the desired high-performance devices. Despite their simple and similar molecular structure the hitherto reported, thienoacenes show different properties in OFET devices. The smallest members of the series, i.e the syn and anti isomers have been compared based on their crystal structure and their properties are rather diverse. The crystal of anti isomer also displays excellent elasticity. We have reported a new, simple yet amazing synthon which is an excellent precursor for the synthesis of a wide variety of thienoacenes. An advantage of this synthon is its ability to give isomerically pure acenes in excellent yields. Using this synthon we have synthesized a "Nonacene" having all syn oriented thiophenes and we are also using it for the synthesis of ladder polymers.

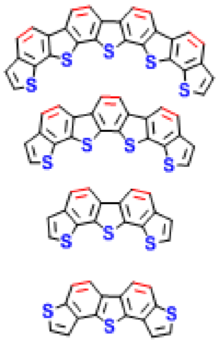

Fig : 1

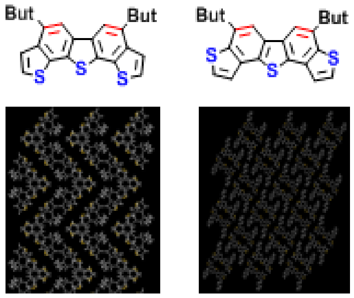

Fig : 2

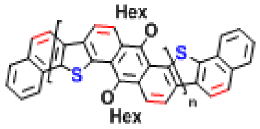

Fig : 3

Fig:1 Isomerically pure Thienoacene, Fig: 2 Different Crystal packing of Two Isomerically pure pentacene,Fig: 3 Ladder polymer

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PREA-OL-03

Enhancing Piezoelectric Properties of Poly(vinylidene) Fluoride and their Copolymers

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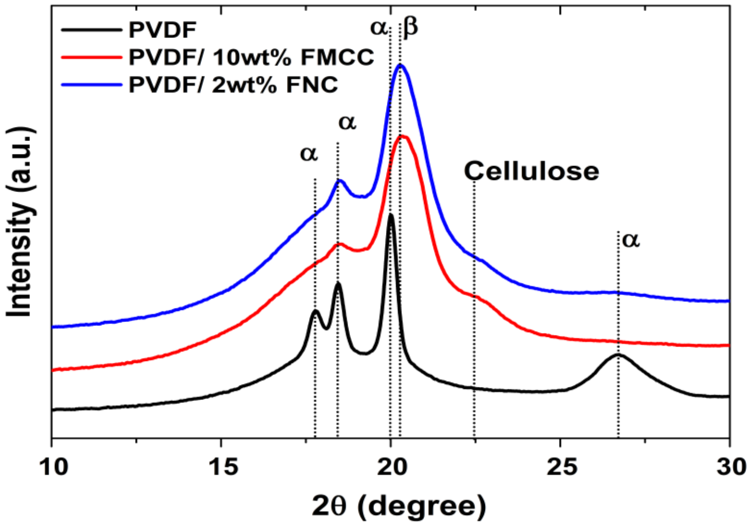
Abstract

Piezoelectric polymers have potential applications in small self-powering devices and as actuators, sensors etc. Applications in internet of things, security, environmental and implantable medical devices could make themimportant materials of future.[1]Melt-processed poly(vinylidene) fluoride (PVDF) shows thermodynamically stable non-polar phase (α-phase). To realize the piezoelectric properites of PVDF, it is very essential to crystallize PVDF in its electroactive phases (β and γ).[2] Herein, we report use of fluorine modified cellulose as a β/γ phase initiator in the PVDF. The fluorine modification on cellulose helped to reduce the phase seperation, and the favorable interactions between PVDF and fluorinated cellulose led PVDF to crystallize in the electroactive phases. We also investigated the effect of particle size and found that nanocrystal has greater effect over microcrystals. This could be attributed to the enhanced specific surface area of nanocrystals leading to enhanced interactions. Further, we found that the fluorinated nanocrystalline cellulose also improved the extent of polar phase in PVDF co-polymers.[3]



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PREA-OL-04

All solid-state polymer electrolyte for lithium metal batteries by cationically initiated crosslinking process

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Abstract

In the field of lithium-ion battery (LiB), solid-state electrolytes are envisaged as a reliable alternate to existing carbonate-based liquid electrolytes [1,2]. However, many constraints have restricted their introduction into the industrial scale production line. The most known reasons are poor ionic conductivity, low Li^+-ion transport properties and extreme processing conditions. Researchers have proposed several possible industrial scale solvent-free processessuch as in situ preparation of polymer electrolytes [3] using free radical and/or ionic polymerization technique. Even though many research activities are directed towards polymerization processes that transforms a liquid mixture in to a 3D-crosslinked polymer network, still the industrial scale production of polymer electrolytes for LiBs is an oasis. In this respect, we are proposing the synthesis of all solid state polymer electrolytes from epoxide based oligomers using thermally induced cationic ring opening polymerization (CROP, see **Figure 1**). CROP has not been convincingly employed in the field of LiBs, and we have developed an all solid-state polymer electrolyte that exhibit ionic conductivity above 0.2 $mS.cm^{-1}$ at ambient conditions. The polymer electrolyte exhibits an anodic stability above 5V vs. Li/Li^+ and excellent cycling at elevated temperature for several hundreds of cycles. The results achieved in our labs confirms that lithium salt catalyzed thermally induced CROP is an industrially up scalable technique with enormous potential for the production of all solid-state polymer electrolytes.

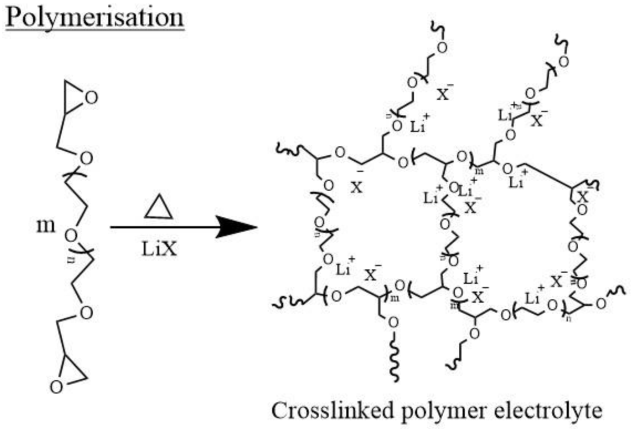

Figure 1: schematic representation of a crosslinked polymer electrolytesynthesised by CROP technique.

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PREA-OL-05

Application of Cellulose Nanocrystals as Ionic Conductor for Fabrication of Solid Electrolyte Membrane for Direct methanol Fuel Cells

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Abstract

The study reports the use of bio-filler: cellulose nanocrystals (CNCs) in the area of fabrication of solid electrolyte membranes for direct methanol fuel cells (DMFCs). CNCs were synthesized by hydrolysis process by using three types of acids H_2SO_4, HNO_3 and HCl. The acids used in hydrolysis had effect on the shape, size and morphology of CNCs, which affected the properties of electrolyte membranes also. Poly (vinyl alcohol) (PVA) and chitosan were used as the polymer matrix. Crosslinking of PVA and chitosan provided the stability to the membranes. CNCs are incorporated in the polymer matrix to improve the ion conductivity. The methanol permeability of prepared membranes was ~10^{-8} cm^2 s^{-1}, which is significantly lower than the base PVA membrane. Along with it, the membranes had good thermo-mechanical properties, low swelling characteristics and higher ion conductivity. Among the three types of CNCs, HNO_3 hydrolysed CNCs based membrane showed better performance in water uptake, ion conductivity and swelling, while HCl CNCs based membrane had better methanol barrier properties. As the methanol permeability of HNO_3 CNCs based membrane was almost equal to HCl CNCs based membrane and it was superior in other properties, so it can be concluded that HNO_3 CNCs based membrane can be a suitable and sustainable option for solid electrolyte used in DMFCs.

Acknowledgements: The authors are thankful to the Department of Chemicals and Petrochemicals (GoI) funded Centre of Excellence for Sustainable Polymers, IIT Guwahati and Central Instruments Facility, IIT Guwahati for utilizing their research facilities.

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Abstracts for Invited, Short and Oral Lectures Under the Theme Soft Materials and Rheology (SMR)

SMR-IL-01

Anomalous temperature dependence of melt rheology of PLA ionomers

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Abstract

It is well known that the polar ionic groups of an ionomer associate to form nanoclusters within the non-polar matrix of the backbone polymer. These self-assembled nanoclusters remain intact even at high temperatures beyond the softening/melting point of the polymer where they serve as transient crosslinks thereby qualitatively modulating rheology of the polymer. Thus for example, ionomer melts typically exhibit high zero shear viscosity and enhanced melt elasticity. However, the temperature dependence of their rheological properties is not known to show any unusual behavior. In this presentation, we will demonstrate for the first time an anomalous inverse temperature dependence of the rheology properties of star telechelic ionomers of poly(D,L-lactide). Using atomistic MD simulations and SAXS data we argue that this surprising behavior arises because of the temperature dependent dynamics of association-dissociation of the ionic clusters. The inverse temperature dependence has significant implications on melt processibility of PLA.

SMR-IL-02

Network formation and disruption in supramolecular gels - insights obtained from linear and non-linear rheology

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Abstract

Assembly, characterization of supramolecular gels and their exploration for various applications have proliferated over last few years. Given the requirements of mechanical stability, rheology is often used to determine the mechanical response of these gels. In this work, we investigate rheology of few model supramolecular gels of ureido-toluene, and of non-proteinogenic amino acids. In addition to the characterization of frequency response, we observe the large amplitude oscillatory shear (LAOS) rheology of these systems. We show that the response can be interpreted in terms of networked systems or soft glassy systems, depending on the gel.

SMR-IL-03

Carboxymethyl Cellulose-based Double Network Hydrogels
With Tunable Network Architecture

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Abstract

Polymeric hydrogels continue to find wide range of applications in drug delivery, tissue engineering, bio-implants, scaffolds, due to their softness, biocompatibility, water permeability, stimuli responsiveness, self healing etc. However, one of the major drawbacks of hydrogels is the lack of mechanical strength. In view of this, "Double Network Gels" (DN) are becoming very important. In this work, we report on DN hydrogel consisting of a tightly cross linked carboxymethylcellulose (CMC) and a loosely cross linked poly(hydroxyethylacrylate)-*co*-Stearyl methacrylate [CMC-PEHA-*co*-SM-DN]. Compressive strength of the CMC-PEHA-*co*-SM-DN gel was found to be 280 times more than that of CMC-SN (single network) gel and with an increase in SM concentration, DN gels showed better recovery after deformation. Stress relaxation measurements showed the ability of DN gels to recover even after continued deformation. The biocompatibility and the cell viability of DN gels arise from the presence of bioactive polysaccharide (CMC) units in it. The network structure could be tuned by varying the ratio of co-monomers in the second network which contributed to the dissipation of energy during deformation. These gels show great promise in implants which addresses the issue of prolonged stress at the implant-site and can expand their life span.

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SMR-OL-01

A Highly Stretchable, Tough, Self-Healing and Thermoprocessable Polyacrylamide Chitosan Supramolecular Hydrogel

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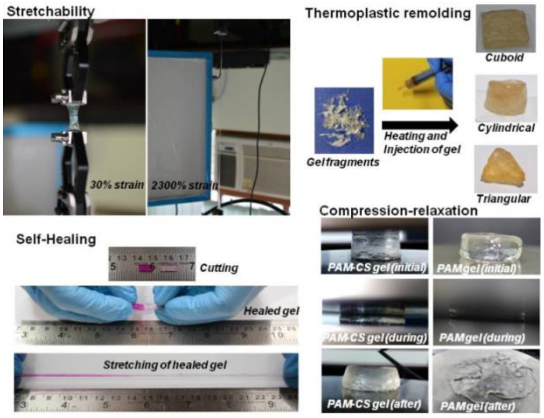
Abstract

Hydrogels have great potential for applications in fields such as tissue engineering[1], drug delivery, and actuation. However, most of the hydrogels do not possess simultaneously a high mechanical strength and toughness (stretchability) that could enormously expand the scope of these applications. Combining these two properties is not trivial as they typically are mutually exclusive[2]. Herein, we have synthesized a hybrid hydrogel by polymerizing AAM in the presence of very short chain Chitosan (a biopolymer) in neutral medium (water) without any covalent cross linker. Although these hydrogels contain ~ 81 % water, they can be stretched up to 30times their original length compared to a physical gel of polyacrylamide(PAAm), which can only withstand a stretching of 1.3 times its original length. Thehybridphysical hydrogelis nearly 6650 times tougher, 370 times higher tensile strength with better stiffness than that of parent PAAmhydrogel. They can also withstand a compressive strain of 95% without fracture and recovertheir original shape after removal of the strain. These gels exhibit high fracture energy (2338 ± 150J/m^2)and pronouncedhysteresis during loading-unloading cycle indicating the presence of effective energydissipation mechanism contributing to toughness. The hydrogel can be reprocessed and healed by heating at elevated temperature. The polymer hydrogel showed a combination of unique properties, which may lead it to find an application in biological systems.



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SMR-OL-02

Application of nanoindentation and nanoscratch techniques in extracting viscoelastic and tribological properties of Soft Material Surfaces

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Abstract

Soft materials are gaining significant attention these days due to their potential applications in various engineering, physical and chemical sciences. For instance, polymer thin films[1], hydrogels, soft colloids particles[2], biomaterials typically of dimensions 10 nm to 10 µm find applications in electronic displays, contact lenses, drug delivery, and regenerative engineering respectively. Macroscale characterization techniques such as simple fragmentation test, scratch[3], and dynamic tests are available to estimate the viscoelastic and tribological properties of soft materials. However, these techniques cannot be successfully applied when the material is confined to a particular direction. In this work nanoindentation, nanoscratch techniques are applied to extract the mechanical properties of polymer thin films and colloidal particles. The residual impression left on the surface of the polymeric material after nanomechanical tests are shown in Figure in 1(a) and 1(b). Both load control (varies from 80 µN to 1000 µN) and depth control (varies from 50 nm to 1500 nm) tests are performed on different materials. Systematic image analysis has been done to measure the contact area at different time intervals. The viscoelastic properties such as storage modulus, loss modulus, and tribological properties such as coefficient of friction and instantaneousscratch hardness are reported. A new model to predict the time-varying hardness is proposed.

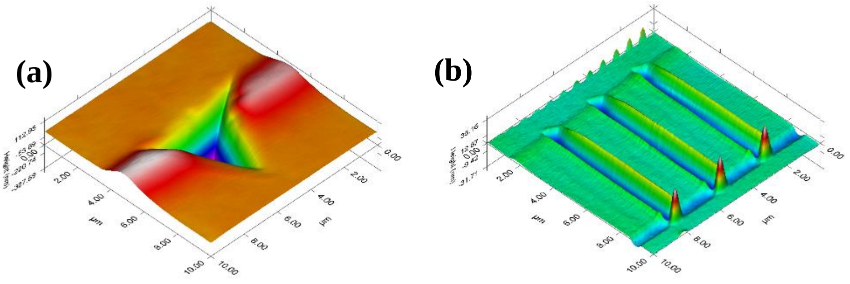

Figure 1. Scanning probe images showing the residual indentation and scratch Impression b left on the surface of the polymeric materials

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SMR-OL-03

Rheological Fingerprints' of Shear Thickening Fluids for Energy Damping Systems

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Abstract

Shear thickening fluids (STFs) are amongst the new class of smart materials developed over a decade to explore its exceptional energy dissipating property associated with a rise in fluids' viscosity[1]. This unique characteristic is a result of particles' rearrangements under shear in presence of Newtonian liquids[2].Several physical and chemical properties of both suspended particle and the liquid medium independently stimulate the uniqueness of the liquid-solid transition[3]. The current work investigates the fundamentals of the mechanism involved in transition and forces of interaction by detailed rheological experiments under various modes.The research presents the occurrence of shear thickening as well as shear thinning in colloidal particle suspensions. Fumed silica in PEG 400 at 20 wt% and surface functionalized silica in PEG 400 at 62 wt% shows a shear thinning behaviour with high yield stress.The varying particle concentration in different colloidal suspensions displayed discrepancy in the flow behaviourleading to further investigation of suspensions in non-linear region, to individually determine the elastic and viscous domain contributions. Large amplitude oscillatory shear experiments[4] (LAOS) showed highest energy dissipation per cycle per volume for 20 wt% fumed silica-suspension as well as great amount of stored elasticity. This contradicts its shear thinning behaviour obtained in steady rheology. Similar results were found for silane modified silica-suspension.In conjunction with LAOS, the effect of silicas' shape polydispersity on the structural deformation and regeneration characteristics of suspensions was demonstrated bythe three interval thixotropic test[5](3ITT). The regeneration of particle structure after each disruption phase carried out 3 times in succession was observed to be greater than the previous phase.

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Abstracts for Invited, Short and Oral Lectures Under the Theme Theory, Simulation and Modelling of Polymers (TSMP)

TSMP-IL-01

Theory of Driven Polymer Translocation through Nanopores

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Abstract

The translocation dynamics of polymers though nanopores driven by external forces is a far-from-equilibrium process, which can be understood based on the tension propagation (TP) theory of Sakaue [1]. In particular, the coarse grained Brownian Dynamics TP theory within the iso-flux (IFTP) assumption [2] allows a self-consistent derivation of analytic equations of motion for the dynamics, including an explicit form for the chain length dependence of the average translocation time [3]. In this talk I will discuss the fundamentals of the IFTP theory and its various applications theory to translocation dynamics of long semi-flexible [4] and end-pulled polymer chains [5]. Time permitting I will also discuss recent works trying to elucidate the role of hydrodynamics and electrostatic interactions on translocation of rod-like molecules in finite and infinite cylindrical nanopores [6].

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TSMP-IL-02

Glass Transition in Polymers from a Molecular Dynamics Viewpoint

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Abstract

To describe physical properties, simulated systems must be correlated to reality in the most effective way. Experimentally, materials are usually in thermodynamics equilibrium. Therefore, they are simultaneously in chemical, radiative, thermal and mechanical equilibria. The two formers are implicitly attained during simulation. The thermal equilibrium is reached using efficient thermostat algorithm. However, mechanical equilibrium is not reached easily. A specific procedure is thus carried out: the volume of the cell with periodic boundary conditions is varied until a minimum in energy is attained. At the bottom of the well, the internal pressure due to interactions inside the polymeric systems equals the stress imposed by the cell, mechanical equilibrium is attained. We show that if it is not achieved, some discrepancies in the final properties can be obtained. We thus disclose how reaching this state is important to calculate mechanical properties and to get reproducible glass transition temperature (T_g). Based on the ensuing accurate results, we argue that atomistic simulation acts as a *slow motion*, or overcranking, used by high-speed cameras to reveal slow-motion [1], paving the way to interesting opportunities in the description of the glass transition from an atomistic viewpoint. More specifically, it offers the significant opportunity to show that the transition from the amorphous state to the glass phase may be detailed in terms of the degrees of freedom freeze.

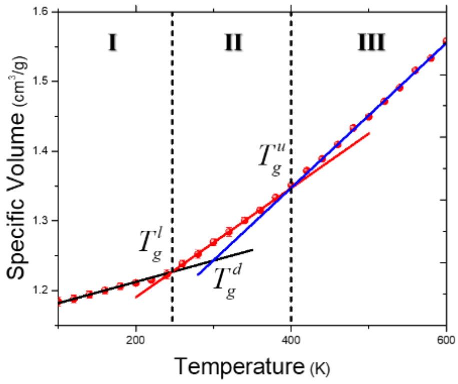

Figure: Specific volume with respect to the temperature (K) for PE.

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TSMP-IL-03

Conformational Transition in Dendritic Polymers

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Abstract

Dendritic polymers are highly branched, acyclic polymers centered on a multifunctional core, resembling a Caylee tree. Compared to linear polymers of the same molecular weight, dendrimers are highly soluble with decreased melt viscosity and low crystallinity. Unlike dendrimers, hyperbranched polymers are devoid of a distinct core with well-defined generations of growth. The conformational properties of these polymers are explored in the framework of optimized Rouse-Zimm theory and with molecular dynamics (MD) simulations. A structural transition is observed in the higher generation dendrimers with a change in the bond orientation angle and strength of excluded volume interactions. This structural transition is a characteristic feature of the topology of dendrimers. This implies that the core of dendrimers is dense, while the terminal groups are distributed throughout the core and the periphery. A similar conformational transition is observed in a MD simulation study as a function of solution pH.

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TSMP-IL-04

Computer Simulations of Novel Polyelectrolyte Membranes for Fuel Cells and Flow Batteries

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Abstract

Recent experiments on polyelectrolyte membranes show that perfluoroimide acid (PFIA) has a higher electrical conductivity than widely used Nafion. We have performed classical molecular-dynamics simulations to study the structural properties of both materials, and the proton and water transport in the corresponding membranes. Our simulations showed the formation of large continuous and connected water clusters in PFIA at high hydration levels which promotes conductivity. Both PFIA and Nafion were percolated at the same hydration levels although PFIA had lesser connected volume as compared to Nafion. The diffusivity constants for hydronium ions and water increase with increasing hydration and increasing temperature and were comparable to that if Nafion. The simulated diffusive conductivity values of PFIA were higher than those for Nafion due to larger number of charge carriers in PFIA. Interestingly, we observed a higher total number of water molecules in the first coordination shell around hydronium in PFIA than in Nafion. This should aid in more hydrogen bonding between hydronium and water in PFIA which, in turn, should help in structural diffusion. Finally, we discuss our preliminary results of the proton transport in Nafion membranes filled with the graphene oxide nanoflakes and doped with ionic liquid.

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TSMP-IL- 05

Kinetics of conformational changes in polyelectrolyte systems

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Abstract

Equilibrium phase behaviour of charged-polymer (polyelectrolyte) systems has been well-studied over past several decades. Interest in the kinetics of conformational changes in such systems, however, has been sporadic, but has received recent attention given their relevance to biological problems like protein-folding or biomedical processes like drug-delivery. Our group has been working on studying the time-dependent, inhomogeneous profiles of physical variables, such as mass and charge densities and osmotic stress, related to such kinetic processes. We will present our understanding that we have developed on this topic over the past two years, especially for two systems - polyelectrolyte gels, and single, isolated, polyelectrolyte chains. Our study considers important issues like charge-regularization and role of elasticity and electrostatics to modulate the spatially varying osmotic forces, which drive these diffusive conformational changes. The major results we have obtained include estimation of effective modulus of charged gels, time-dependency of the size of a gel or a single chain as a function of its charge content, temperature, density of cross-links, and chemical affinity of the polymer and the solvent, relaxation time of swelling as function of the above parameters. The non-linear theory we propose addresses arbitrary deformation, which is in accessible to prevalent linear theories.

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TSMP-IL-06

Molecular Dynamics Study of Interactions between a Zwitterionic Thiophene Polymer and Surfactants

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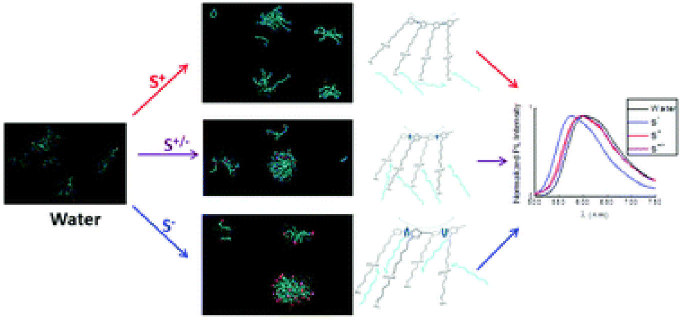
Abstract

Water-soluble conjugated polythiophene (PT)-based polyelectrolytes are an important class of conjugated polymers receiving great attention as active materials in optoelectronic devices and biosensing.[1] PT derivatives show unique chromic features that can be used as rapid and versatile detection tools as the colour of PT solutions can vary from deep violet (λmax ~ 550 nm) to bright yellow (λmax ~ 400 nm).[2] These changes in π–π* transitions are related to conformational changes of the backbone from planar to nonplanar so an understanding of the structural properties of PTs is essential. The optical and structural properties of a zwitterionic PT (P3SBDEAHT) and its interaction in water with surfactants have been investigated.[3] Molecular dynamics simulations were used with experimental methods to closely examine the interactions taking place between P3SBDEAHT and a range of differently charged surfactants. Different surfactants were studied to evaluate the effect of the head group and chain length on the self-assembly. Experimental data emphasize the importance of polymer–surfactant electrostatic interactions in the formation of complexes. Nevertheless, MDS data have shown that nonspecific interactions also play an important role. These interactions seem to be responsible for the spatial position of the surfactant tails in the complex and the consequent breaking-up of P3SBDEAHT aggregates.



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TSMP-IL-07

Aggregation characteristics, thermodynamics, dynamics and mechanism of polyelectrolyte-neutral block copolymer micellization in aqueous solution

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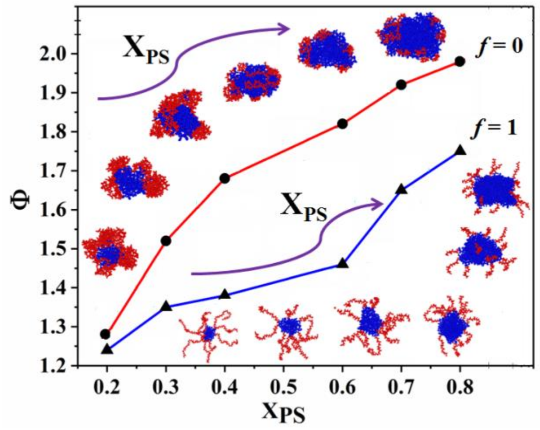
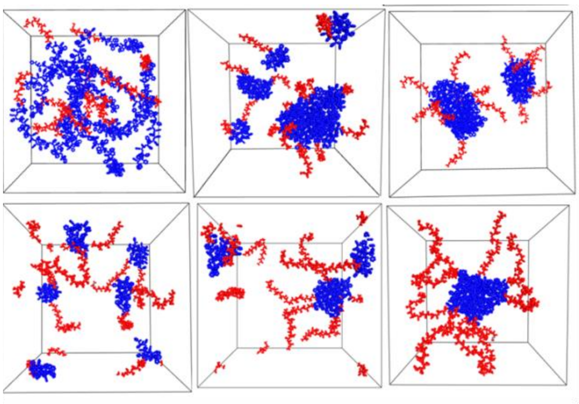
Abstract

Micelle characteristics, intermolecular structure, thermodynamic behavior and dynamics of micellization process of symmetric and asymmetric polyelectrolyte-neutral block copolymer, in aqueous solution was studied via atomistic molecular dynamics simulations as a function of the copolymer composition (X_{PS}) and the fractional charge (f). Simulations show favorable copolymer-water interaction responsible for micelle formation and solvation influenced by hydrogen bonding interactions. The core shows power-law dependence with respect to number of units with an exponent 0.56 in excellent agreement with scaling relations and experiments. Increase in X_{PS} results in a linear increase in micelle size and change in shape from spherical to prolate. Structural and thermodynamic analysis confirm the existence of micelle in osmotic regime, in agreement with mean-field theory. Micellization kinetics, dynamics and diffusion were investigated by the molecular simulation approach for the first time in the field. Asymmetric micelle follows a combined approach of unimer insertion and cluster fusion mechanism while interestingly symmetric micelle follows exclusively unimer insertion process. Micelle formation takes a longer time for copolymers having charged (ionized) block ($f > 0$) and relatively short core block ($X_{PS} < 0.5$) in qualitative agreement with DPD simulations on uncharged copolymer micelles. Hydrophobic insoluble blocks show slower relaxation than soluble blocks. The relaxation of PAA-water h-bonds is slower for charged system as compared to uncharged system. Other detailed characterizations not easily possible by experiments will also be presented.





TSMP-IL-08

The glass forming ability in binary mixtures: Role of mixing entropy

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Abstract

When a liquid is cooled very fast, it avoids crystallization due to suppression of nucleation and enters the supercooled liquid regime and on further cooling undergoes glass transition at **Tg**. The glass forming ability (GFA) is the tendency of the system to avoid crystallization and undergo vitrification. In this talk I will discuss about the properties which contribute to the GFA. I will present a study of different binary mixtures where we have shown that although all of them have a global crystalline minima some undergoes crystallization and some are stable in their supercooled liquid state[1]. Our study suggest that the stability against crystallization comes from the frustration between the locally favoured structure and the global structure. This frustration is manifested best when a global structure is a mixed crystal where a single species contributes to both the crystal form and where the two crystal forms have large difference in some order parameter related to that species. I will then present the study where we have taken one of the glass forming systems and studied it at different compositions [2]. The global minima in all the compositions are a mixed crystal thus in
all these systems the frustration between the locally favoured structure and the global structure are similar. However we found that depending on the composition, the barrier to crystallization and thus the glass forming ability varies. We have also shown that the pre crystalline liquid undergoes a demixing process. This variation in the GFA of the different compositions have been connected to the loss of mixing entropy in the process of crystallization. Our study further reveals that the stability of a system against crystallization comes both from kinetics and thermodynamics.

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TSMP-IL-09

Role of Polymer-Pore Interactions in Translocationdynamics

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Abstract

The transportof a polymer through a nanoporeplays an importantrole in severalbiologicalprocesses, such asthetranslocationof DNA and RNA acrossnuclearpores, transportofproteinthroughmembranechannels, andvirusinjection. The basicquestionconcernsthedependenceofthetranslocation time on thesystemparameters such asthe polymer chainlength, sequence, porelengthandporewidth, externaldrivingforce, and polymer poreinteraction. Driventranslocationprocessis an out ofequilibriumphenomenaandcannotbecapturedfromtheoreticalcalculations. In ourworkweinvestigatetheinfluenceof polymer-pore interactions on thetranslocationdynamicsusingLangevindynamicssimulations. Oursimulationresultsshowthestrengthandspatialdistributionofinteractionscanstronglymodifythetranslocationdynamics. We also showthatthedynamicsofinteractionof a polypeptidewiththenanoporecanbetunedbyalteringthe pH gradientsacrosstheporethatcan alter thecaptureandescape rate ofthepolypeptidethroughtheproteinpore. Oursimulationresultsarequalitativelyexplainedbyfreeenergycalculations. Ourcoarse-graineddescriptionofthetranslocationdynamicsexplicitlyconsidersthe individual contributionofthefilling, transfer, andescapestagetothetranslocation time in oursimulationsthatisdifficulttoobtainfromtheexperiments.

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TSMP-IL-10

Bacterial chromosome organization: special crosslinks, confinement effects and molecular crowders play the pivotal roles

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Abstract

Using a coarse-grained bead-spring model of bacterial chromosomes of *C. crescentus*(and *E. coli)*we show that just 33 (and 38) effective cross-links in 4017 (and 4642) monomer chain at special positions along the chain contour can lead to the large-scale organization of the DNA polymer, where confinement effects of the cell walls play a key role in the organization. The positions of the 33/38 cross-links along the chain contour are chosen from the Hi-C contact map of *C. crescentus and E. coli*. We represent 1000 base pairs as a coarse-grained monomer in our bead-spring flexible ring polymer model of the DNA. Thus a 4017/4642 beads on a flexible ring polymer represents the *C. crescentus/E.coli* DNA polymer with 4017/4642 kilo-base pairs. Choosing suitable parameters from our preceding study, we also incorporate the role of molecular crowders and the ability of the chain to release topological constraints. We validate our prediction of the organization of the bacterial chromosomes with available experimental data and also give a prediction of the approximate positions of different segments within the cell in 3D.

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TSMP-IL-11

Role of Particle Based Simulations in Industrial application of Soft Materials

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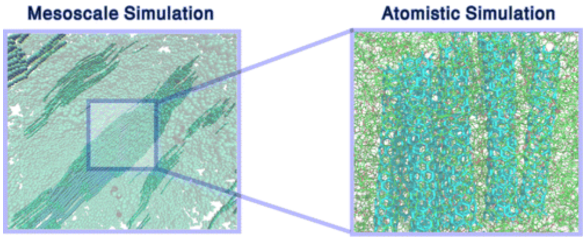
Abstract

In this talk I intend cover various application areas of soft materials for which particle-based simulation methods like molecular dynamics, coarse graining, mesoscale simulations were applied, and some cases developed to address relevant problems toward industrial applications. Choice of simulation methods are highly specific for soft materials as per the length (size) and time scale of the observable one would like to resolve. So, during my talk, I shall be addressing different methods as per the length and time scale and will connect to the final observable (properties-prediction) of the problems. I intend to present some building blocks of iterative Boltzmann inversion coarse graining (IBI-CG) and mesoscale dissipative particle dynamics methods (DPD) and show how the interaction potentials are optimized for certain applications.

I have plan to cover application areas starting from fuels, lubricants, kinetic hydrate inhibitors, gels, rubber to drug delivery vehicles. In each of these application areas I intend to show how we have attempted issues which helped the related industries in designing new additives (for lubricant), kinetic inhibitor (gas hydrate, pipe line flow assurance), gel formation, glass transition of rubber-composites and delivery vehicle for cancer chemotherapy drug.



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TSMP-IL-12

Nanostructure and Dynamics of Polymer Electrolyte Membranes: Insights from Molecular Dynamics simulations

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Abstract

The Perfluorosulfonic acid and Benz-imidazole family of Polymer Electrolyte Membranes (PEM) have been extensively investigated for proton conduction in low and medium temperature fuel cells. In this talk, I will provide a broad overview on the utility of classical Molecular Dynamics (MD) simulations (using all atom force-fields) to calculate, predict and validate membrane nanostructure and dynamics of molecular/charge transport in various fuel cell operating conditions. The caveats of molecular modeling and simulation of such large complex macromolecular systems will be briefly discussed. The influence of membrane humidity, effect of dopant type and concentration and pendant side chain length will also be presented. The properties elucidated from the simulations will largely focus on Pair Distribution Functions (to examine inter-molecular interactions), radius of gyration and diffusion coefficients in several PEM environments. Finally, the limitations of classical MD simulations to describe the structural diffusion of protons and hence the need for computationally expensive ab initio MD simulations methods will be highlighted.

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TSMP-OL-01

Crystallization of Binary Polymer Blends Studied by Dynamic Monte Carlo Simulation

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Abstract

Polymer blends are known to be one of the exciting materials to prepare nanoscale devices via self-assembly. The thermodynamic and mechanical properties largely depend on their mutual miscibility. Miscible blends usually give a single glass transition temperature, whereas immiscible blends produce two distinct glass transition temperatures. Since the components in the blend are chemically dissimilar, they phase separate via macrophase separation. We report dynamic Monte Carlo simulation results on the crystallization of A/B binary polymer blends with varying composition, wherein both the components are crystallizable. We model A-polymer as high melting component and hence its crystallization precedes the crystallization of B-polymer upon cooling from a homogeneous melt. The morphological development is controlled by the interplay between crystallization driving force (attractive) and de-mixing energy (repulsive) between the components [1]. With increasing the composition of B-polymer, macrophase separation, crystallization and lamellar thickness follow a non-monotonic trend [2]. This non-monotonic trend is attributed to the composition-heterogeneity in the blend. When one component is relatively less compared to the other, its mobility is reduced affecting transition temperature during crystallization. As a result, transition happens at a relatively lower temperature (viz., enhanced thermal driving force). Isothermal crystallization reveals that the crystallization behavior and crystal morphology strongly depends on the mode of cooling. Two-step, compared to on-step isothermal crystallization provides better crystalline structures. Finally, some recent results on thin film crystallization on patterned substrate will be discussed.

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TSMP-OL-02

Role of Multidentate Carbonate Donor in $MgCl_2$ supported Ziegler-Natta Olefin Polymerization Catalysis: A DFTStudy

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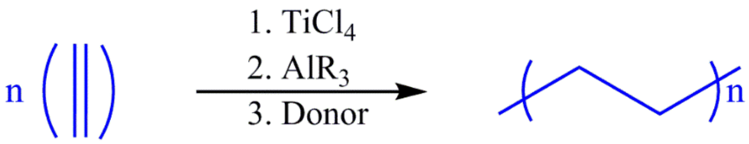
Abstract

Full quantum chemical calculations using density functional theory (DFT) have been donein order to understand the role ofmultidentate carbonate as a potential donor in Z-N catalyst system. In this regard, firstly, four different donor coordination possibilities such as mono, di, tri and tetra, to the $MgCl_2$ surface have been investigated. It has been observed that tridentate coordination possibility has stabilized the surface more in comparison to other coordinations. In order to validate the effectiveness of the multidentate donor, three different industrial relevant donor classes such as phthalate, diether and succinate have also been used. These results indicate that multidentate donor stabilized the surface two folds in comparison to the other existing donor catalyst systems. Moreover, the effect of multidentate donor has also been investigated for the insertion and the termination steps with respect to other donor catalyst systems. These results suggest that the multidentate donor significantly influences the catalyst performance. Furthermore, the regio- and stereoselectivebehaviour of propylene monomer on the titanium growing polymer chain has also been investigated and it has been observed that the multidentate is equally effective as other donors. Therefore, the current chemical calculations provide new insight into the nature of donor interactionwith the $MgCl_2$ surface.



Abstracts for Invited, Short and Oral Lectures
Under the Theme
Functional Polymers and Composites (FPC)

FPC-IL-01

Polythiophene-graft-polyelectrolytes for Different Optoelectronic Applications

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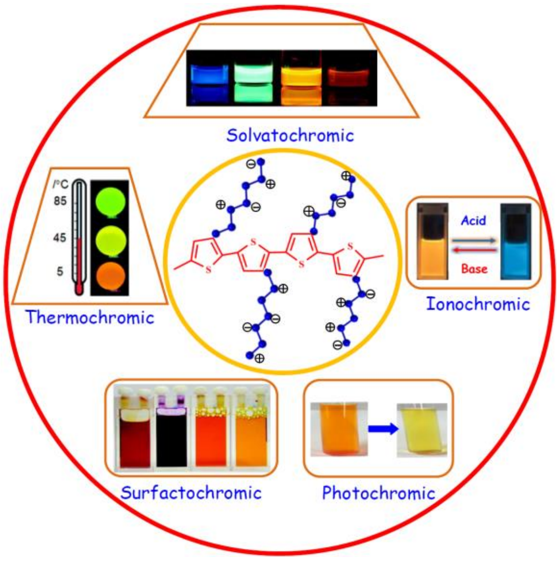
Abstract



In the field of materials science, conjugated polymers having fluorescence property are the stunning candidate for the fabrication of multifunctional smart polymeric materials. mong the entire conducting polymers, polythiophene is a well-known conjugated polymer showing tuneable fluorescence property and electrical conductivity, arising from the different conformational states of the conjugated chain. On the other hand, polyelectrolytes are polymers whose repeating units bear ionic groups. The pendent ionic groups of polythiophene-graft-polyelectrolyte dissociate in aqueous solution, making polythiophene soluble in water that opens a scope to alter its aggregation style in several self-organized patterns for fundamental and application based works. So, we have firstly synthesized a new water soluble cationic polythiophene for specific detection of highly toxic cyanide ion much below the level of lethal dose (limit of detection limit is 4.4 ppb) in pure water even in presence of other ions using the fluorescence property. We have synthesized a water soluble polythiophene-graft-polyampholyte which shows reversible fluorescence turn "on/off" behavior with sequential addition of differently charged ionic surfactants at different pHs of the medium. In another attempt we have successfully able to tune the optical and electronic properties of ampholytic polythiophene with its self-assembled nature utilizing the position of iodide ion by varying pH or by adding polyanionic RNA. We have designed a water soluble uracil anchored cationic polythiophene where the electronic structures of π conjugated backbone is successfully manipulated by light irradiation, to get superior optoelectronic properties and to regulate light induced thermo responsiveness in presence of halide screening agents.

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FPC-IL-02

SYNTHESIS OF FUNCTIONAL SMART HYBRID MATERIALS

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Although technological and scientific importance of functional polymers have been well established over the last few decades, the most recent focus that attracted much attention are stimuli-responsive polymers. This group of materials is of a particular interest due to their ability to respond to internal and/or external chemico-physical stimuli that is often manifested by large macroscopic responses. Aside for scientific challenges of designing stimuli-responsive polymers, the main technological interest are numerous applications ranging from reactive surfaces to drug delivery and separation systems, or from chemo-mechanical actuators to other applications that have been extensively explored.[1]Here, different approaches to prepare devices based on thin layers of smart hydrogels will be presented. For instance, temperature responsive films with LCST or UCST behavior were combined with pH responsive hydrogels.[2] Their application in sensors and actuators were demonstrated. To increase the scope of such hydrogels a novel dual crosslinking system combining photocross-linkable covalent bonding with special molecular recognitions sites was introduced.When the noncovalent bond was broken or formed, the swelling ratio of the polymer gel will be changed significantly. Further, an alternative way to synthesize mesoporous Al_2O_3 by using hydrogels as porogenic material is presented. Hydrogels can easily be patterned by light and used to imprint their structure onto alumina opening a new approach to fabricate patterned Al_2O_3. Followed by a nanocasting process mesoporous alumina samples were synthesized.[3, 4]

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FPC-IL-03

Foam processability of Multiphase polymers with supercritical fluids

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Abstract

High potential of microcellular PP, its blend, composite and nanocomposite in automotive industries motivated to make a comparative study on foamability of blends, composite and nanocomposites of PP. In case of blends, foaming of PP/HMS PP blends and PP/crosslinked or uncrosslinked elastomer blends was studied. In general the foam density reduced with increase of branch content of PP irrespective of conditions. DSC analysis of the foams which was foamed at a constant pressure and varying temperature revealed a presence of threshold foaming temperature beyond which the melting point of foams increase significantly. However, increase in pressure did not prove to be sensitive in changing the melting point of the polypropylenes. On the other hand, PP/elastomer blend foams the elastomer particle size played a very key role on foamability of blends, such as smaller particles gave better foam nucleation and homogeneous cell formation. Blends interface acted as the nucleating site for foaming (captured by SEM) and interfacial interaction of raw materials had very important role either in development in blend morphology as well as in foamability. The introduction of crosslinked elastomer into the polypropylene matrix improved the foamability of polypropylene up to a certain limit and then deteriorated. The absolute and specific tensile modulus of foams obtained from the optimized foaming parameters combinations showed an increasing trend with the rise in cell density; whereas, the tensile strength of foams was not sacrificed significantly. In case of composites, PP/fiber system has been considered in present study. Although, the incorporation of fiber increased the foamability of PP; a significant insight could be observed for the uncompatibilized and compatibilized composites in terms of polymer-fiber interaction, which eventually governed the foamability. The compatibilized composites showed lower density foams with smaller cell sizes as compared to the uncompatibilized composites. The effect of rheological influence on the development of microstructure in polypropylene/clay nanocomposites vis-à-vis foamability of the nanocomposites was identified. The fingerprint characteristics of nanocomposites have an enormous role on foam structure development. With the increase in clay loading, cell density increased; furthermore, with an increase in saturation time, there was a phenomenal decrease in expansion ratio of neat polypropylene due to CO_2-induced crystallization which could be mitigated by the incorporation of nanoclay into the polypropylene matrix. Therefore, nanoclay could be exploited as the inhibitor of CO_2-induced crystallization. The objective of introducing HNT and CNT was to facilitate the heterogeneous nucleation for foaming and improvement of melt strength of polypropylene.

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FPC-IL-04

Polymer – Metal/Semiconductor Nanocomposite Thin Films: *In situ* Fabrication and Applications

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Abstract

Polymer-metal and polymer-semiconductor nanocomposite thin films are versatile materials that combine the unique characteristics of the components, and manifest mutualistic effects. The facile, mild and eco-friendly soft-chemical protocol developed in our laboratory, for the *in situ* generation of metal, alloy and semiconductor nanostructures in polymer thin films will be described;[1] the fabrication procedure exploits chemistry within a polymer matrix. The talk will focus on the specific advantages of the fabrication methodology,[2] crystal-to-crystal transformation at the nanoscale,[3] unique nanostructures that can be generated,[4] and a range of analytical[5] and catalytic[6] applications of these versatile polymer based nanocomposite materials.

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FPC-IL-05

Manufacturing of Nanomaterials from Bio-Wastes and Production of Eco-Friendly Bio-nanocomposites

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Abstract

Green chemistry started for the search of benign methods for the development of nanoparticles from nature and their use in the field of antibacterial, antioxidant, and antitumor applications. Bio wastes are eco-friendly starting materials to produce typical nanoparticles with well-defined chemical composition, size, and morphology. Cellulose, starch, chitin and chitosan are the most abundant biopolymers around the world. All are under the polysaccharides family in which cellulose is one of the important structural components of the primary cell wall of green plants. Cellulose nanoparticles (*fibers, crystals and whiskers*) can be extracted from agrowaste resources such as jute, coir, bamboo, pineapple leafs, coir etc. Chitin is the second most abundant biopolymer after cellulose, it is a characteristic component of the cell walls of fungi, the exoskeletons of arthropods and nanoparticles of chitin (*fibers, whiskers*) can be extracted from shrimp and crab shells. Chitosan is the derivative of chitin, prepared by the removal of acetyl group from chitin (*Deacetylation*). Starch nano particles can be extracted from tapioca and potato wastes. These nanoparticles can be converted into smart and functional biomaterials by functionalisation through chemical modifications (*esterification, etherification, TEMPO oxidation, carboxylation and hydroxylation etc*) due to presence of large amount of hydroxyl group on the surface. The preparation of these nanoparticles include both series of chemical as well as mechanical treatments; crushing, grinding, alkali, bleaching and acid treatments. Transmission electron microscopy (*TEM*), scanning electron microscopy (*SEM*) and atomic force microscopy (*AFM*) are used to investigate the morphology of nanoscale biopolymers. Fourier transform infra-red spectroscopy (*FTIR*) and x ray diffraction (*XRD*) are being used to study the functional group changes, crystallographic texture of nanoscale biopolymers respectively. Since large quantities of bio wastes are produced annually, further utilization of cellulose, starch and chitins as functionalized materials is very much desired. The cellulose, starch and chitin nano particles are currently obtained as aqueous suspensions which are used as reinforcing additives for high performance environment-friendly biodegradable polymer materials. These nanocomposites are being used as biomedical composites for drug/gene delivery, nano scaffolds in tissue engineering and cosmetic orthodontics. The reinforcing effect of these nanoparticles results from the formation of a percolating network based on hydrogen bonding forces. The incorporation of these nano particles in several bio-based polymers have been discussed. The role of nano particle dispersion, distribution, interfacial adhesion and orientation on the properties of the eco friendly bio nanocomposites have been carefully evaluated.

FPC-IL-06

Improvement of polymer gas barrier properties through (nano)composites approaches: mechanisms and key-factors

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Abstract

The optimization of polymer barrier properties is currently of crucial importance for a wide range of applications from packaging to building or even energy applications. To meet the requirements of these applications, polymer matrices are often combined with impermeable (nano) fillers. This presentation will enlighten, from the detailed study and characterization of different and selected nanocomposite film series, the particular role of the filler shape, filler location and dispersion state as well as the crucial influence of the filler/matrix interfacial properties on the gas diffusion and final barrier properties. The interest of combining different filler shapes and different nanocomposite preparation routes (e.g. preformed nanofiller dispersion and *in situ* generation of nanofillers) will be discussed. The indirect effects of fillers, such as a modification of the polymer matrix microstructure will be investigated. Finally, the potentiality of modeling approaches based on numerical simulation techniques such as finite element method (FEM)will be demonstrated and the importance of 3D simulation strategies for the understanding and prediction transport properties in the most complex nanocompositestructures will be addressed.

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FPC-IL-07

Conducting Polymer Guest in Porous Coordination Polymer Host

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Abstract

Metal-Organic Frameworks (MOFs), in general, are not electrically conducting due to the insulating nature of the organic linkers and poor orbital overlap between the metal ion and the heteroatom of the linker which does not allow the effective delocalization of electrons across the framework. Though the examples of electrically conducting MOFs and/or their composites are reported, those combining electrical conductivity with fluorescence, leading to multifunctional MOFs, are rare. Herein, we have demonstrated a Cd-based fluorescent MOF to host pyrrole monomers which were then assembled into polymer chains. Polypyrrole chains inside the nanochannels of MOF are confined in such a way that the non-covalent π⋯π/N-H⋯π interaction lead to the formation of percolating conducting paths resulting in the electrical conductivity enhancement by ~9 orders of magnitude.[1] Further, Hall-effect measurements revealed the composite to be an n-type semiconductor with magnificently high-carrier density (η) of $\sim 1.5 \times 10^{17}$ cm^{-3} and mobility (μ) of ~8.15 cm^2 V^{-1} s^{-1}. Also, the florescence of the pristine MOF was almost retained in the composite in the form of associated exciplex-type emission. Such observation on MOF-conducting polymer system will direct the rational designing of such materials for optoelectronic applications.

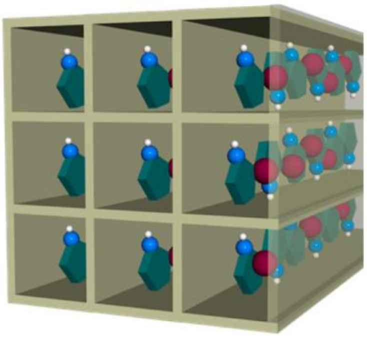

Figure 1: Schematic representing polypyrrole chains assembled inside the nanochannels of the Cd based MOF.

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FPC-IL-08

Porous structure studies on the composite membrane of polyether sulfone incorporated with functionalized multiwalled carbon Nanotubes

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Thin film composite membranes of functionalized multiwalled carbon nanotubes (MWCNT) with polyether sulfone as the membrane matrix were prepared by classical phase inversion process. Unlike the asymmetric membranes that result from the pristine polyether sulfone, the porous structure of the composite membranes is different and unique. Capillary flow porometry as well as small angle neutron scattering (SANS) studies reveal interesting morphology. SANS analysis reveals smaller pore diameters than the results obtained from capillary flow porometry. The cross sectional image of cold fractured membrane from scanning electron microscopy (SEM) shows the asymmetric nature of membranes. The composite membranes show higher pure water flux as compared to the pristine polyether sulfone membrane and so couled be used for efficient removal of heavy metal ions. The CNTs impart higher thermal stability to the composite membranes as shown by Thermo gravimetric analysis (TGA). Interestingly, the conducting properties of membranes as measured by the LCR meter shows significant increase.

Keywords: Multiwalled Carbon nanotubes, Asymmetric, morphology, Small Angle Neutron Scattering.

FPC-IL-09

Toughened Epoxy -Nanocomposites for Structural Applications

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Abstract

The incorporation of nanofillers into epoxy matrix is gaining significant interest in the structural composite application, where strength, stiffness, durability, lightweight, design, and process flexibility are required such as in aerospace and automobile industry. The inherent brittle nature of the epoxy matrix can be improved by the incorporation of nanofillers in the matrix. The realization of nanofiller reinforced epoxies with high toughness requires a homogeneous dispersion and strong interfacial interaction between the nanofiller and the polymer matrix. Generally nanoparticles have a tendency for agglomeration because of the weak van der Waals force of attraction. Surface modifications of nanofillers are an effective way to improve interfacial interaction between the nanofillers and the epoxy matrix, which in turn leads to better filler dispersion, and enhanced mechanical performance in the nanocomposites.Apart from surface modification, nanofiller geometry of a composite also plays a crucial role in determining the mechanical performance of the composites. It is therefore significant to determine the influence of shape on the properties of the composites made with nanofillers. By judiciously selecting nanofillers of different geometry and size, and modifying the surface of these fillers with suitable polymers, tremendous improvement in fracture toughness and mechanical strength can be achieved. In our work, the surface of multi-walled carbon nanotubes (MWCNTs) and GOs were modified by grafting with carboxyl terminated poly(acrylonitrile-co-butadiene) rubber (CTBN) and hydroxyl terminated poly(ethersulfone) (PES). Incorporation of PES and CTBN grafted MWCNTs in epoxy matrix composites imparted tremendous improvement in fracture toughness when compared to pristine and acid modified MWCNT/epoxy composites in addition to the improvement in mechanical characteristics. The TiO_2(B)-NWs shows the highest mechanical properties and comparable thermal properties when compared to TiO_2 nanoparticle. The optimum properties of this system are attributed to the particle shape or particle dimension that has been described by the aspect ratio wherein the elongated filler shows the highest aspect ratio hence improving the bonding between resin and filler.

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FPC-IL-10

Synthesis and Characterization of Sulfonated Semi-fluorinated Aromatic Polytriazoles: Superior Proton Exchange Membrane Properties

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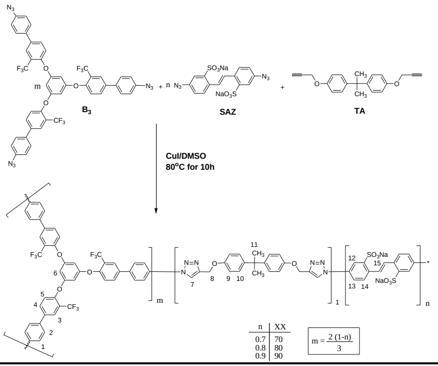
Abstract

Proton exchange membranes (PEMs) are one of the important components of fuel cells and act as solid electrolytes [1]. In this regard, Dupont's Nafion®, sulfonated tetrafluoroethylene based copolymers are commonly used materials because of their outstanding oxidative and chemical stability along with high proton conductivity. However, deterioration in the proton conductivity and mechanical strength at temperature above 80 ^{o}C, and high preparation cost of Nafion® urge the necessity to develop alternative polymers. From this view, our group has prepared different semifluorinated sulfonated co-poly(ether sulfone)s (S (SPIs) and co-poly(ether triazole)s and their properties have been investigated thoroughly.[2] In our work, we found that incorporation of $-CF_3$ groups in the sulfonated copolymers not only help in solubilizing these polymers in selected solvents but also enhances their oxidative stability and helped in getting better phase separated morphology which is responsible for higher proton conductivity.[2,3] In a recent work, we have incorporated a branched unit (**Figure 1**) in copolytriazoles that resulted in improved PEM properties. This work will descuss the effect of this unit (B_3) on the physical properties and proton c and will be compared with their linear analogues. [4,5]



n	XX
0.7	70
0.8	80
0.9	90

$m = \frac{2(1-n)}{3}$

Scheme 1. Reaction scheme of synthesis of the polymers

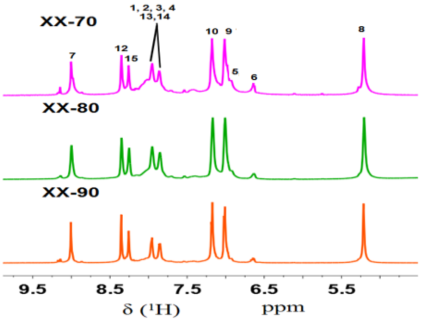


Figure 1. ^{1}H-NMR spectra of the polymers

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FPC-IL-11

Epoxy-resins for Aerospace Applications

Abhijit Som

Abstract is waiting

FPC-IL-12

Graft To, Graft Through and Direct immobilization of polymers on surfaces

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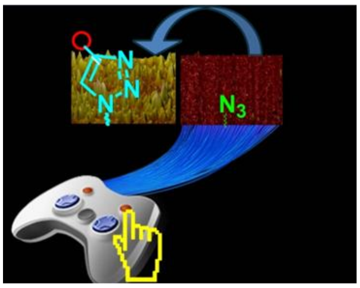
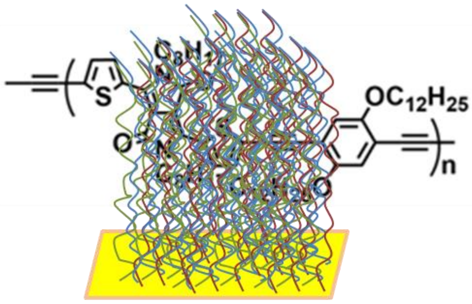
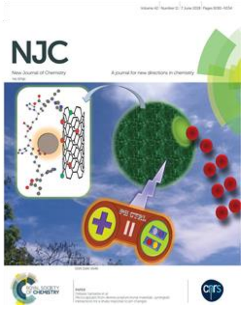
Abstract

Polymers are immobilized on various surfaces for solar cell and molecular electronic device fabrications, biosensor development etc. Although spin coating or Langmuir-Blodgett film formation techniques have been used routinely, more reliable techniques like self-assemble monolayer (SAM) formation technique has been invoked for better results. In this case, a suitable end group is necessary to immobilize to a specific surface. For example, trimethoxysilane functional group may be used to immobilize to silicon and ITO surface or thiol group may be used to immobilize to gold surface. To immobilize polymers to surfaces using SAM formation technique, a graft from, graft to, graft through or direct methods of immobilization can be used. In our recent review article, we highlighted various aspects of immobilization of polymers on surfaces.[1]

In the presentation, we like to highlight our recent results related to synthetic methodology and applications of polymer-immobilized surfaces. Particularly, results related to different methods like graft to, graft through[2] or direct mode of immobilization[3] will be presented. A comparative result related to immobilization of conjugated or semi conjugated polymers[4] using conventional spin coating and more recent SAM formation technique will be presented briefly. A special emphasis will be given on the application potential of those materials. Finally, our recent results on special immobilization techniques on surfaces like leather or leather like materials will be presented.







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FPC-SL-01

Hyperbranched polyimides and their nanocomposites with MWCNTs-COOH/NH_2

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Abstract

A new triamine TAPPSPB was synthesized and successfully polymerized into hyperbranched polyimides (HBPIs) with commercially available dianhydrides BTDA and PMDA by A_2+B_3 method. The structure of the amine and the resulting hyperbranched polyimides were characterized by FT-IR, ^{1}H-NMR, and ^{13}C-NMR analysis. The T_g and $T_{5\%}$ temperature of the HBPIs were in the range of 229-256 ^oC and 430-474 ^oC respectively. HBPI/MWCNT nanocomposites were prepared using TAPPSPB, commercially available dianhydrides and amino functionalized MWCNT by the conventional two step method by varying the percentage of MWCNT (1, 3, 5, and 7 wt %). The T_g and $T_{5\%}$ temperature of the nanocomposites were in the range of 260-266 ^oC and 481-493 ^oC respectively. The results from DSC and TGA show that the T_g and the thermal stability of the HBPI/MWCNT nanocomposites are higher than that of pure HBPIs. The dielectric constant and dielectric loss of the HBPIs and nanocomposites were in the range of 3.05 – 3.31 and 0.64 – 0.83 at 1 MHz respectively. SEM studies revealed that the MWCNT are evenly dispersed throughout the polymer matrix in the nanocomposites. X-ray diffraction studies shows that the synthesized HBPIs and nanocomposites are amorphous in nature.

Keywords: hyperbranched polyimides, A_2+B_3, carbon nanotubes, thermal and electrical properties

FPC-SL-02

Blocked Isocyanates: A view on Equilibrium of Blocking and Deblocking Reactions, Catalysis, New Blocking Agents and Applications in Non-Cured Products

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Abstract

Blocked isocyanates are economically valuable polyurethane raw materials; its concept was first disclosed on 1949[1]. They are technically advantageous over free isocyanates and are used to obtain the performance of two-component polyurethanes in one-component thermally curable systems. Understanding the relationship between reaction parameters of blocking and deblocking reactions is very important in the context of production and use-at-end of these materials. However, this complexity was not resolved until 2016. Similarly, though many reviews on this subject have been published[2-4], none of them addressed blocked isocyanate concept used for applications other than one-component polyurethane products. In this short review presentation, it is intended to describe the new developments made on full spectrum of the reaction through the equilibrium. It is also intended to highlight the use of blocked isocyanates in many synthesis which not aim coatings materials or any heat-curable polyurethane products for which they were originally introduced. Additionally, disclosure on new blocking agents, catalysts and applications of blocked isocyanates are also put forward.

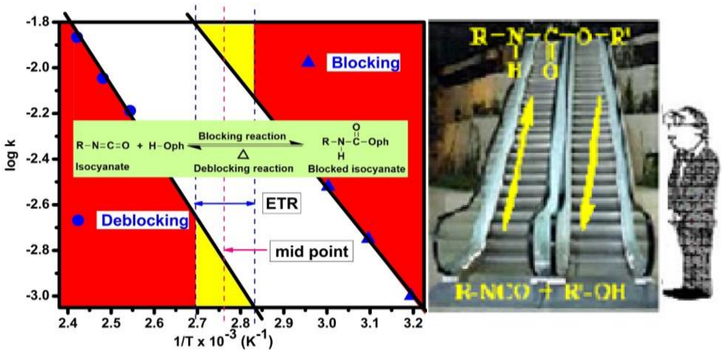

Figure 1. Concept of blocked isocyanate

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APMP-SL-03

Enthalpy based reaction kinetics determination study for bench scale ethylene polymerization in hexane media

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Abstract

Kinetics of olefin polymerization for polypropylene heterogeneous catalysts is important to understand for heat and mass transfer determination during reaction. Molecular level model based on single particle olefin polymerization focuses on reaction constants determination, particle growth, polymerization rates, concentration and temperature profiles, polymer microstructure and particlemorphology [1-4]. Development oftransport phenomena based model requiresmany experiments to be carried out under different experimental conditions and dealing with complex mathematical equations. We have carried out reaction kinetics determination for ethylene polymerization to predict amount of polyethylene formed in a 4 L semi batch (continuous feed) STR reactor using enthalpy based model. Computation of polymerization rate using various mathematical techniques (curve fitting method, MATLAB etc.) has been developed based on reactor and heating media temperature with respect topolymerization time. Heat transfer coefficients were determined for reactor fluid (hexane) and jacket fluid (Diethylene Glycol) for reaction temperature of 80°C. Value of propagation rate constant (K_p) based on developed model was in the range of 1000 to 2500 L/mol.s for lab polymerization reactor. These value are in accordance with value suggested in literature which is 2000-4000 L/mol.s [1] based on transport phenomena based models. Value of decay constant K_d was found in range of 0.1 to 0.27 min^{-1} and initial rate of polymerization rate is in range of 10-25 Kg/g h. Enthaly based model can be quick tool to determine rate constants for comparison of various polymerization conditions and catalyst types basedon propagation and decay constants value from industrial context.

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FPC-SL-04

Polymer Composites for Structural Applications

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Abstract

Composites are a macroscopic combination of two or more materials, with a distinct interface between the individual constituents. Structural composites have fibers as the principal load carrying members whereas the surrounding matrix keeps them in desired location and orientation. The matrix, usually a thermoset polymer, also acts as a load transfer medium between the fibers, and protects them from environmental damages. Because of their low density, high strength to weight ratios and high modulus to weight ratios, polymer matrix composites are being used as primary load bearing structures in aerospace, automotive, and other industries.

In this paper, an 'out of autoclave' composites manufacturing method, viz., Resin film infusion (RFI), is presented. In this process, polymer resin, e.g. epoxy, is cast in film form and sandwiched between two reinforcement layers. These layers are cut to shape, laid on the tool, and vacuum bagged. The rest is a standard vacuum bagging process at ambient pressure and elevated temperature. When heated resin becomes fluid, it flows and wets out the reinforcement. Latent curing agents premixed in the resin, act at an elevated temperature and cured parts are made. A range of products realized through this method for defence applications will be discussed.

Composites realized through RFI method have also been hybridized with nanomaterials. Methods have been optimized to disperse nanomaterials such as Carbon nanotubes, Nanofibers, Nanosilica etc. in Glass/Carbon-epoxy composites. Loading fractions of nanofillers for an efficient reinforcement, yet retaining the ideal processing parameters has been optimized and scaled up for large structures.

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FPC-OL-01

Chemical Modification of Polyisoprene Using Hypervalent Iodine Reagents

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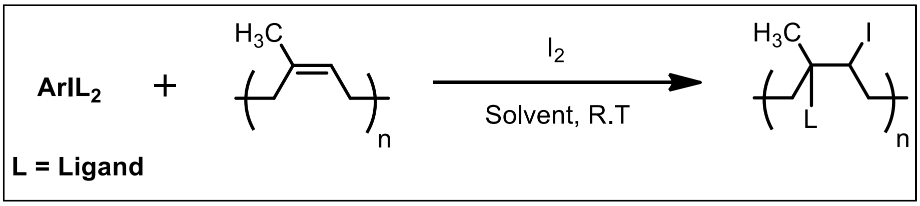
Abstract

Rubber is one of the oldest naturally occurring polymersknown to mankind. The chemical modification of natural rubber, including its functionalization yielding soluble materialswith altered properties and enhanced performance are topics that have gained significant attentionboth from industry and academia.[1-3]Herein, we present anefficient functionalization strategy to modify polyisoprene using hypervalent iodine(III) reagents[4]that easily undergo homo- and heterolytic cleavage that afford species able to react with a variety of unsaturated compounds, including polymers with backbone or pendant double bonds. All reactions werecarried out at room temperature and the products were characterized by ^{1}H, ^{13}C NMR and IR spectroscopy, GPC, DSC, and TGA. The results indicate successful modification of polyisoprene, which opens a new avenue to previously inaccessible or difficult to make functional and reactive materials.



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FPC-OL-02

Preparation of polyethyleneamine(PEI) based thin film composite nanofiltration membranes with modulated charge and performance

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Abstract

The problems of polyethylene(PEI)-based thin film composite (TFC) nanofiltration (NF) membranes are the low permeate flusx, and low separation efficiency of divalent anion (monovalent counter ion). This is due to the high thickness and positive charge of polyamide active layer. In this work control of polyamide thickness, charge and performance of PEI-based NF membranes is reported. It has been shown that the active layer thickness as low as 12-40 nm could be obtained by controlling the diffusion of PEI towards the interface during interfacial polymerization. The charge of the membranes could be varied from negative to neutral to slightly positive by varying the initial concentration of PEI in the aqueous phase and keeping the concentration of acid chloride at fixed value. The pore size of the membranes could also be varied by varying the concentration of PEI. The NF membranes of neutral charged exhibited high rejection of both divalent cation and divalent anion with permeate flux as high as ca. 90 Lm^{-2}h^{-1}at applied pressureof 5.2 bar. Figure 1A and 1B shows the permeate water flux and salt rejection efficiency of different membranes prepared with varying the concentration of PEI with fixed concentration of trimesoyl chloride.[1]

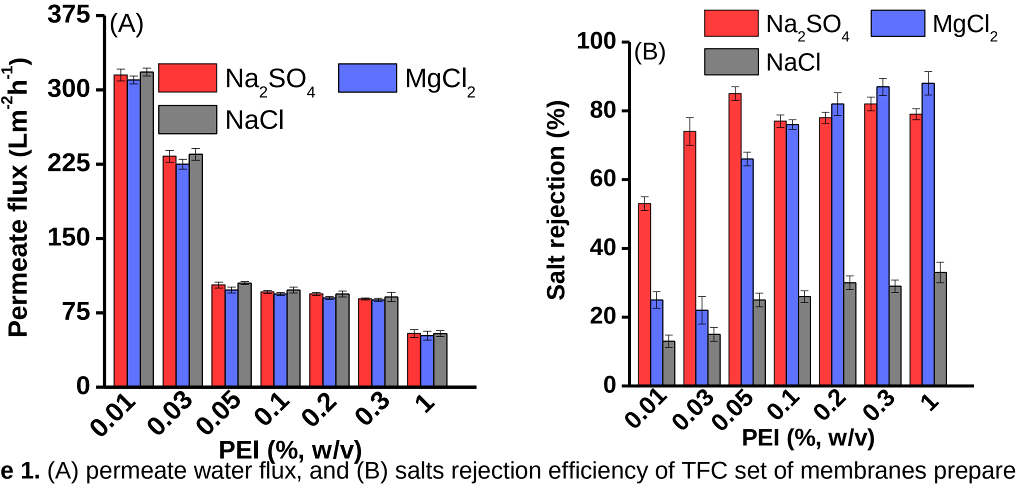

Figure 1. (A) permeate water flux, and (B) salts rejection efficiency of TFC set of membranes prepared with varying concentration of PEI. The concentration of salt was 1500 mg/L for the separate feed, and applied pressure was 5.2 bar for experiments.

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FPC-OL-03

Magnetic Field Assisted Alignment of Proton Conducting Channels in Polymer Electrolyte Membrane

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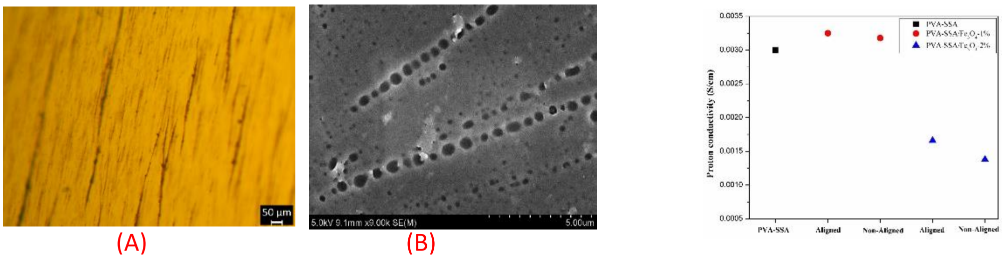
Abstract

External magnetic field was employed to create ion conducting channels in proton conducting poly(vinylalcohol)-sulfosuccinic acid (PVA-SSA) membranes. Magnetic field promotes the alignment of the magnetic moments of the iron oxide nanoparticles in PVA-SSA matrix and the strong dipole-dipole interactions between the neighbouring particles lead to the formation of larger size spherical aggregates in the polymer matrix. The spherical aggregates aligned parallel to the direction of the field forming ordered chain-like anisotropic superstructures during the evaporation of water to form free standing films. The introduction of iron oxide nanoparticles in the PVA-SSA matrix lead to increase in water uptake levels and swelling volume of the membranes. Although the particle concentration (0.1wt%, 1 wt% and 2 wt%) is the same in both the sets (aligned and non-aligned) of the membranes, the membranes with homogenous distribution of the particles show higher water uptake levels and hence swelling and the membranes with magnetically aligned particles showed moderate water uptake and controlled swelling. Animportant reason is due to the decrease in the number density of particles per unit area during the alignment process along the magnetic flux lines. All the nanocomposite membranes, despite their higher water uptake and dimensional change compared to neat PVA-SSA, possessed good flexibility unlike the brittle nature of fully swollen PVA-SSA membranes. Appreciallble proton conductivity was obtained with both aligned and non-aligned membranes and the difference in their condutivity was studied.



(A) (B) (C)

Figure. (A)Optical microscope and (B) SEM image of magnetically aligned PVA-SSA/1% Fe_3O_4membrane (C) Proton conductivity plot.

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FPC-OL-04

Poly(ε-Caprolactone-*co*-δ-Valerolactone) Copolymer as an impact modifier for PLA

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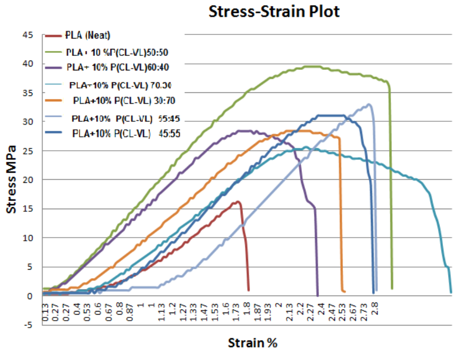
Abstract

Polylactic acid (PLA) is a widely used bio-based aliphatic polyesters. PLA posseses good mechanical properties comparable to other synthetic polymers; however, one of its principle drawback is its brittleness and low heat distortion temperature (HDT). This has limited the widespread applications of PLA. In order to improve its properties, different strategies have been explored, namely, elastomer blends, copolymerization and use of additives and plastisizers[1-3]. However, to obtain PLA with a good balance of toughness and stiffness while retaining its transparency and bio-degradability continues to be challenging. Poly(ε-caprolactone) (PCL) and Poly(δ-valerolactone) (PVL) are two of the most important biodegradable aliphatic polyesters. In the present work, random co-polyesters containing ε-caprolactone and δ-valerolactone [Poly(CL-VL)] with different compositions were prepared by ROP using tin octoate catalyst. The co-polymers were characterized by IR, NMR spectroscopy, gel permeation chromatography (GPC), differential scanning calorimetry (DSC) and scanning electron microscopy (SEM). Poly(CL-VL) copolymers were melt mixed with PLA (Mw = 112000 g/mol, PDI = 1.6, Tg = 55^{o}C, Tm = 163^{o}C) synthesized by ROP using a twin screw extruder. The effect of biodegradable copolymer additive (10 wt.%) was studied on the morphology of PLA matrix by SEM and mechanical properties. The morphological studies showed the cavities representing the disperse phase that is localization of copolymer particles regularly dispersed within the PLA matrix. The effect of these additives with different compositions on the toughness of PLA was also studied.



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FPC-OL-05

Synthesis and Characterization of Stimuli Responsive Polymer Grafted Organically Modified Mesoporous Silica and its Application in Targeted Drug Delivery

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Abstract

Mesoporous silica is considered one of the efficient material for drug delivery application due to its biocompatibility and uniform pore volume. In order to carry the required drug in the pores it is an important challenge to choose efficient gatekeepers and to graft it onto the surface of mesoporous silica. In the present work,grafting of poly N-isopropyl acrylamide (PNIPAM)was performed via surface initiated reversible addition-fragmentation chain transfer (RAFT) polymerization. RAFT functionalities were anchored to the surface of mesoporous silica then N-isopropyl acrylamide was polymerized onto the surface of the mesoporous silica. The resultant mesoporous silica were characterized using field emission scanning electron microscopy (FESEM),transmission electron microscopy (TEM), thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), nitrogen adsorption isotherms (BET) and solid state NMR. The PNIPAM can control the access of the guest molecules to and from the mesoporous silica due to its thermoresponsive behaviour. Thus to study the thermoresponsive nature of PNIPAM dye and drug loading experiments were carried out and was finally characterized by confocal laser scanning microscopy.

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FPC-OL-06

Rheokinetic studies and compressive response of high performance polybenzoxazine syntactic foams

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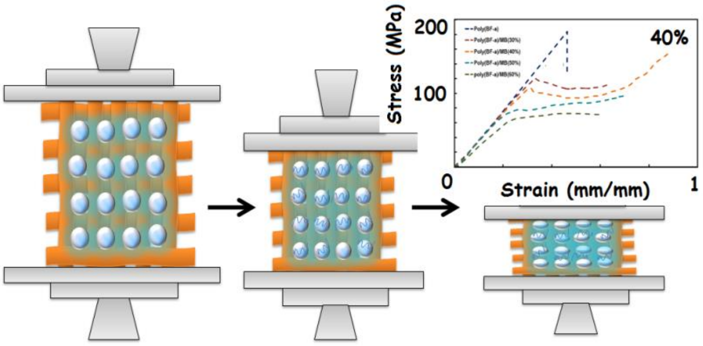
Abstract

The high-tech aerospace industry is in a continual search of materials with high thermal stability, robust mechanical response and most importantly low density, which directly translates to benefits in the form of low fuel consumption. In this context, syntactic foams offer their excellent candidature and are hence trending as light-weight construction materials with high specific structural properties, especially as "core component" in sandwich structures. Surprisingly, the potential of benzoxazines for this purpose has not yet been duly explored. Polybenzoxazines are finding increasing usage in demanding applications where high temperature stability is required, especially in the field of aerospace. In this work, thermally stable Bisphenol-F based polybenzoxazine (PBF-a) syntactic foams containing varying volume fractions (30-60%) of hollow glass microballoons (HGM) were prepared and their mechanical response in the quasi-static regime was established. The effect of glass microballoons on the curing profile of benzoxazine resin was studied using both non-isothermal differential scanning calorimetery (DSC) and rheometry. Temperature-sweep experiments were performed to arrive at the optimal processing window of the benzoxazine-glass microballoons formulations, particularly in terms of viscosity, gelation temperature and time. Thermally accelerated ring opening polymerization of the benzoxazine resin led to complete curing of the syntactic foam formulations. As expected, the density of the syntactic foam specimens decreased with increasing microballoon content. The specific compressive strength and toughness of the PBF-a/HGM samples was highest in samples containing 40% volume fraction of glass microballoons. The thermal degradation behaviour of the PBF-a/HGM was obtained from thermogravimetric analysis (TGA).



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Abstracts for Invited, Short and Oral Lectures Under the Theme Advanced Processing and Manufacturing of Polymers(APMP)

APMP-IL-01

Methodology of Polymer Research in Solvay

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Abstract

The purpose of the talk is to introduce how research is done in an industrial set up like Solvay, what are the areas we are interested (in polymers), and how we are preparing to face the future in terms of business. This talk could clear many doubts students and postdocs have about research in a major polymer industry like Solvay, while also providing a connection between the themes of MACRO with polymer research in industries.

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APMP-IL-02

Synergistic surface engineering by reactive compatibilization ofhydrophilic and hydrophobicaqueousemulsion and dispersion polymer blends

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Abstract

Blends of mutually incompatible hydrophilic and hydrophobic aqueous polymeric emulsions and dispersions have been reactively compatibilized to prepare single pack, mechanically robustcoating systems. The polymers and the coatings are chemically and physically characterized using FTIR, GPC and DSC. The effect of reactive compatibilization on phase morphology and interface characteristics are studied using microscopy (SEM and AFM) and surface energy measurements. Interestingly, synergistic improvements of surface properties with a gradual trend toward a direction of super-hydrophobicity is observed. These blends can have potential for very interesting coating applications with a number of functional attributes.

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APMP-IL-03

Overview of Heterogeneity Associated with 3D Printing of Polymeric Materials

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Abstract

Plastic components are conventionally processed by injection molding (IM). There is a growing interest in the industry to process such applications using additive manufacturing (3D printing), since it, offers ease of fabricating complex designs without elaborate machinery. This talk provides an overview on various 3D printing technologies available worldwide, such as stereolithography (SLA), selective laser sintering (SLA), fused deposition modeling (FDM), PolyJet, Thermoplastic Jetting, 3D multiJet fusion, continuous liquid interface production (CLIP), big area additive manufacturing (BAAM), etc. FDM has the widest choice of commercially available engineering thermoplastic that can meet different functional properties and it is therefore an interest for this study. FDM is a kind of 3D printing system that fabricates parts from polymeric resins by stacking layers of semi-molten filament upon a build platform. It is anticipated, that such stacking layers of materials, leads to creation of air gaps, which subsequently leads to difference in part performance. For applications, such as electrical and electronics one of the important consideration is electrical safety. This change in processing method (i.e. IM to 3D printing), is anticipated to alter electrical safety evaluation. A case study is finally presented, to study electrical insulation characteristics of parts, specifically dielectric strength of 3D printed specimens and Analytical methods are presented to quantify the part breakdown due to application of electric voltage.

APMP-OL-01

Controlled Polymer Synthesis Using Process Analytical Tools

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Abstract

Controlled polymer synthesis requires efficient analytical tools and feedback systems to archive a cost effective process and with the desired polymer properties. Improved production processes enable faster, safer and high quality products.Polymerization typically is a multistep process where molecular properties such as molecular weight, particle size and reaction completion need to be monitored and controlled simultaneously. In this paper we intend to highlight some spectroscopic tools such as NIR (near infrared), MIR (mid infrared) and Raman spectroscopy for polymerization control. The paper highlights examples of solution polymerizations and similar other reactions. During analytical method development at a lab scale,several parameters were studied like signal response to monomer depletion, molecular weight/viscosity buildup or formation of new covalent bonds. Calibration models were designed using statistical tools such as partial least square method (PLS) or multivariate regression analysis.Kinetic data was also derived using these spectroscopic tools.

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APMP-OL-02

Foam morphology development in polypropylene / γ-irradiated elastomer blends and their mechanical performances

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Abstract

Acomparative study amonga series offoams of polypropylene/gamma irradiated elastomer blends was done by virtue of varying the irradiation dose and elastomer particle size. The effects of gamma irradiation of blends directed towards the crosslinking of elastomer (Vamac Ultra IP). Foaming was done in a high pressure autoclave at three different temperaturesusing supercritical CO_2 as a blowing agent. The cell structure development mechanism was established and the irradiation dose optimization was done. The elastomer particle size played a very key role on foamability of blends. Blends interface acted as the nucleating site for foaming and interfacial energy of raw materials had typical role either on development of blend morphology oron foamability.Furthermore, the density of foams decreased with increasing foaming temperature abiding by the general phenomena of foaming.The introduction of crosslinked elastomer into the polypropylene matrix improved the foamability of polypropylene.For evaluating the mechanical performances (tensile and impact test) of foams in the next stage,foaming of blends was carried out at three different conditions, which were determined to be optimized on the basis of 1) lowest cell density, 2) highest cell density and 3) highest volume expansion ratio by using Taguchi method followed by ANOVA in anotherinvestigation. The absolute and specific tensile modulus of foams with optimally irradiated elastomer showed an increasing trend with the rise in cell density might be due to the molecular microstructural changes; whereas, the tensile strength of foams was not sacrificed significantly. The absolute and specific impact strength of the foams also exhibited the increasing trend.

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Abstracts for Sponsor Talks

Sponsor Talk

Characterisation of Chitosan Molecular weight distribution by Multi-Detection Field-Flow Fractionation and SEC-MALS

Y. Gonzalez-Espinosa[1], B. Sabagh[2], E. Moldenhauer[2], P. Clarke*[2] and F. Goycoolea[1]
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Abstract

Molecular weight determination of chitosan is commonly conducted using intrinsic viscosity measurements, light scattering and/or size exclusion chromatography (GPC/SEC)[1]. All of these techniques require complete dissolution of the polymer to avoid inaccurate estimation of molecular weight (MW) due to the presence of intermolecular aggregates[2]. Recent studies have reported the use of asymmetric flow field flow fractionation (AF4) to characterise the MW distribution of chitosan[3-5]. However, the full experimental conditions used have been vaguely reported, making the methods difficult to reproduce. We present here a method for determination of the MW of chitosans by AF4 coupled with MALS and DRI detectors. The method allows the separation of the dissolved polymer from the aggregate fraction, making possible the accurate determination of molecular weight distribution. We also evaluated the effect of different experimental conditions on the results obtained and compared them with results from SEC-MALS-DRI under identical solvent conditions. We analysed a set of chitosan samples from different sources (crustaceans, squid and fungi) and of varying degree of acetylation (DA ~1 to ~50%). AF4-MALS-DRI results revealed that although aggregates are significantly minimised when using a good solvent, some still remain, and are only eliminated by filtration through small pore sizes (~0.2 µm). This represents a limitation for chitosan, as filtration can lead to high amount of the material being retained in the filter. The method described here has the advantage of allowing us to identify and separate the aggregates and to accurately determine the MW distribution for a wide range of chitosan types.

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Sponsor Talk

Viscoelastic response of bidirectional carbon fiber/epoxy composite

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Abstract

Dynamic mechanical analysis is a great tool for material characterization under shear, extensionalor mixed flow field, be it transient or dynamic mode. Eachdeformation field reveals unique information.Sometimes it is the material property which limits method that can be used for characterization.

Bidirectional composites are known for their anisotropic property. Using dynamic mechanical analysis, distinct viscoelastic response towards specific fiber orientation can be obtained.

Reference

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Sponsor Talk

Silicon, Silanes, Silicones and You: Ordinary and Extraordinary Applications of Silicon and Silicon-Containing Compounds

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Abstract

Worldwide sales of silanes, silicones and other organosilicon compounds exceed US$ 40 billion annually and the industry continues to grow[1]. Where are these products used? How are they used and by whom? This presentation will show that silicon-containing compounds are present in, or are used to process, a wide variety of industrial, medical and consumer products that satisfy basic human needs in a modern society. Yet, there is little awareness of the ubiquity and utility of these compounds even among members of the chemistry community. The presentation seeks not only to increase awareness, but also to impart appreciation of the enhancement of value in the final products that arise from the use of silicon-containing additives. Emphasis will be placed on the applications and the fundamental principles or properties, which enable the use of silicon compounds in the ordinary and extraordinary applications that will be illustrated.

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Sponsor Talk

Fluorescence & Absorption Spectrometer and Application

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Abstract is waiting

Sponsor Talk

Numerous Applications of Polyurethanes (PU) and Structure and Property Relationship in PU Foams

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Abstract

Polyurethanes were first developed during World War II as an alternative to natural rubber,

and today have found their way into thousands of applications in homes and businesses throughout the world. Polyurethanes describe a class of materials valued by consumers for their high performance and durability. Polyurethane foam used in furniture, insulation, and bedding may be the most easily recognizable product.

Physical and chemical properties of polyurethanes depend upon the type of isocyanates and the active hydrogen containing components used, number of reactive group present in the raw material, molecular mass and the structure of both reactive component and the stoichiometry used. Typical properties of polyurethane for which it is preferred candidate in many applications include easy processability, good flexibility, abrasion resistance, good adhesion and availability in wide range of hardness and densities. How the structure of the monomers used, effect the properties of the final polymer produced for a certain kind of application will be discussed in the presentation

Also, how one can obtain the required specific properties and tailor make the product by incorporating a small amount of comonomer during the synthesis, will be described.

Sponsor Talk

Fundamentals and Applications of Small/Wide Angle X-ray Scattering (SAXS/WAXS) Beamline System

Bhavidas Charles

Abstracts of Presentation on "Fundamentals and applications of Small/Wide Angle X-ray Scattering (SAXS/WAXS) beamline system" from Xenocs, SA ; France at SPSI-MACRO 2018

- Xenocs system for Material Characterization
- "Small/Wide Angle X-ray Scattering (SAXS/WAXS) systems" offered by Xenocs, SA; France.
- Several Models offered by Xenocs and its advantages over applications.
- Key Attributes and configurations required for a SAXS/WAXS system.
- Detailed configuration and advantage of Xenocs SAXS beamline system
- Comparison of Xenocs SAXS system with Synchrotron platform.
- Upgrades, options and accessories for SAXS system.
- Applications of SAXS/WAXS in different samples.
- Users in India.

Sponsor Talk

Polymers in Healthcare Aspects

Ashok G.

GE healthcare

Abstract is waiting

Abstracts for Poster Presentation

CPSA-01

Polymorpholinones: Design, Synthesis and Characterization

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Abstract

A new class of monomers, Morpholin-2-ones (**Mono** $_{\mathbf{(H)}}$, **Mono** $_{\mathbf{(DODEC)}}$, **Mono** $_{\mathbf{(UDOH)}}$), were synthesized using low-cost industrial chemicals through simple and metal-free synthesis strategy for the generation of biodegradable polymorpholinones. The organocatalytic ring-opening polymerization of N-substituted morpholin-2-ones would provide a general strategy to prepare a family of functionalized poly(aminoesters). Considering the novelty of the synthetic approach, kinetic studies of the polymer, **Poly** $_{\mathbf{(H)}}$ generated from **Mono** $_{\mathbf{(H)}}$ were performed. Interestingly, the polymer was quite soluble evenly in non-polar as well as polar solvents, but **Poly** $_{\mathbf{(H)}}$ with a high degree of polymerization (DP=75) was insoluble in highly polar solvents like water.

Due to the wide range solubility of **Poly** $_{\mathbf{(H)}}$, we were inquisitive to know the change in the behaviour of the polymer as we attach a long chain hydrophobic and hydrophilic moiety to the parent monomer **Mono** $_{\mathbf{(H)}}$ to obtain sequentially **Mono** $_{\mathbf{(DODEC)}}$ and **Mono** $_{\mathbf{(UDOH)}}$ and finally polymerized to get **Poly** $_{\mathbf{(DODEC)}}$ and **Poly** $_{\mathbf{(UDOH)}}$ respectively. Furthermore, we were curious to investigate the solubility and self-assembly behaviour of the specified polymers **Poly** $_{\mathbf{(DODEC)}}$ and **Poly** $_{\mathbf{(UDOH)}}$ in various solvents with a broad range of polarity. Owing to these exciting observations, this biodegradable poly(morpholinones) containing amines in the polymer backbone and pendant groups are expected to possess expanding roles spanning from biomedical applications such as drug delivery to environmental applications such as the removal of heavy metals.

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CPSA-02

Controlled Grafting of Polyaniline on Carbon Quantum Dots for the Fabrication of Supercapacitor Electrode Material

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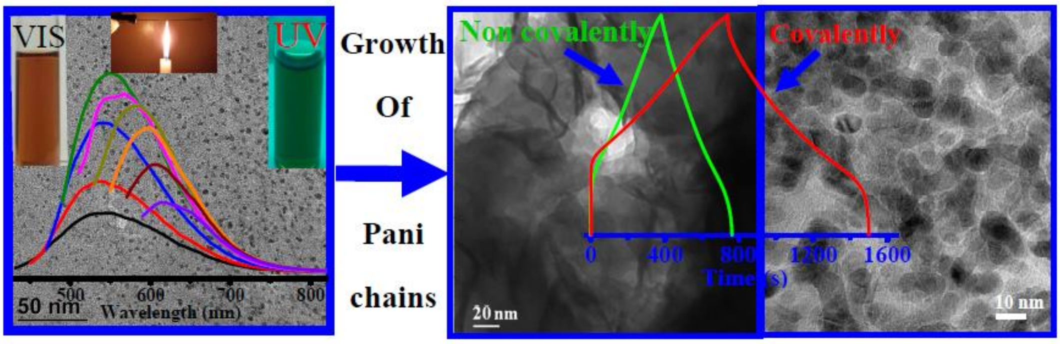
Abstract

A general approach for controlled synthesis of polyaniline (PANI) chains after initiated from oligomeric aniline, N,N'-bis(4'-aminophenyl)-1,4-quinonediimine (APQD, in the emeraldine state) state will be presented. The oligomeric aniline compound present in the emaraldine state is anchored on carbon nano dots prepared from readily available source like candle soot. The kinetics of polymerization indicates grafting of PANI chains only from the oligomeric moieties attached on the CND surface under optimized conditions which are eventually working as seeds. The carbon quantum dots prepared from candle soot are thoroughly characterized by UV-Vis and Fluorescence spectroscopy. The oligomeric aniline and PANI coated CNDs are thoroughly characterized by FT-IR, Raman Spectroscopy and FESEM/HRTEM/AFM and WAXS techniques. FESEM and HRTEM techniques show gradual development of distinct nanosized CND-g-PANI particles. The analysis of electrochemical properties of CND-g-PANI shows tremendous storage properties with a maximum of 972 F/gm of specific capacitance (1A/g) and about 92% retention of capacitance after 2000 charging/discharging cycles compared to 483 F/g in case of non covalently grafted CND/PANI composite material. The electrochemical properties are characterized both using two electrode and three electrode cells and a comparison of these two techniques will be discussed. An appreciably high energy density of 17.7 Wh/Kg in 1A/g has been obtained. The observed electrochemical properties are attributed to the formation of nano structured polyaniline on carbon quantum dots in a controlled fashion.



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CPSA-03

Inverse Micro-Emulsion Entrapped Catalyst for Conducting Solvent Free, Ambient Temperature Highly Controlled ATRP of 2-Dimethylaminoethyl Methacrylate

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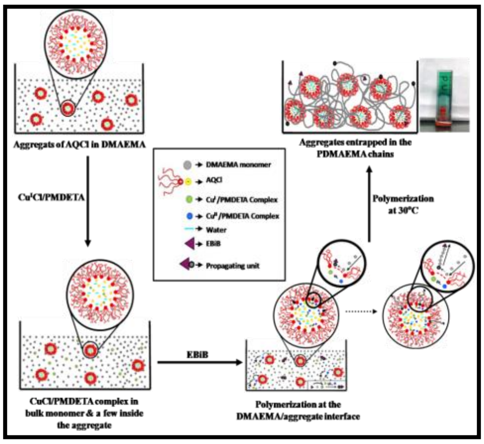
Abstract

Living poly(2-dimethylaminoethyl methacrylate) (PDMA) has been synthesized by Atom Transfer Radical Polymerization (ATRP) of 2-dimethylaminoethyl methacrylate (DMA) in bulk at 30°C using CuCl/*N,N,N',N',N''*-pentamethyldiethylenetriamine (PMDETA) catalyst.[1],[2] Addition of catalytic amount of tricaprylylmethylammonium chloride (Aliquat®336)(AQCl) keeps the deactivator cupric complex soluble throughout the polymerization. The solubility of the charged cuprous/cupric complexes in bulk DMA is proposed through their entrapment within the ionic core of the reverse micelle like aggregates formed by AQCl in DMA medium, as observed from dynamic light scattering analysis.[3] The polymerization kinetics and molecular weight development indicate a significantly controlled polymerization only when AQCl is present. Improved control over the polymerization in presence of AQCl is attributed to the improved solubility of the deactivator cupric complexes through entrapment within the aggregate core. Synthesized PDMA molecules have been successfully chain extended with different methacrylate monomers in one pot for the synthesis of various stimuli responsive, multifunctional di- or triblock copolymers.[4] An adventitious role of water molecules in respect of kinetics and control over polymerization is noted when moist monomer or AQCl is taken for reaction. The structure and molecular weight of the synthesized polymers have been characterized by ^{1}H-NMR, gpc and MALDI-TOF MS techniques.



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CPSA-04

Comparative Self-Assembly Study of Two Distinctive Lactones Derived Thiobarbiturate Nanostructures and Their Stimuli Responsiveness

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Abstract

Synthesis of Amphiphilic biodegradable unique molecular architecture from polylactones (polycaprolactone, polylactide) derived Thiobarbiturate homopolymers (PCL-BBT, PLA-BBT) and their characterization are discussed here, where lactones are hydrophobic and barbiturate is hydrophilic in nature. To produce the compounds, Friedel-Crafts acylation and ring opening polymerization (ROP) techniques are applied. ^{1}H NMR, ^{13}C NMR and FT-IR spectroscopy confirm the product formation. These newly designed homopolymers are able to self-assemble in aqueous solution. Diffraction Light Scattering (DLS) and Critical Aggregation Concentration (CAC) studies are carried out to confirm the formation of aggregate in solution. To investigate the morphology of these homopolymers, Transmission Electron Microscopy (TEM) and Transmission Electron Cryomicroscopy (CryoTEM) studies have been done. Encapsulation of both hydrophobic (Nile Red) and hydrophilic (cationic, Rhodamine B; anionic, Fluorescein) dye into the homopolymers helps us to authenticate the reversibility of the aggregates. Dye release study in octanol-water system implies the stimuli responsiveness of these innovative nanostructures. After analysing the results, it reveals that, irrespective of the backbone the barbiturate moiety is responsible for the self-assembled nanoaggregates and the fascinating properties.

Structures of lactones derived Thiobarbiturate

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CPSA-05

Terpolymer conetwork based anion exchange membrane and its application for desalination and diffusion dialysis in acid recovery

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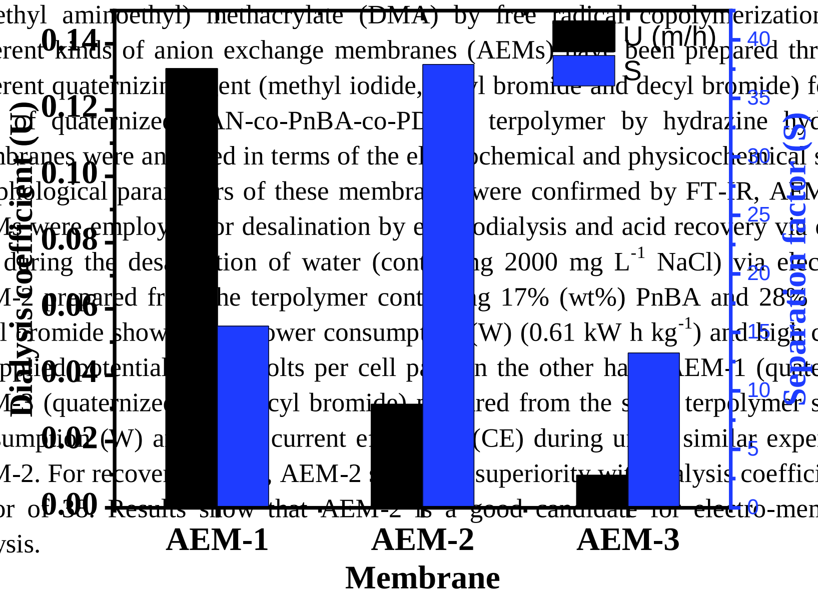
Abstract

We have synthesized random terpolymer of the mixture of acrylonitrile (AN), n-butyl acrylate (nBA) and (2-dimethyl aminoethyl) methacrylate (DMA) by free radical copolymerization using AIBN initiator. Three different kinds of anion exchange membranes (AEMs) have been prepared through quaternization by varying different quaternizing agent (methyl iodide, butyl bromide and decyl bromide) followed by crosslinking of each type of quaternized PAN-co-PnBA-co-PDMA terpolymer by hydrazine hydrate. The performance of the membranes were analyzed in terms of the electrochemical and physicochemical system. Structural, chemical and morphological parameters of these membranes were confirmed by FT-IR, AFM, SEM and TEM analysis. The AEMs were employed for desalination by electrodialysis and acid recovery via diffusion dialysis. It is observed that during the desalination of water (containing 2000 mg L^{-1} NaCl) via electrodialysis (ED) the membrane AEM-2 prepared from the terpolymer containing 17% (wt%) PnBA and 28% (wt%) PDMA quaternized with butyl bromide showed [illegible] power consumption (W) (0.61 kW h kg^{-1}) and high current efficiency (CE) (96%) at an applied potential of [illegible] volts per cell pair. On the other hand, AEM-1 (quaternized with methyl iodide) and AEM-3 (quaternized with decyl bromide) prepared from the same terpolymer shows a relatively higher power consumption (W) and [illegible] current efficiency (CE) during under similar experimental condition compared to AEM-2. For recovery of [illegible], AEM-2 shows superiority with dialysis coefficient of 0.031 m/h and separation factor of 38. Results show that AEM-2 is a good candidate for electro-membrane processes and diffusion dialysis.



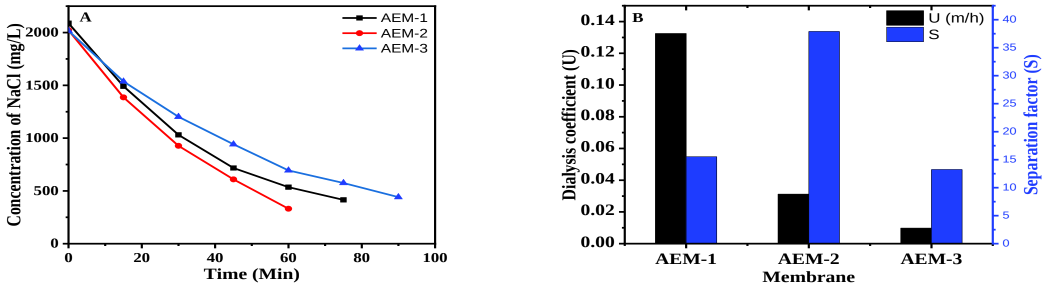


Fig.1 (A) Concentration of NaCl (mg/L) vs Time (min) during desalination of water and (B) Dialysis coefficient (U) and Separation factor (S) for different anion exchange membranes.

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CPSA-06

Stable PVDF/Copolymer Based Blend Anion Exchange Membrane Via Phase Inversion Method For Water Purification

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Abstract

Non solvent induced phase inversion process has been employed for the prepration of anion exchange membrane (AEM). A fabric supported AEM was prepared from the miscible blend of polyvinylidene fluoride (PVDF) and poly (methyl methacrylate) -*co*- poly (chloromethyl styrene) by phase inversion method followed by post treatment with tertiary diamine. Different membranes were prepared with different composition of PVDF/copolymer ratio. These membranes were used for water purification such as desalination as well as removal of fluoride ion via electrodialysis (ED) process. The copolymer and the blend mixture were characterized by ^{1}HNMR, ATR-IR spectrscopy and TGA analyses. The electrochemical properties of the membranes such as ion exchange capacity (IEC), transport number (t^-), ionic conductivity (K^m) were evaluated. The membranes showed temperature stability up to 60 ^{o}C and pH stability upto 10. A membrane prepared with blend containing 69.5%, w/w copolymer and 30.5% w/w PVDF exhibited best electrochemical properties with IEC 1.85 meq g^{-1} K^m 3.02 mS cm^{-1}, and t^- 0.98. This AEM also showed 0.978 KWh kg^{-1} power consumption and 94% current efficiency during desalination of water (NaCl concentration 2000mg/L) at 2 V/cell pair applied potential.

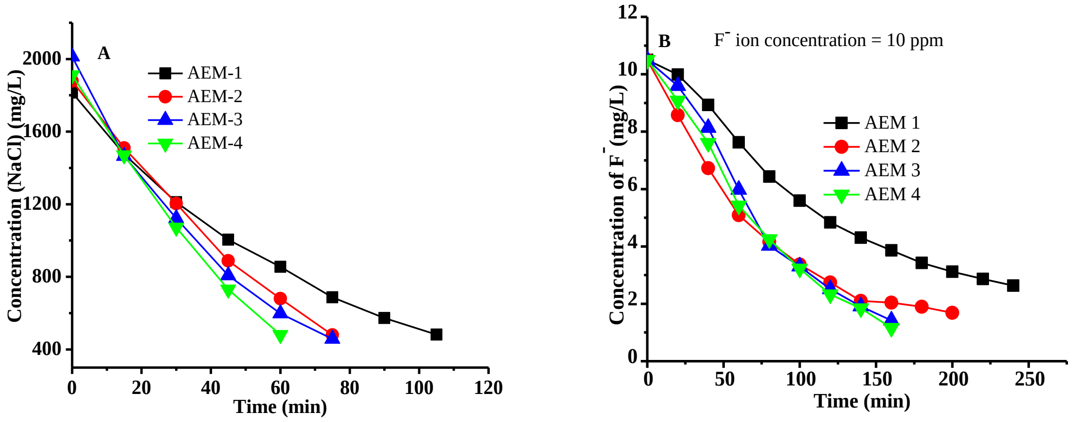

Fig.1 (A) Variation of NaCl concentration with time and (B) variation of fluoride ion concentration with time in diluate compartment by ED process using the prepared AEMs.

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[1] Mondal, R.; Pal, S.; Bhalani, D. V.; Bhadja, V.; Chatterjee, U.; Jewrajka, S. K. Desalination 2018, vol.445, 85-94.

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CPSA-07

Immobilization of single site catalyst on inorganic oxide support for preparation of Disentangled Ultra High Molecular Weight Polyethylene (DUHMWPE)

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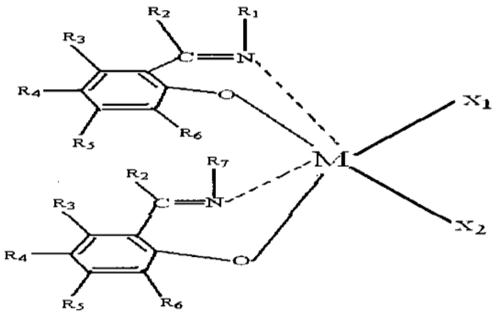
Abstract

Single site homogenous catalyst has been reported in literature for the synthesis of disentangled ultra high molecular weight polyethylene (DUHMWPE)[1]. Homogeneoues catalysts are highly sensitive to moisture and imurities present in the solvent and feed and also known to frequebt fouling of polymerization reactor. Anchoring of the homogenous catalyst physically on a support known to reduce the catalytic efficiency & catalyst leaching in to the polymerization medium. To over come these drawbacks, we have report single site heterogeneous catalyst chemically immobilized on an inorganic oxide support (Formula I)[2]. The supported catalyst has shown good activity towards ethylene polymerization to produce DUHMWPE. The synthesis of supported single site catalyst involveds (1) Functionalization of inorganic oxide to introduce amine group followed by generation of Schiff base imine ligand on the support through reaction with hydroxy aldehydes. (2) Lithiation using *n*-butyl lithium and subsequent reaction with $TiCl_4$ to obtain the immobilized catalyst. The immobilized FI catalyst was evaluated for the polymerization of ethylene using methylaluminoxane (MAO) / poly-methylalumoxane (PMAO) as co-catalysts by variation of reaction parameters and produced DUHMWPE with molecular weight (ASTM) of 1 to 13 million g/mole, improved bulk density of 0.09 to 0.17 g/cc), high crystallinity (> 90% XRD) & having fibrous / porous morphology (SEM).



Formula I Single Site Heterogeneous FI catalyst chemically immobilized on an inorganic oxide support

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CPSA -12

Rational synthesis of multi-arm polymers and copolymers of lactide using an arm-first approach

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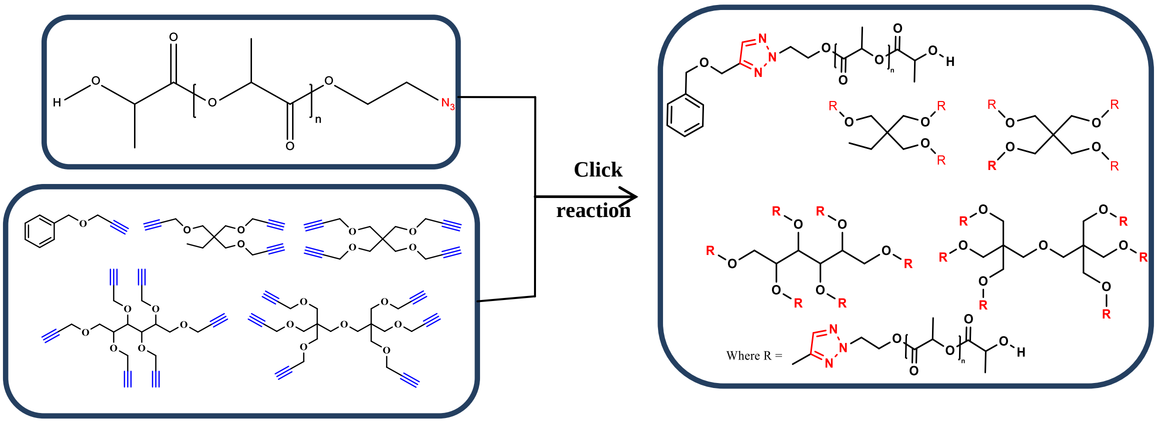
Abstract

Multi-arm star shaped polymers have attracted significant attention in the literature. Their unique macromolecular architectures result in useful functional, rheological and mechanical properties and exhibit good degradation and controlled drug release properties. Star polymers contain one central core which is also referred as a branching point from which linear arms radiate and form branched molecular architecture. "Arm first" method is one of the important approaches for the synthesis of multi-arm star polymers. This method provides high level of structural control. In this method, the core (multifunctional coupling agent) and the arm (linear polymer with terminal reactive group) are independently prepared with a high degree of control and characterized prior to performing the coupling reaction of the core with the arm.

Click chemistry has been widely exploited in synthetic polymer chemistry for the synthesis of well defined macromolecular architectures. Herein, we report the synthesis of multi-armed star branched polymers and copolymers of L-lactide and glycolide via copper catalyzed azide-alkyne cycloaddition (CuAAC) reaction of azide terminated polymers and copolymers of lactide and glycolide with alkyne derivatives of trimethylol propane (TMP), pentaerythritol (PET), pentaerythritol (DPE), sorbitol, respectively. This method provides access to well defined multi-arm star polymers of lactides and glycolides. The cores, arms and the resulting star polymers were characterized by HRMS, FT-IR and NMR, MALDI-TOF and GPC to establish the fidelity of structures as well as the controlled nature of the polymers synthesized.



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CPSA-13

A New Approach for the Synthesis of Miktoarm Star Polymers Through a Combination of Thiol-Epoxy 'Click' Chemistry and ATRP/Ring Opening Polymerization Techniques

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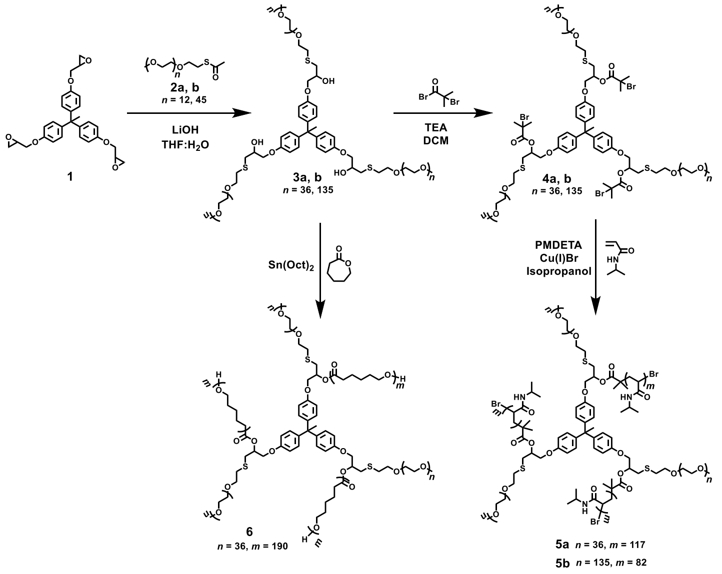
Abstract

Miktoarm star polymers[1] are class of macromolecules in which different polymer chains are attached to the core. Such polymers have aroused much interest due to their intriguing properties such as smaller radii and lower viscosity compared to their linear counterparts[2] and self-assembly behaviour.[3] These find potential applications in the arena of controlled drug release system, as viscosity modifiers, and so on. A new synthetic approach will be presented for synthesis of certain A_3B_3-type of double hydrophilic or amphiphilic miktoarm star polymers using a combination of "grafting onto" and "grafting from" methods. Acetyl protected polyethylene glycol (PEG) thiols (M_n = 550 and 2000 Da) were utilized to generate A_3-type of homoarm star polymers through an *in-situ* protective group removal and a subsequent 'click' reaction with a tri-epoxide core. The secondary hydroxyl groups generated upon the thiol-epoxy reaction were then esterified with □-bromoisobutyryl bromide to install ATRP initiating sites. Atom transfer radical polymerization (ATRP) of *N*-isopropylacrylamide (NIPAM) using the 3-arm homo polymer fitted with ATRP initiating sites adjacent to the core afforded double hydrophilic A_3B_3-type of $(PEG)_3(PNIPAM)_3$ miktoarm star polymers. Furthermore, the generated hydroxyl groups were directly be used as initiators for ring opening polymerization (ROP) of ε-caprolactone to prepare A_3B_3-type of amphiphilic $(PEG)_3(PCL)_3$ miktoarm star polymers.



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CPSA-14

Nonionic block copolymer surfactant for the synthesis of latex particles

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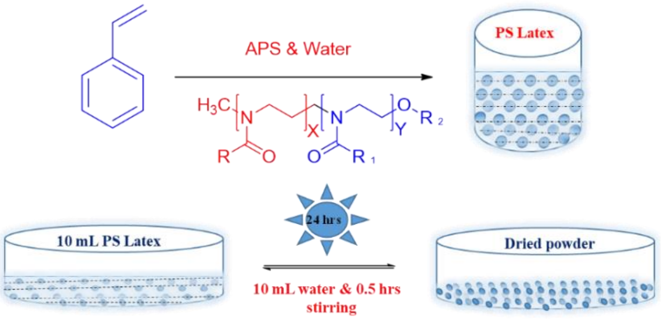
Abstract

A series of poly(2-oxazolines) block copolymers with methyl, butyl and phenyl pendants were synthesized by living Cationic Ring Opening Polymerization (CROP) method.[1] The hydrophobic and hydrophilic segments in copolymer was designed to match the HLB.[2] So that it can self-assemble in aqueous solution into micelle. Block copolymers were characterized using FT-IR and NMR. The critical micelle concentration (CMC) of the prepared block copolymer was estimated by using UV-Visible spectroscopy with iodine as less intrusive probe.[3] The block copolymers that showed clear breakpoint in CMC measurements are used as nonionic surfactant in the emulsion polymerization.[4] A number of polystyrene latexes were synthesized by varying the amount of surfactant and while maintaining the styrene content. The prepared latex were stable, which are subsequently dried under the natural resource, i.e. sun and redispersed into the same amount of water. The size of as prepared latex and redispersed latex particles were determined by (DLS) dynamic light scattering. The particles sizes are in the range of below 500 nm and redispersed latexes are also of comparable size as that of the original latex. The difference between the pristine and redispersed latex particle is <20 nm.



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CPSA -15

Evidence of cooperativity among van der Waals interactions in functionalized siloxane copolymer

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Abstract

Cooperativity of van der Waals interactions in bio-molecules and supramolecular assemblies has drawn significant scientific attention due to its offering of seamless opportunities to generate new materials.[1] However, the potential of such cooperativity in synthetic polymers is very limited. In silicon based polymers, experimental evidence of very weak Si/X (F, N, O) interactions was reported on fluoro substituted silicon catenated polymers highlighting the significance of these weak interactions in directing rod-like helical conformation and its application as chemo sensor.[2] In this study, we demonstrate a strategy to achieve cooperativity via enhancement of weak interactions in a designed siloxane copolymer. Segmentation of siloxane copolymer with specific alkyl chain length (C18) induces cooperativity in van der Waals interaction amongst the alkyl chains resulting in interdigitated as well as end-to-end packing. The cooperativity of hydrophobic interactions is also evident from difference in differential scanning calorimetry (DSC) studies that reveal high dissociation energy of designed block siloxane copolymer as compared to its control counterpart i.e. a compositionally similar random siloxane copolymer. Small-angle X-ray diffraction (SAXD) results also provide evidence for difference in the crystallization pathways of two polymers. The concomitant involvement of the main chain siloxanes towards building of such hierarchical packing was also evident from the temperature dependent Fourier-transform infrared spectroscopy (FTIR) studies of the copolymers. The dynamic relation of cooperativity and physical properties in the siloxane polymer was further substantiated using "sergeants-and-soldiers" experiment by disturbing the symmetry of alkyl chain.[3]

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CPSA -16

Grafting of modified alpha cyclodextrin with polyurethane embedded in Hydrogel for Sustained Drug Release and Healing of Melanoma

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Abstract

We develop an injectable hydrogel based drug delivery carrier for long term drug release by assembling various generation of cyclodextrin (CD) followed by hydrophobic layers to sustain the drug delivery rate for better cancer treatment[1]. Three different generations of CDs are designed through urethane linkages using small spacer HMDI to create a large hydrophilic core which is covered with hydrophobic layers of polyurethane through grafting to maintain the hydrophilic hydrophobic balance of the whole superstructure[2]. Drug release becomes significantly sustained from the intricate superstructure following the non-Fickian diffusion process resulting massive cancer cell killing as compared to low killing rate from the pure material arising from its burst release. Cellular studies have been translated into animal model showing the efficacy of newly developed injectable hydrogel. The superstructure is found to be a good biomaterial and is applied to albino mice to treat their tumor, generated through melanoma cell line. Drug embedded superstructure is inoculated in injectable hydrogel and is placed at subcutaneous, below the tumor site, and completely heal the melanoma. No side effect is observed, as opposed to conventional/control system, arising from the sustained release of drug from the superstructure as evident from histopathological studies of sensitive body organs and biochemical parameters. Thus, new design of vehicle heal tumor by enhancing the bioavailability of drug and specific interaction without having any side effects.

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CPSA -17

Periodically Grafted Liquid Crystalline Polymers

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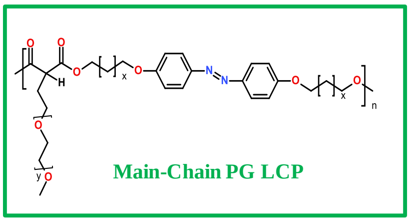
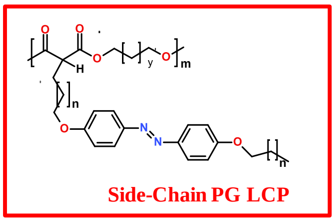
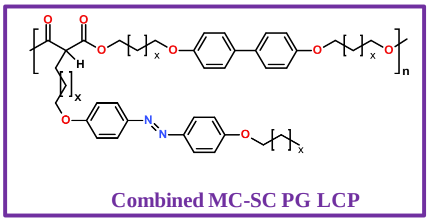
Abstract

Liquid crystalline polymers could be of different architectures; mesogenic units that impart the liquid crystalline property could be present either on the polymer backbone or as a pendant unit. The nature and property of the mesophase formed evidently depends on the architecture, among other factors; the precise conformation of the polymer chain and its organization in bulk is rather difficult to probe experimentally, and the mesophase structure is most often examined in terms of the organization of the mesogens. An interesting question that arises is: could the polymer be architectured to control the nature of the mesophase formed?


Main-Chain PG LCP


Side-Chain PG LCP


Combined MC-SC PG LCP

During the past decade, we have demonstrated that immiscibility between long segments, in suitably designed polymers, can be utilized to control the polymer chain conformation;[1-3] zigzag folding of the polymer chain was shown to permit the segregation and collocation of immiscible segments in periodically grafted amphiphilic copolymers (PGAC), often leading to the formation of lamellar morphology assisted by the crystallization of either one or both the segments. In the presentation, I shall describe our recent efforts to understand the behavior of a new class of periodically grafted liquid crystalline polymer (PGLCP); I shall explore the influence of various structural parameters, such as the location of the mesogen (pendant versus backbone), nature and length of the pendant immiscible segment, etc., on the mesomorphic behavior.

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CPSA -18

Effect of layer-by-layer fabricated lanthanum cerium molybdate nanocontainer on corrosion resistance of AZ91D magnesium alloy

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Abstract

Magnesium alloys, being one of the light weight engineering materials, have attracted more and more attentions as preferred alternative structural material for various applications. But, their low corrosion resistance are quite questionable which constraint their applications. Hence, the corrosion protection of magnesium alloys becomes a crucial topic in the area of research. In this context, incorporation of the **"Smart Nanocontainers", fabricated via layer-by-layer (LbL) technique**, in the coating matrix has triggered considerable attention towards anticorrosive coatings with self-healing ability. The layer-by-layer (LbL) technique involves an assembly of alternating layers of oppositely charged **weak and/or strong polyelectrolyte polymers** and corrosion inhibitor onto the outermost surface of dense template nanoparticles resulting in **"Nanocontainers" which can provide lasting and even "smart" release of the inhibiting species on demand.**

In present work, a novel lanthanum cerium molybdate nanoparticles, synthesized by conventional method, has been used as a core of the nanocontainer formulation to get the **dual advantage** for the anticorrosive Nanocontainer. The lanthanum cerium molybdate nanocontainers were fabricated with corrosion inhibitor benzotriazole and **pH-responsive polyelectrolyte polymer layers of polypyrrole (strong cationic polyelectrolyte) and polyacrylic acid (weak anionic polyelectrolye)** by means of hydrothermal method and ultrasonic irradiations respectively where the inhibitor encapsulated between the strong and weak polyelectrolyte layer. The so synthesized Nanocontainers has been designed to respond for the external stimuli "pH of an external environment".

Synthesis of Nanocontainers is followed by characterization by instrumental techniques viz. ICP-AES, Particle Size And Zeta Potential Analyzer, FTIR, XRD, TGA, SEM, TEM, and UV-VIS Spectrophotometer for desired aspects. Anticorrosive performance of the synthesized nanoparticles and nanocontainers in **epoxy-polyetheramine resin** were evaluated by electrochemical corrosion analysis (EIS) and salt spray methods for AZ91D magnesium panels. The results obtained indicate that the incorporation of loaded nanocontainers into a coating improves its corrosion protection as compare to system of epoxy-polyetheramine resin with nanoparticles and neat epoxy-polyetheramine resin without destroying the coherence of coating. Hence, justifying the significance of using lanthanum cerium molybdate as a core and benzotriazole as an inhibitor for dual enhanced performance.

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CPSA -19

Synthesis and anticancer effect of TEMPO functionalized polyurethane denderimers

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Abstract

Polyurethane dendrimers, generation number upto four, functionalized with stable 2, 2, 6, 6-tetramethylpiperidin-1-yloxyl (TEMPO) groups were prepared and structures of the compounds were confirmed by ^{1}H NMR, ^{13}C NMR, FT-IR, and HR-MS spectroscopy techniques. The TEMPO radical exhibited a triplet with nitrogen hyperfine splitting constant of 14.4 G, at g = 2.0026 in the EPR spectra. The absolute molecular weights of dendrimers were determined using SEC-MALLS technique and the chromatogrammes confirmed narrow dispersity of the dendrimers. The antioxidant effect of TEMPO fuctionalized dendrimers was evaluated *invitro* in A549 lung adenocarcinoma cells and normal L132 lung cells and the studies demonstrated the efficacy of polyurethane dendrimers which significantly reduced the level of free radicals and its mediated cellular damage in both L132 normal lung cells and A549 lung adenocarcinoma cells. The studies includes assessement of cell cytotoxicity, cell morphological studies, measurment of intracellular reactive oxygen species, SOD, CAT, GSH and GPx.

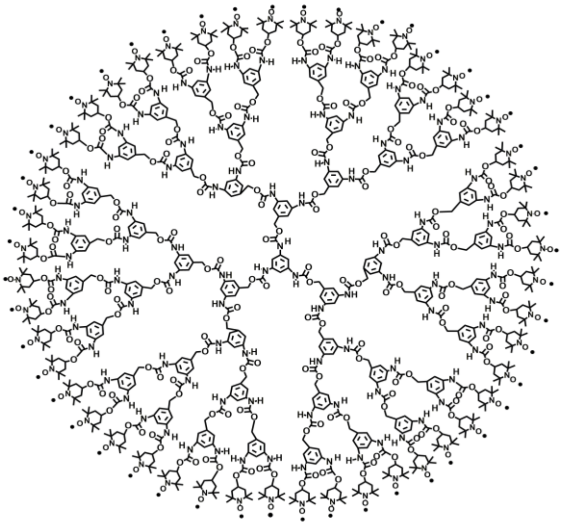

Fig.1 Structure of G4 Dendrimer

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CPSA -21

Novel Homogeneous Single Site Catalysts & Polymerization Process for Disentangled Ultra-High Molecular Weight Polyethylene (D-UHMWPE)

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Abstract

Disentangled ultra-high molecular weight polyethylene (DUHMWPE) is a specialty polyethylene which exhibits outstanding physical, chemical & mechanical properties along with excellent ease of processibility. The well-known catalyst for producing DUHMWPE is FI type catalyst which has pentafluoro-aniline moiety in its ligand framework, thus making the catalyst very costly. Besides, rapid reaction kinetic profile exhibited by FI catalyst poses a challenge in regulating molecular weight of the polymer, especially in the region of 1-6 million g/mol. The uncontrolled polymerization leads to fouling of polymerization unit and on surface of stirrer shaft/paddle assembly. In the present study, we have reported a novel family of transition metal based homogeneous single site catalysts which is highly efficient to produce DUHMWPE with improved reaction kinetic control and molecular weight regulation properties[1].

The single site catalyst was synthesized from a Schiff base imine ligand, obtained from an aromatic diamine like meta phenylene diamine and substituted salicylaldehyde like 3-tert-butyl salicylaldehyde or 3,5-ditert-butyl salicylaldehyde etc., followed by chelation with transition metal halides like titanium tetrachloride. A non-cryogenic process[2], i.e., polymerization process at ambient temperature and high pressure, which is economically viable as well as industrially feasible, has been adopted to produce DUHMWPE. Under optimized process conditions, the catalyst exhibits good kinetic profile, enabling proper regulation of molecular weight in the range of 1 to 10 million g/mole. The resulting DUHMWPE exhibits distinct and unique properties like low bulk density (0.05 to 0.08 g/cc), high crystallinity (> 90% by XRD) and fibrous and porous morphology (SEM).

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CPSA -23

Environmentally Benign Approach To Conductive Polystyrene-Polypyrrole Nanocomposites

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Abstract

A facile, environmental friendly and water mediated approach for preparing conductive polystyrene-polypyrrole (PS-PPy) composites by the assembly of positively charged PS latex particles and water sonicated pyrrole, followed by in-situ oxidative polymerization using ferric chloride as an oxidant. The PS latex was prepared by surfactant-free emulsion polymerization using a cationic free radical initiator, which created the positive charges on the surface of the PS particle. The interaction between PPy and PS chains were characterized by using X-ray diffraction, thermogravimetric analysis, Fourier transforms infrared spectroscopy,UV–Vis spectroscopyand scanning electron microscopy. Scanning electron microscopy images showed PPy was homogeneously dispersed in the spherical nanopartciles of PS with diameters of several hundreds of nanometers and the formation of conductive-filler network at a relatively low filler content. A significant improvement in the conductivity of composites was observed as a function of PPy loading which is due to the presence homogeneously dispersed PPy in the polymer matrix. This study suggests that the composites have the potential to be used for suitable electronic applications with desired electrical properties.

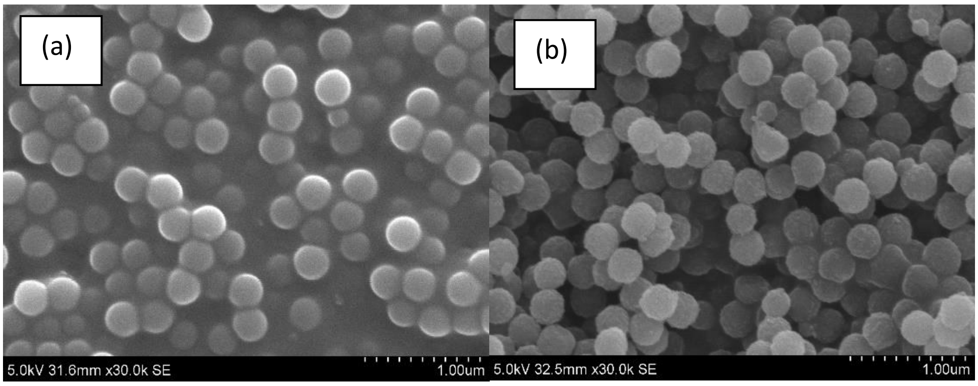

Figure-1. SEM image of (a) PS nanoparticles and (b) PS-PPy composite.

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CPSA -24

RAFT mediated grafting of di-block copolymers on the silica nanoparticle surface

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Abstract

In this work, we have grown a series of heterocyclic di-block copolymer chains of N-vinyl imidazole (NVI) and N-vinyl-1,2,4-triazole (NVT) of varying chain length on silica nanoparticle (SINP) by using reversible addition fragmentation chain transfer (RAFT) polymerization through *grafting-from* approach to develop a designer nanoparticle. In a multistep synthetic process, well-defined heterocyclic di-block copolymer grafted SINP was synthesized with tunable chain length from RAFT agent anchored SINP surface using NVI and NVT as monomers. Spectroscopic and thermal analysis confirmed surface grafting of the block co-polymer of NVI, NVT on SINP surface and the amount of grafted block co-polymers were also quantified. The approach is metal-catalyst free and provides pNVI-*b*-pNVT-*g*-SINP, pNVT-*b*-pNVI-*g*-SINP in a simple manner in comparison to other controlled radical polymerization technique for surface modification of SINP.

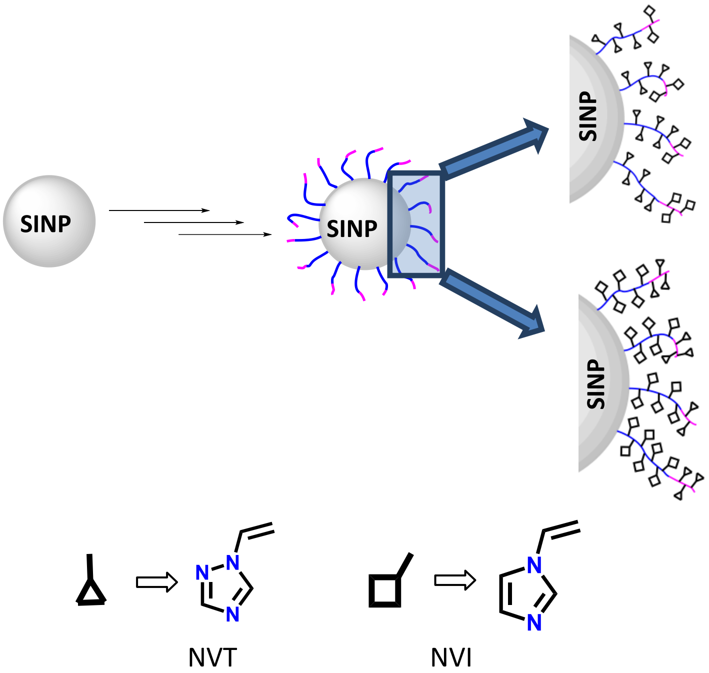

Fig: A multistep approach to develop designer nanoparticles.

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CPSA -25

Design, Synthesis and Applications of Functional Mesoporous Molecular Materials

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Abstract

In recent years, functional mesoporous materials (pore size: 2-50 nm) have gained significant research interest because of their extremely high surface area and large pore volume. These materials have many applications in the areas of separation, adsorption, chemical sensor, catalysis and synthesis of host–guest functional material.[1,2] Furthermore, they are also useful for optical sensor applications, energy storage and information processing and as Magnetic Resonance Imaging (MRI) contrast agents.[3] Among them, mesoporous polymer (MP) nanomaterials has potential use in electronics, controlled drug release and heterogeneous catalysis,[4] while mesoporous carbon (MC) materials are used as an adsorbent of bio- and organic- molecules, catalyst supports, component of Li ion batteries and component of fuel cells.[5]

A facile approach has been developed for the production of functional mesoporous molecular materials via surface-confined reversible deactivation radical polymerization (SC-RDRP). Fine-tuning the reaction conditions led to synthesis of materials with wide range of pore geometry and shape. Functionality of thus developed molecular materials can be controlled by choosing an appropriate functional comonomer alongside a base-monomer. %incorporation of the functional monomer can be controlled by controlling the initial $[\text{base-monomer}]_0/[\text{functional monomer}]_0$ feed ratios. Thus developed materials were characterized by different microscopic (scanning electron microscopy, tunneling electron microscopy and atomic force microscopy) and spectroscopic (NMR and IR spectroscopy). Finally, thus developed materials were tested for their potential applications as materials and biomedical field.

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CPSA -26

Organo-clay Hybrid Hydrophobic Spherical Styrene Divinyl benzene Crosslink beads for High performance Carbon Dioxide Capture

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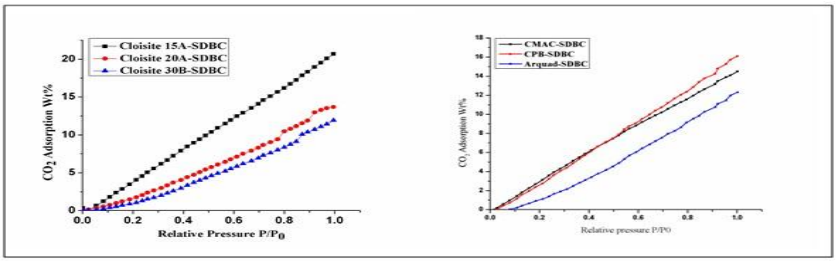
Abstract

We report here the carbon dioxide sorption properties for a series of cloisites and quaternary bulky ammonium salts containing crosslink hybrid materials. These materials were prepared copolymerizing styrene divinylbenzene in presence of various cloisites and quaternary bulky ammonium salts through suspension polymerization in one pot in order to obtain uniform spherical beads. The homopolymer formed during the polymerization was separated from the hybrid. The synthetic strategy is user-friendly, cost-effective, and can be easily scaled up for production and shows good mechanical strength. The microporous polymeric spheres containing organo-clay (cloisite) showed a high surface area of ~80 - 370 m^2 g-1 with a microspheres size ~4.4 nm. These polymeric spherical beads were hydrophobic and thermally stable up to 300°C. It showed high carbon dioxide uptake (up to ~20.7 wt % at 273K /1.0 bar)in case of cloisite containing hybrid material, and (up to ~16.4 wt % at 273K /1.0 bar), in case of quaternary ammonium salt(bulky groups) due to lone pair electrons of heteroatom, which might sharpen the interaction between the CO_2 molecules and polymeric matrices through local-dipole/quadruple interaction. It showed the good capacity to store CO_2, which is attributed to the presence of quaternary ammonium groups in the hybrid materials and presence of large amount of narrow microspheres (~4.4 nm) in hybrid material. The equilibrium CO_2 capacities of the prepared spherical beads were due to the interaction between the quaternary ammonium salt and the negatively charged oxygen atoms of CO_2 occurred and showed potential applications in gas adsorption and separation.



CO_2 Adsorption by Cloisite-SDBC   Quaternary ammonium salt (bulky groups)-SDBC

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CPSA -27

Judicious Reduction of Supported Ti Catalyst Enables Access to Disentangled Ultrahigh Molecular Weight Polyethylene

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Abstract

The seven decades old and continuously evolving field of olefin polymerization also have some remaining challenges.[1] Heterogeneous Ziegler-Natta and homogeneous metallocene catalysts are known to produce ultrahigh molecular weight polyethylene (UHMWPE) in the entangled state. On the other hand, only two single-site homogeneous catalysts are reported to yield disentangled UHMWPE (dis-UHMWPE).[2] The disparity between the two types of catalysts and the two states of the polymer can be bridged if a heterogeneous single-site catalyst that yields dis-UHMWPE is made accessible. Here, a single-site heterogeneous catalyst system has been developed with a two-stage activation strategy. After the second activation with excess modified methylaluminoxane (MMAO-12), titanium centre uniformly exists in Ti(III) state, which has been analyzed using XPS.[3] The catalyst system was found to be highly active in ethylene polymerization and produced dis-UHMWPE.[4] The Mw and MWD of the nascent PE were estimated by HT-GPC. The presence of dis-entangled state was confirmed by the appearance of two separate melting peaks in DSC curve, after annealing and isothermal crystallization for a stipulated time. Further, the disentangled state of the nascent PE and its Mw and MWD were authenticated by rheological investigations.

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CPSA -29

Multi-Stimuli Responsive Zwitterionic Ionic Liquids/Poly(ionic liquid)s and Their Tunable Hierarchical Nanoaggregates

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Abstract

Smart stimuli-responsive polymeric materials has tremendous potential for a variety of interesting applications including drug delivery, catalysis, sensing and making responsive nanomaterials.[1] Most of the reports in this area are focused on the development of nonionic homopolymers/copolymers that are responsive to either single or dual stimuli. In this direction, a new class of zwitterionic ionic liquid (ZILs) monomers with coexisting imidazolium bromide ionic liquid and zwitterionic imidazolium alkyl carboxylate moieties with different alkyl spacer groups are designed and synthesized. RAFT polymerization of these ZIL monomers produces a series of multi-stimuli responsive poly(zwitterionic ionic liquid)s (PZILs) of controllable molecular weights and low dispersities. Near the isoelectric points (~pH 5.7), PZIL solutions undergo a phase transiton form transparent to turbid containg hierarchical nanoaggregates (NAs) of various morphologies such as small sphere, large sphere, flower-like, dendrite-shaped, and dendritic fibrillar-like depending upon the pH and chemical structures of PZIL. PZILs exhibit triple-stimuli-responsiveness toward pH, temperature, and anions as demonstrated by solubility phase transition in aqueous solution. The obserevd upper critical solution temperature (UCST)-type cloud point can easily be tuned by changing various parameters such as molecular weight, concentrations, structure of PZILs, nature and concentration of anions and solution pH.[2]Further, as an extention of this work, a series of different zwitterionic ionic liquids (ZILs) containing various aliphatic/arometic substituents are also synthesized to understand the structure-property relationship in detail. ZILs show high thermal stabilities and interesting glass transition temperature behaviors. ZILs in water form pH-tunable nanoaggeragtes of various shapes and shows UCST-type thermoresponsiveness.[3]

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CPSA -30

Fluorescent Perylene-Bridged Ionic Amphiphilic Polymers: Synthesis, Self-Aggregation and Responsive Behaviours

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Abstract

Water-soluble fluorescent polymers have attracted great attention among polymer and materials research community because of their enormous important applications in biosensing, bioimaging, tissue culture, chemical sensors, optoelectronic device designing etc. This report describes an easy and new way of synthesizing fluorescent amphiphilic perylene-bridged ionic polymers. The two-step synthesis involves the preparation of poly(1-vinyl imidazole) (PVim) or poly(ionic liquid)s (PILs) by thiol-mediated radical polymerization using cysteine followed by their tethering with perylene dianhydride. In the case of Perylene-PVim, the iconic character is introduced by the post-modification of pendent imidazole group with HCl or 1-bromoalkanes. The resultant water-soluble Perylene-PVim or Perylene-PILs polymers are amphiphilic in nature due to the presence of hydrophilic ionic polymer block and hydrophobic perylene moiety. Self-assembly of these fluorescent amphiphilic polymers into micelles or miceller aggregates in aqueous solution is studied by DLS, UV-vis,fluorescence spectroscopy and microscopy. An attempt is also being made to study the interesting stimuli-responsive behaviours of these fluorescent amphiphilic polymers in aqueous solution.

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CPSA -31

Novel Ionic Liquid-Based Photoinitiators for Aqueous Free-Radical Polymerization

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Abstract

Photopolymerization is a well-accepted technique that has huge applications in coatings, adhesives, printing inks, photoresists, and biomaterials. There are many commercially available radical and cationic photoinitiator that are routinely used for the photopolymerization of vinyl monomers. Photo-induced controlled radical polymerization has also been the recent focus because of its mild reaction conditions. Recently, our research dealt with the development of new stimuli-responsive ionic liquid (ILs)/poly(ionic liquid)s. In this context, we have designed and synthesized some phosponium ILs that act as novel photoinitiators for polymerization of different monomers such as *N*-isopropylacrylamide (NIPAM), 2-(Dimethylamino)ethyl methacrylate (DMAEMA) under UV irradiation (λ = 310 nm) in aqueous medium. These ionic liquid photoinitiators and the obatined polymers are well-characterized by different instrumental techniques. The kinetics of this polymerization has also been studied. The mechanism of this photopolymerization is proposed to proceed through free-radical pathway, which is established through end-group analysis by MALDI-TOF-MS, EPR and some control experiemnts. As an extension, it is shown that phosphonium poly(ionic liquid)s can also be used as photoinitiator for grafting it with PNIPAM. The thermoresposnsive behaviours of the formed graft copolymer is also studied by turbidimetry and DLS.

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CPSA -32

Synthesis of block copolymer of 2-acrylamido2-methyIpropanesulfonic acid and methyl methacrylate via RAFT methodology and explore its application.

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Abstract

Controlled radical polymerization has been the focus of intense research during the last decade. Reversible addition−fragmentation chain transfer (RAFT) polymerization has been the focus of intensive research over the past few years since this methodology allows the synthetic tailoring of macromolecules with complex architectures including block, graft, comb, and star structures with predetermined molecular weight, terminal functionality, and narrow molecular weight distribution. Our attention to the acrylamido family of monomer and investigated the RAFT polymerization of 2-acrylamido2-methyIpropanesulfonic acid (AMPS). AMPS were polymerized in DMF via using Xanthate based RAFT agent and AIBN was used as initiator to initiate the polymerization reaction at 70^{o}C under nitrogen atmosphere. Further, synthesized polymer was characterized by using various analytical techniques such as FTIR, ^{1}HNMR, ^{13}CNMR, XRD, SEM. Absolute Molecular weight of synthesized poly-(2-acrylamido2-methyIpropanesulfonic acid) was calculated using GPC and % conversion of polymer was calculated by ^{1}HNMR. Application of the synthesized polymer will be explored in different fields of biomedical and others.

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CPSA -34

TEMPO Driven Mild and Modular Route to Functionalized Microparticles

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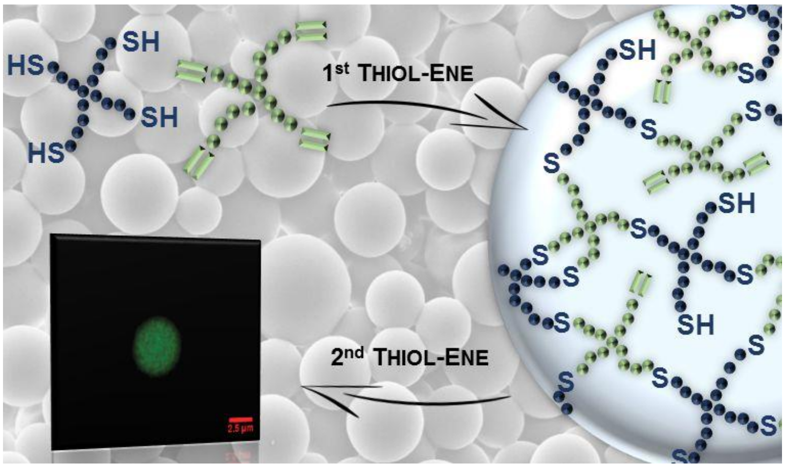
Abstract

Thiol-ene click chemistry is widely used for synthesis of hydrogels, dendrimer, microfluidic devices and for construction of macromolecular architecture. Thiol-ene reaction can be catalyzed using several methods, for example, using a photo initiator or a thermal initiator and by base (such as triethylamine and diphenylphosphine). The synthesis of cross-linked polymeric microspheres (3.8 – 15.0 µm) via (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) initiated thiol-ene dispersion polymerization at ambient conditions is reported for the first time. The initiating ability of TEMPO for the thiol-ene reaction is validated by electron paramagnetic resonance (EPR) and ^{1}H nuclear magnetic resonance (NMR) spectroscopy on model reactions between 1-octadecanethiol and two electron deficient enes, *n*-butylacrylate and divinyl sulfone. Critically, the TEMPO resonance observed in the EPR spectra decreases with time when TEMPO is mixed with thiol and an electron deficient ene. The ^{1}H NMR spectra evidence formation of up to 90% of thioether under ambient conditions. Based on these model reactions, a variety of cross-linked polymeric microspheres were synthesized with excellent morphological stability using poly(vinyl pyrrolidone) (PVP) as surfactant. The ability of the microspheres for a second TEMPO initiated thiol-ene reaction was demonstrated by the ligation of fluorescein-5-maleimide (an ene) to the microspheres' surface containing excess of thiol functionality and by ligation of cysteine (containing a thiol group) to the microspheres' surface containing an excess of ene functionality. The synthesized polymeric microspheres were characterized using scanning electron microscopy, differential scanning calorimetry, Fourier-transform infrared spectroscopy, zeta potential, and X-ray photoelectron spectroscopy.



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CPSA -35

Synthesis, Characterization and Thermal studies of new thermo-responsive glycopolymers and their Copolymers with *N*-isopropyl acrylamide

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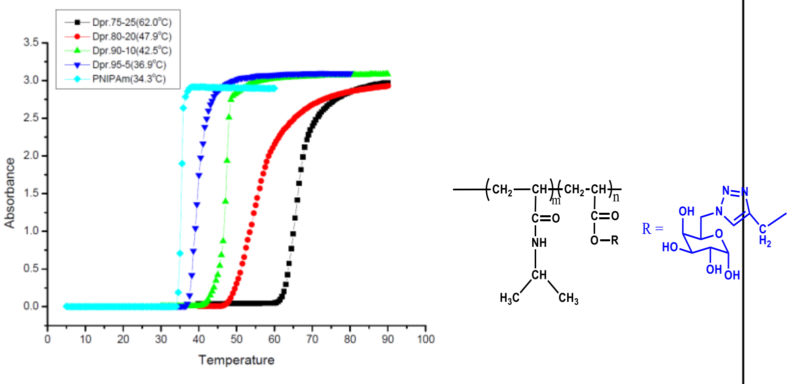
Abstract

Galactose containing glycomonomer was prepared by copper catalyzed azide-alkyne cyclo-addition reaction of 1,2,3,4 di-isopropylidene 6-azido D-galactose and propargyl acrylate. The synthesized monomer was characterized by NMR, IR, MS techniques. The monomer was subjected for homopolymerization and copolymerization with *N*-isopropylacrylamide (NIPAm) in different composition by free radical polymerization using 2, 2'-azobis-isobutyronitrile (AIBN) as an initiator. The composition of the copolymer was determined with ^{1}H-NMR spectroscopy. On acid hydrolysis, water-soluble deprotected polymers were obtained. The polymers were characterized by NMR, IR, TGA, DSC, GPC and thermal analytical techniques. The protected and deprotected copolymers showed a sharp cloud-point temperature. A linear correlation was obtained between the lower critical solution temperatures and the concentration of glycomonomer in the copolymers. The TGA curves clearly revealed two weight loss processes in the degradation behavior of the copolymers whose sharpness and intensity was varied with composition. DSC experiments were also run for deprotected polymers and the resulting Tg data are plotted.



Cloud point measurements of Glycopolymer

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CPSA -36

Functional Fluoropolymers: Design, Synthesis and Applications

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Abstract

Fluoropolymers are niche products exhibiting unique properties such as exceptional thermal and chemical stabilities, inertness to acids and common solvents, low inflammability, low dielectric constants and dissipation factors. Consequently, fluoropolymers play an important role in the development of new materials for advanced applications in aeronautics and aerospace, building industries, petrochemicals, automotive industries, Li-ion batteries, high performance membranes, and microelectronics. Poly(vinylidene fluoride), PVDF, one of the most representative examples of fluoropolymers, possesses high resistances to weathering, ageing, temperature and chemical aggressions, and is ferro- and piezoelectric. The development of efficient Reversible Deactivation Radical Polymerization (RDRP) techniques for VDF (and other fluoroolefins) can broaden the range of applications of VDF-based (co)polymers. However, RDRP of VDF has not been very successful as that of other vinyl hydrogenated monomers. Until recently, only Iodine Transfer Polymerization (ITP)[1] and Reversible Addition-Fragmentation Chain Transfer (RAFT)[2] polymerization were able to afford some control on the polymerization of VDF. To go beyond the limits of the RAFT and ITP of VDF, Cobalt-Mediated Radical Polymerization (CMRP)[3] was also examined and shown to be the most efficient RDRP technique to control the polymerization of VDF. This contribution will present a detailed account of an overall strategy to synthesize VDF-based novel fluorinated (co)polymers via radical (co)polymerization of 2-trifluoromethyl monomers with VDF, leading to various "smart" coating materials exhibiting tunable hydrophobicity,[4] anti-corrosion properties.[5]

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CPSA -38

PEGylated Polyurethane Dendrimers Containing Bis-indole Groups: Synthesis and Cytotoxicity Evaluation

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Abstract

Blocked isocyanate-terminated, bioactive bis-indole based polyurethane dendrimers of generation G0 – G3 were subjected to urethane interchange reaction with polyethylene glycol monomethyl ether and the reactions yielded PEGylated polyurethane dendrimers. The structures of the polymers were confirmed using FT-IR and ^{1}H-NMR techniques. The absolute molecular weights of the polymers were determined using SEC-MALLS technique and the values were found close to the theoretically calculated values. The PDI of the polymers were found between 1.24 and 1.49 and these values are on par with 1.46 of polyethylene glycol monomethyl ether used. Cytotoxic response and MTT assay of all the dendrimers were evaluated in A549 lung adenocarcinoma cells over a period of 24 hrs and found that PEGylated G-3 polyurethane dendrimer was highly cytocompatible.

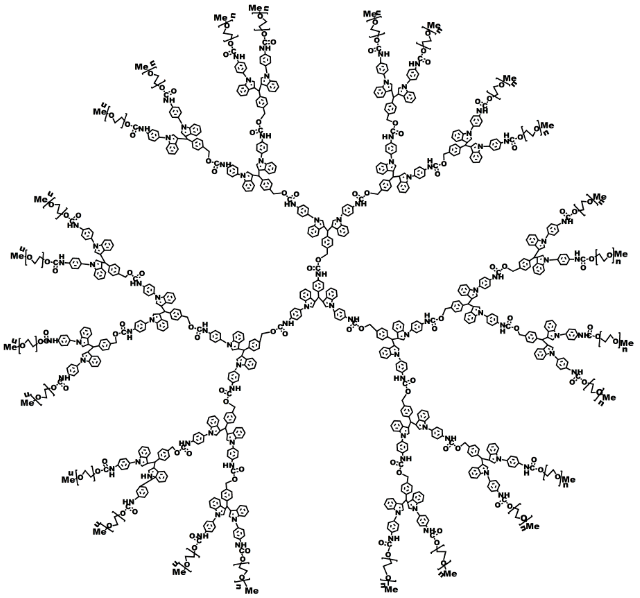

Fig.1. Structure of PEGylated G3-polyurethane dendrimers with bis-indole groups.

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CPSA -40

Dextran and poly (oleic Acid) based copolymer as nifedipine carrier

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Abstract

Polymeric micelles are mostly considered as carriers for drug delivery, as some drugs are poorly soluble in water and not able to reach into the targeted sites, which influence the effectiveness and potential toxicity of the "free" drug.[1] Herein, we have synthesized pH-responsive supramolecular graft copolymeric micelle from dextran and poly (oleic acid) through RAFT polymerization with controlled M_n and narrow polydispersity.[2] The formation of copolymer has been confirmed with ^{1}H NMR spectral analysis. Critical micelle concentration (CMC) of the copolymer has been determined by fluorometrically and conductometrically. Dextran-g-OA copolymer demonstrates spherical morphology at CMC, while rod like assembly has been evidenced beyond CMC. The copolymer is non-cytotoxic, and shows sustained release characteristics for nifedipine.

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CPSA -41

Study on the synthesis of fluorescent polyesters by consuming different secondary amine with coumarin in its backbone

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Abstract

A series of water insoluble polyesters were developed by using s-triazine, *N, N'* biphenyl amine and N-methyl amine with coumarin in its backbone. The synthesised polymers displayed significant fluorescence. All the polyesters were characterised by IR and ^{1}H NMR spectral techniques. The solubility properties of all the polyesters were checked by using polar and nonpolar solvents. The inherent and reduced viscosities were performed by Ubbelohde solution viscometer and intrinsic viscosity was measured by using Huggins and Kramer's equations ranging from 0.396-0.699 dl/g in DMF at 25^{o}C. The stability of synthesised polymer is upto 550^{O}C measured by TGA and DSC. All the polyesters were showing excellent fluorescence property. Unique fluorescence property of these polyesters makes them valuable in high performance material and Polymers combined with fluorescent probes have been widely used in chemosensor, biological imaging and PH/temperature sensor for their unique favorable mechanical properties and good workability.

Key Words: Coumarin, Polyesters, s-Triazine, Chemosensor, fluorescence.

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CPSA -42

Polymerization of Styrene using Pincer Type Redox active Nitrogen Donor Cobalt Complexes as Catalysts

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Abstract

Pincer type of redox active non-innocent ligands have received much attention in modern co-ordination Chemistry to understand new forms of reactivity and catalysis study.[1] Thus a number of pincer ligand systems have been developed and their metal mediated polymerisation reactivity of olefins and other saturated monomer has been explored.[2] Since Ziegler–Natta-type catalysts were developed, the field of transition metal catalyzed olefin polymerization has continued to grow worldwide in both industry and academics. Earlier early transition metal complexes has been used for polymerization reaction. Later on, it is tuned to late transition metal complexes when the first report came in 1995 by Brookhart and co-workers.[2] Then onwards there has been an intense search for new generation catalysts for the polymerization of olefin and other unsaturated monomer in both academic and industrial research laboratories, especially those containing late transition metals.[3] With the aim of studying the catalytic properties of the late metal complexes for styrene polymerization, we have been exploiting the synthesis and reactivity of redox non-innocent pincer type NNN-donor cobalt complexes and used as catalyst precursors for the polymerization of styrene with the activation of methylaluminoxane (MAO). Herein, we present the novel examples of this type of transition metal complexes exhibited excellent activity for styrene polymerisation even at room temperature with high conversion, which is very much beneficial in terms of energy savings.(Figure 1).

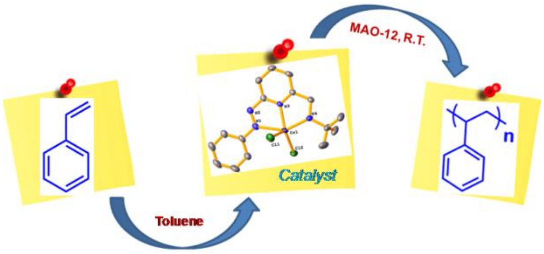

Figure 1. Schematic representation of the work.

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CPSA -43

High performance polymeric molecule containing aromatic pendant group

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Abstract

Ten compounds have been synthesized in a series of s-triazine analogues which, in addition to indole carboxylic acid and different secondary amines as substituents on the C-6 position of s-triazine ring. High-performance aromatic polymers based on aromatic rings are desirable not only because of their high primary bond strengths, but also their rigid polymer chains offer increased resistance to bend and thermal softening. The choice of s-triazine nucleus is based on its high thermal stability derived from its molecular symmetry and aromaticity. Modification of monomer structures by introduction of aromatic pendent groups or heterocyclic rings into the polymer backbone provides good solubility and thermal stability. All the polyamides showed good thermal stability and most of them were readily soluble at room temperature in polar solvents. Its analogues, cyanuric acid and cyanuric chloride are important starting compounds for various materials with wide range of applications in textile, plastic, pharmaceuticals and rubber industries. These compounds are also used as pesticides, dyestuffs, optical bleaches, explosives and surface-active agents. Finally, various aromatic amines derivatives were allowed to reacts and the product were characterized by conventional and instrumental methods. Their structures were determined as well important properties were studied. All the final compounds were structurally elucidated based on IR, ^{1}H NMR, ^{13}C NMR, TGA, DSC fluorescence and elemental analysis.

Keywords: s-triazine, indole carboxylic acid, 2^{o} amine, fluorescence, TGA

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CPSA -44

Bis-Benzilidene and Azo based polymers for NLO and LC applications

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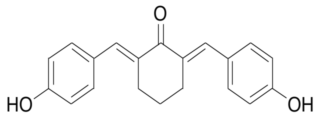
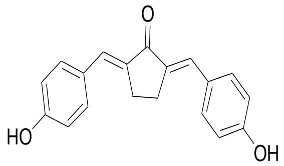
Abstract

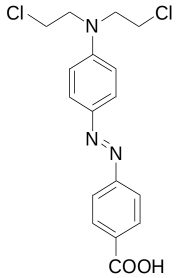
Nonlinear optics (NLO) and Liquid crystals (LC) includes a range of materials such as inorganic materials, organic small molecules and polymers (macromolecules). These materials having applications include optical communication, optical data storage and frequency generation etc. As there were a lot off technical problems with respect to inorganic materials, researchers switched over to polymers to solve some of the problems. There are a lot of activities around the world among researches to find a suitable polymer which can act as a rugged NLO and LC active film for device application. In the search, different synthetic polymeric materials such as Polyamide, Poly(methyl methacrylate), Polyimide and Polyurethane having dipole molecules within the polymeric system been synthesized for NLO as well as LC applications.

Especially for all these polymers, researchers were included a donor and accepter containing moiety linked through an azo or non-azo groups which shows an overall properties w.r.t. NLO. Some of the commonly used moieties are shown in the Fig.1. Even though these small molecules are NLO active, but after including these in to the macromolecules, they have shown enhanced properties llike resulting in the enhancement of thermal stability as well as device stability. Bis-benzilidene moiety has shown excellent properties for NLO as well as for LC. A.B.Samui et al. Synthesized various types of Bis-benzilidene based polymer for studying of LC behaviour. Also researchers were included both Bis-benzilidene and azo for studying of NLO behaviour like second harmonic generation (SHG) which is one of the area for frequency doubling devices. In especially the cross linking ability of Bis-benzilidene boosting this area for device point of view as this can increase the life time of device by aligning the dipoles for longer time which is the key stage for any success of device. Here we would like to present the past and current research of Bis-benzilidene and Azo based polymers for NLO and LC applications.





Eg. 2,6-bis(4-hydroxybenzylidene)cyclohexanone 2,5-bis(4-hydroxybenzylidene)cyclopentanone



4-((4-(bis(2-chloroethyl)amino)phenyl)diazenyl)benzoic acid

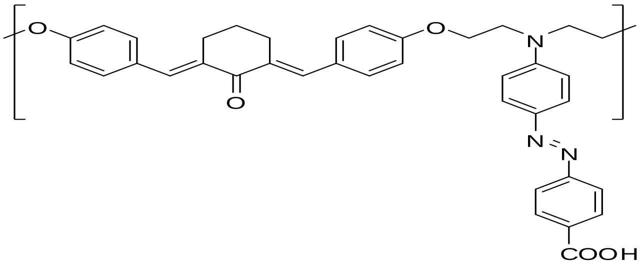


Fig.1

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CPSA -47

Synthesis of Novel Water Soluble Polycarbamate Dendrimer

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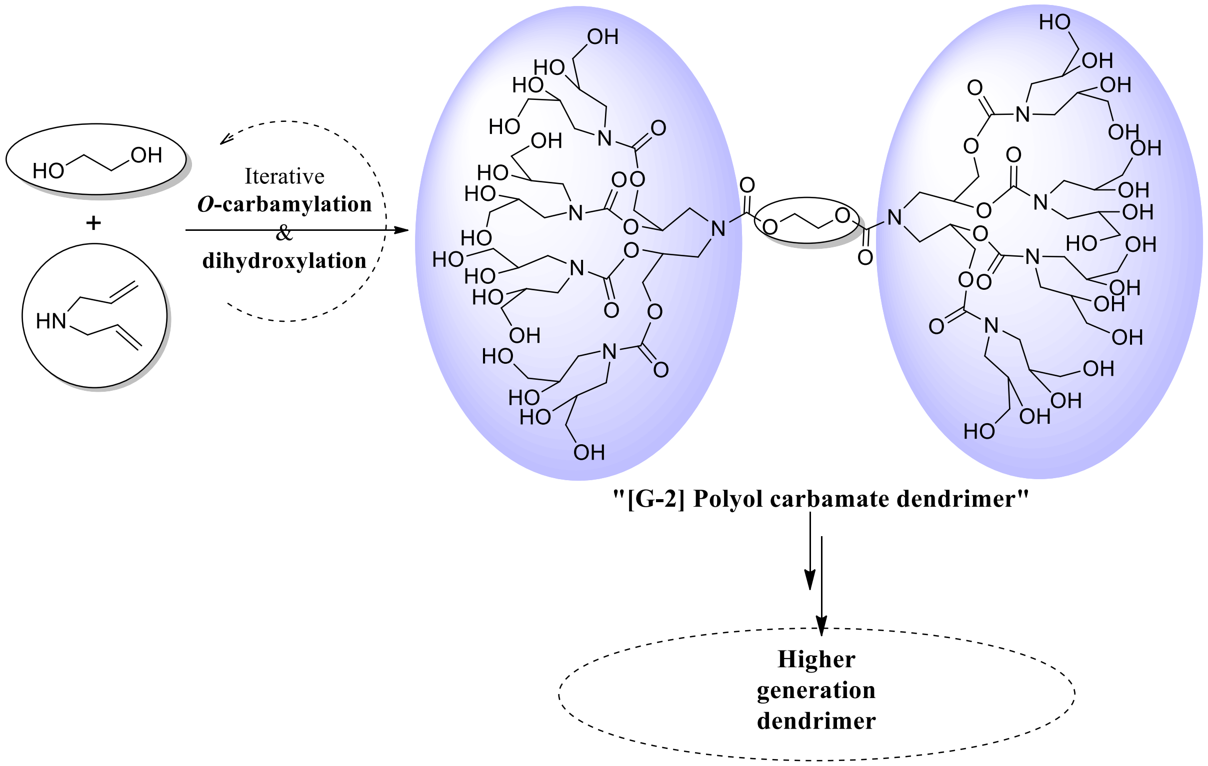
Abstract

A new water-soluble dumbbell shaped polycarbamate dendrimer with hydroxyl periphery has been successfully synthesized. Both divergent and convergent growth processes were adopted to construct the dendrimer possessing diallyl amine as key branching unit. Synthesis involves simple iterative two-step process based on allylation of an alcohol groups through tertiary carbamate linkages followed by dihydroxylation of allyl groups. Dendrimer and dendrons were fully characterized using IR, NMR spectroscopy, size exclusion chromatography and mass spectrometry. Utilization of diallyl branching unit produces dendrimers with numerous hydroxyl functionality even in its lower generations and synthetic strategy provide easy access towards the higher generation dendrimers.

Scheme



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CPSA -48

Redox and Enzyme dual responsive Block Copolymers for Cancer Theraphy

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Abstract

Multidrug Resistance(MDR) is a major hindrance in the field of cancer chemotheraphy which includes efflux of small molecule cancer drugs. Also, it is well known that the cancer drugs available in the market are not specific to targeting cancer cells alone and cause serious side effects both in the short and long run.Redox responsive polymeric nanovehicles have emerged as the solution the aforementioned problems thanks to Enhanced Permeability and Retention(EPR) effect.[1-2] This report is aimed to synthesize a biocompatible and bio-degradable block copolymer with a disulfide linkage that can be reduced and cleaved inside cancer cells to release the cargo and destroy the cells. Boc-protected caprolactone monomer was synthesised through multistep synthesis[3-4] and macroinitiator PEG was modified to possess the redox responsive disulfide linkage. This macroinitiator was used to ring open the monomer to acquire the amphiphilic diblock copolymer. Both the macroinitiator and the block copolymer were characterised through ^{1}H NMR, ^{13}C NMR and MALDI-TOF confirmed that the macroinitiator was pure. Since the polymers can be removed from blood circulation by opsonin proteins if their hydrodynamic diameter is 200 nm or higher[5], size studies were also performed on the synthesised polymers after they were made to self-assemble into micelles. DLS studies and electron microscopy studies revealed that these self-assembled polymers were well below the limit. Dye loading studies were performed with Nile Red. Polymers showed a moderate percentage of dye loading content and dye loading efficiency. Release studies gave a confirmation that the disulfide bond in the polymer is indeed cleavable in the presence of 10 mM concentration of Glutathione and a burst release of the dye was observed within a short period of time. Further studies are to be performed with higher molecular weight polymers and on drug loading . Subsequently, *in vitro* cytotoxicity studies have to be performed in MCF-7 cancer cells. To conclude, these polymers with multiple stimuli response can aid with specifically targeting cancer cell letting aside the healthy cells.

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CPSA -49

Non-phthalate Ziegler-Natta catalyst and polypropylene products

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Abstract

Polyolefin, in particular, polypropylene (PP) is one of the most used plastics in the world with a wide range of industrial and consumer applications. Polypropylene has impressive mechanical properties, combined with high chemical resistances. Moreover, RIL is the global leader in polypropylene business with range of product grades and properties. Current polyolefin market is moving to greener catalyst development. Worldwide existing monoester/diester or diether Zeigler-Natta catalyst system employed aromatic molecules as internal & external electron donors[1,2]. From FDA near future polypropylene grades for food/packaging/medical application devices need to be phthalate free Zeigler-Natta catalyst system.

Further, it seemed that catalyst design, polymer reaction engineering[3], and polymer process technologies were being pushed forward to produce novel polyolefin materials to meet the demands of highly diversified industries.

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CPSA -51

Synthesis and polymerization of 4-hydroxycyclohexane carboxylic acids

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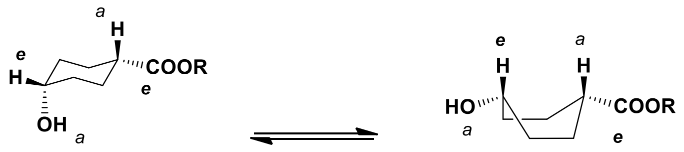
Abstract

Aliphatic polyesters suffer from many property drawbacks, such as brittleness, poor crystallization rate, poor toughness, low glass transition temperature and low melting temperature. The interest in using alicyclic monomers as components of aliphatic polyesters arises because many of their properties lie in between aromatic and linear aliphatic polyesters.[1,2] In general, alicyclic diols are far less volatile than aliphatic diols. Additionally, alicyclic diols containing secondary hydroxyl/carboxyl group have low reactivity in step-growth reaction, and hence, tend to undergo other competitive reactions, such as, elimination of hydroxyl group or cyclization, leading to loss of reactive functionality.

4–Hydroxy cyclohexane-1-carboxylic acid (4-HCHCA) is an AB monomer which can obviate some of the disadvantages associated with the step-growth polymerization of AA+BB monomers, wherein the diol is an alicyclic compound. 4-HCHCA exists in two configurations, namely, e, e *(or a, a)* and *a,e*-isomers. The a,*e* isomer is volatile and can be distilled (b.p. 260°C) (**Figure 1**). It can also be lactonized upon applying heat or on heating with acetic anhydride,[3] (m p of lactone 126-128°C). The *e, e (or a, a)* isomer, on the contrary, does not form a lactone.

a,a (Trans) *e,e (Trans)*



a,e (Cis) (Chair) *a,e (Cis)(Boat)*

Figure 1. Structure of 4-hydroxy cyclohexane carboxylic acid/ester and their conformations

A careful search of the literature reveals that 4-HCHCA has not been used as a monomer for the preparation of aliphatic polyesters. Ability to polymerize (or copolymerize) this AB type monomer could open the way for preparing a host of new polymers and copolymers leading to a diversity of structures with potentially useful properties.

Therefore, the polymerization of 4-HCHCA, an AB type monomer bearing secondary hydroxyl and carboxyl groups, has been studied under a variety of conditions as a route to aliphatic polyesters containing cyclohexyl group in the backbone. Preliminary results suggest that melt polyesterification of 4-HCHCA can give rise to polyesters with an Mn of about 17000 g/mol. Solution polyesterification at a lower temperature at 120^{o}C using toluene as entrainer and transesterification-polycondensation of the corresponding methyl ester using titanium tetra-isopropoxide as a catalyst at 150^{o}C led to polymers with lower values of Mn. MALDI-ToF analysis of the polymer indicates the occurrence of, both, linear and cyclic polymer formation, under the conditions explored. Further work is in progress to improve the efficiency of the reaction and to obtain higher molecular weight polymers and, subsequently, characterize their properties.

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Theme-SPNA

SPNA-01

2,4,6-Tri(thiophen-2-yl)-1,3,5-triazine based conjugated porous polymers for dye adsorption and CO_2 capture

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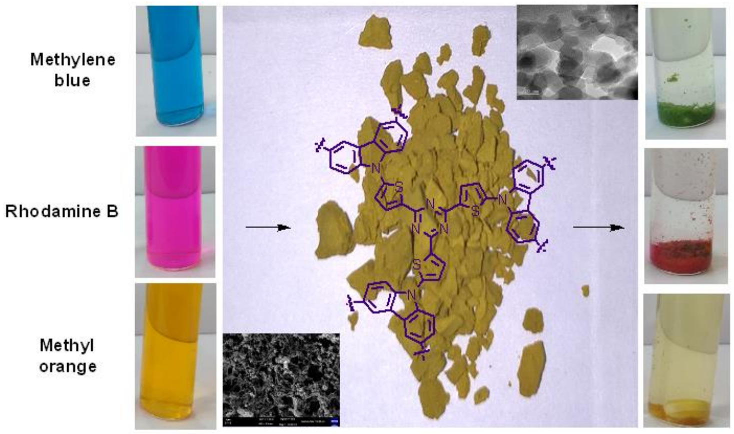
Abstract

A series of conjugated porous polymers (**CPPs)** were synthesized using 2,4,6-tri(thiophen-2-yl)-1,3,5-triazine as the main building block and other nitrogen rich moieties. **CPP1**, **CPP2** and **CPP3** were obtained by Sonogashira-Hagihara coupling of 2,4,6-tris(5-ethynylthiophen-2-yl)-1,3,5-triazine with 3,6-dibromo-9*H*-carbazole, 3,3',6,6'-tetrabromo-9,9'-bicarbazole and tris(4-bromophenyl)amine respectively. **CPP4** and **CPP5** were obtained by $FeCl_3$ mediated oxidative polymerisation of carbazole substituted 2,4,6-tri(thiophen-2-yl)-1,3,5-triazine in abscence and precence of $MeNO_2$, respectively. The porosities and morphologies of all **CPPs** were studied and compared. Amongst all these **CPPs**, **CPP5** displayed highest BET surface area of 1059 m^2g^{-1} and Langmuir surface area of about 1980 m^2g^{-1} and an average pore width of 4 nm. With high surface area, excellent thermal stability and porous structure, **CPP5** exhibited excellent adsorption of organic dyes, methylene blue and rhodamine B and moderate adsorption of methyl orange from their aqueous solution. All the **CPPs** were tested for CO_2 adsorption. **CPP5** with its excellent adsorption properties could be a potential candidate for water purification and treatment.



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SPNA-02

CHARACTERIZATION AND GREEN SYNTHESIS OF PQ

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Abstract

A new monomer bearing dialkyl groups, 3,3-dinonanoylbenzidine, when copolymerized withdiacetyl monomers gave six new alternating conjugated copolymers, poly(2,2-arylene-4,4-bis(4-alkylquinolines))s, which are soluble in organic solvents. The thermal, electrochemical, photophysical, and electroluminescent properties of the new polyquinolines varied with the arylene linkage, including *p*-phenylene, 4,4-biphenylene, stilbene, 5,5-bithienylene, bis(thienyl)vinylene, and 3,7-phenothiazinylene. The new conjugated polymers combined high glass transition temperature (110-254 °C) with quasireversible electrochemical reduction from which 2.72-3.00 eV electron affinities were estimated. The optical band gap varied from 2.19 to 2.86 eV whereas the photoluminescence emission maximum varied from blue-green (477 nm) to deep red (646 nm). Some of the new polymers with alternating donoracceptor architecture showed strong intramolecular charge transfer. Electroluminescence of moderate brightness (up to 209 cd/m2) was achieved with blue-green, green, yellow, orange, and deep red colors depending on the arylene linkage of the copolymer. The new polyquinolines were also demonstrated as useful electron transport materials for the enhancement of polymer light-emitting diodes.

Keywords- PQ, p-phenylene,4,4-biphenylene……..

SPNA-03

Influence of Hofmeister I^- on Tuning Optoelectronic Properties of Ampholytic Polythiophene by varying pH and Conjugating with RNA

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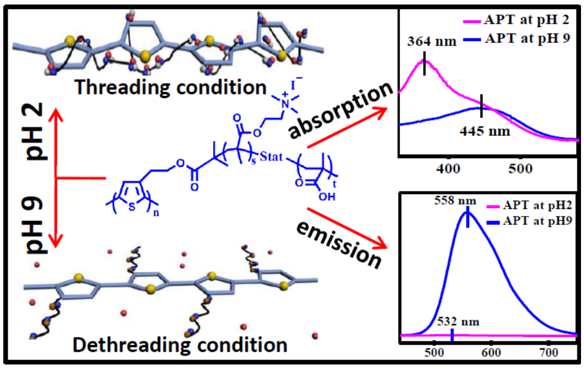
Abstract

A significant tuning of optoelectronic properties of polythiophene (PT) chains due to Hofmeister iodide (I^-) ion is demonstrated in ampholytic polythiophene [polythiophene-g-poly{(*N*,*N*,*N*-trimethylamino iodide)ethyl methacrylate-co-methacrylic acid}, APT] at different pH. In acidic medium, the absorption and emission signals of PT chromophore exhibit appreciable blue shift in presence of I^- as counter anion. The co-operative effect of undissociated -COOH and quaternary ammonium groups immobilize I^- near apolar PT chain causing threading of grafted chains and hence twisting of the backbone attributing to the blue shift. As medium pH is increased, dethreading of PT backbone occurs due to ionization of –COOH group, releasing quencher iodide ions from the vicinity of PT chains resulting red shift in absorption and sharp hike in fluorescence intensity (390 times) for increase of excitons lifetime. With increase of pH, morphology changes from multivesicular aggregate with vacuoles to smaller size vesicles and finally to nanofibrillar network structure. Dethreading is also found when APT interacts with RNA showing significant hike of fluorescence (22 times) for displacing iodide ions forming nanofibrillar network morphology. Threading and dethreading also affect the resistance, capacitance and Warburg impedance values of APT. Molecular dynamics simulation of a model APT chain in a water box supports the threading at lower pH where the iodide ions posing nearer to the PT chain than that at higher pH causing dethreading. So the influence of Hofmeister I^- ion is established for tuning the optoelectronic properties of a novel PT based polyampholyte by changing pH or by conjugating with RNA.



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SPNA-04

Solvent Geometry Dependent Pathway Complexity and Controllable Supramolecular Polymerization

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Abstract

Directional molecular interactions such as H-bonding and others endow an internal order in supramolecular polymers of diverse π-systems. However controlling their growth mechanism and the mesoscopic structure remains an uphill task. Recently, we have shown core-substituted naphthalene-diimide derivatives (cNDI-1/ cNDI-2, Scheme 1) exhibit similar *J*-aggregation in cyclic as well as linear hydrocarbon solvents, but gelation was noticed only in linear alkanes (dodecane, decane, heptane, hexane) in contrast to free flowing solution in their cyclic analogs (methyl-cyclohexane, cyclohexane). Investigation of mechanistic pathway by variable temperature UV-Vis studies indicated highly cooperative supramolecular polymerization pathway in linear hydrocarbons due to the direct participation of linear alkanes in the nucleation process by favorable mixing with the peripheral alkyl chains. In contrast ill-defined polymerization was noticed in Methylcyclohexane (MCH) because of lack of nucleation owing to geometry mismatch. Morphology studies revealed the formation of 1D fibrillar structure in decane whereas in MCH irregular particles were produced indicating an off-pathway aggregation. We have explored this solvent geometry regulated pathway selection for controllable supramolecular polymerization by a chain growth mechanism. Linear polymer produced in decane was sonicated to get small seeds which were used as initiator for controlled supramolecular polymerization of the off-pathway aggregate in MCH. By this method it was possible to synthesize supramolecular polymers with controllable chain length (by varying monomer/seed ratio) and low polydispersity. Chiral seed produced from cNDI-2 was successfully utilized to generate helical supramolecular from the meta-stable off pathway aggregate of achiral cNDI-1 in MCH. The presentation will highlight precise solvent geometry effect on nucleation and thermodynamic properties of supramolecular polymerization and elucidate the impact on controlled seed-initiated supramolecular polymerization.

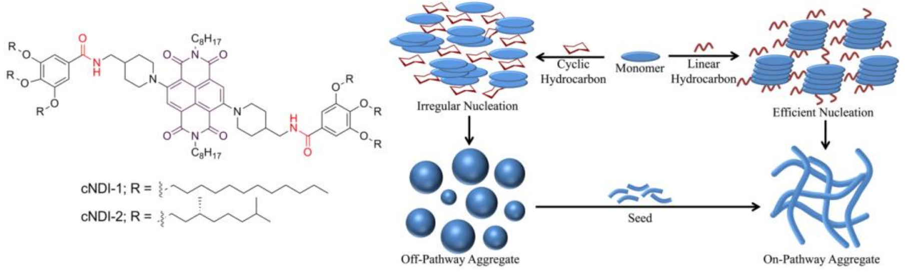

Figure 1. Molecular structure of NDI derivatives (left) and schematic representation of solvent geometry dependent pathway complexity and seeded supramolecular polymerization (right).

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SPNA-05

Directed Assembly of Hierarchical Supramolecular Block Copolymers: A Strategy to Create Donor-Acceptor Charge Transfer Stacks

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Abstract

Organic donor-acceptor complexes have emerged as promising candidates for diverse applications in the area of organic electronics, responsive materials, supramolecular assemblies, etc. The organization of aromatic donor-acceptor molecules into well-defined ordered structures in the solid state is of great importance due to their promising role as active components in organic electronics. In the present work, we have developed the strategy to obtain highly ordered charge-transfer nanostructures, in which donor and acceptor molecules are alternatively arranged with the help of block copolymer based supramolecular assemblies (SMA) (Figure 1). First, the SMA was produced by the association of donor molecules with one of the polymer blocks by noncovalent interaction such as hydrogen bonding. Further, the acceptor molecules were added to the SMA to obtain the CT complexes within the block copolymer domains. The non-covalent interactions between small molecules and block copolymers stabilize the donor and acceptor molecules by forming hierarchical structures (structures-within-structures). In addition, the morphological changes occurred during the donor-acceptor interaction within the SMA system is studied in detail using transmission electron microscope and small angle X-ray scattering.

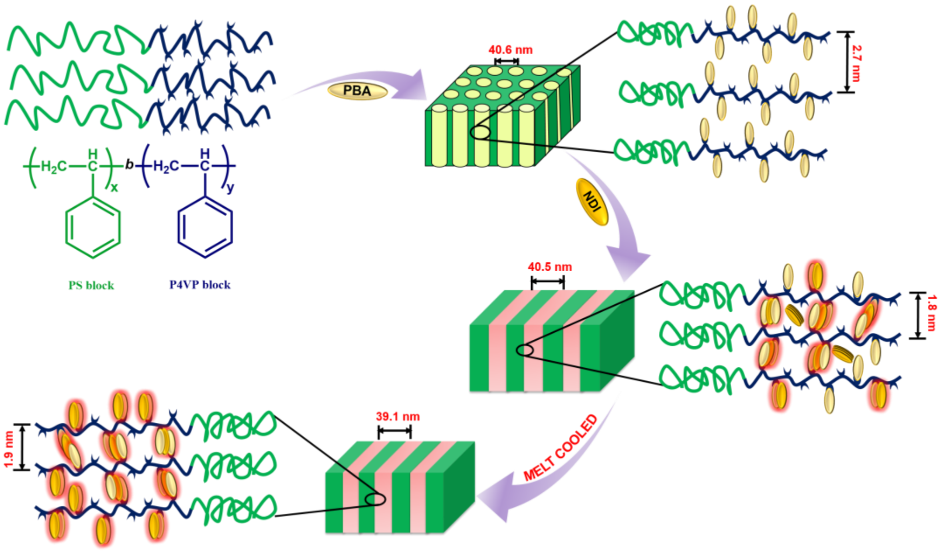

Figure: Schematic representation of the formation of CT complexes within the block copolymer domains using SMA approach.

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SPNA-06

H-bonding Promoted Supramolecular Nanostructures and Impact on Multivalent Bonding

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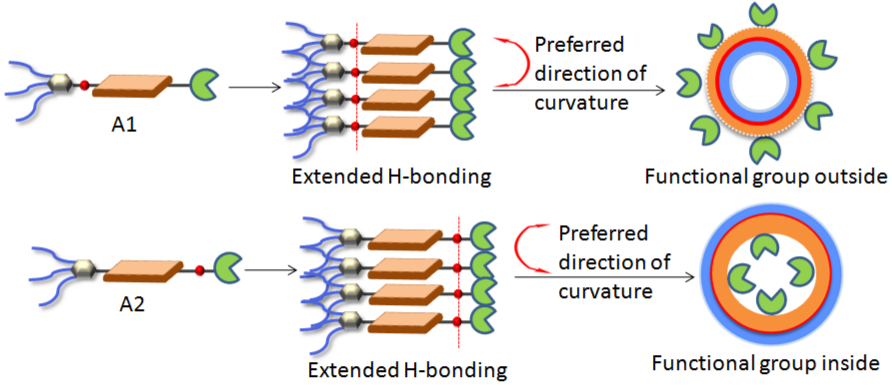
Abstract

It remains a challenging task to control the functional group display at the inner or outer surface of a vesicle at will. Even though it has been attempted using unsymmetric bolaamphiphiles, lack of control in their lateral orientation results in random distribution of the two different hydrophilic head groups in the exo- and endo- wall. We have recently solved this classical problem by H-bonding functional group attached π-Amphiphiles (Scheme 1). Basically, driven by the motivation to form extended H-bonding, both A-1 and A-2 undergo uni-directional orientation and furthermore the propensity of the H-bonded chain to remain at the inner wall implicates display of the functional group attached to the H-bonded arm to converge at the inner wall while the functional group attached with the other arm are displayed at the outer surface.[1] This has been tested with series of unsymmetric bolaamphiphiles having different anionic head groups. Subsequent studies demonstrate the possibilities of precisely tuning the size and surface charge density of such vesicles by systematic variation of the structure of the ionic head groups [2] which was reflected in their ability to inhibit the enzymatic activity of ChT. Most recently, H-bonding regulated functional group display has also been verified[3] by the glycol-cluster effect exhibited by sugar-functionalized similar π-amphiphiles. Hydrazide containing bolaamphiphile produces unsymmetric membrane leading to effective display of the sugar moieties at the vesicular surface which enables much efficient binding with ConA compared to control molecule lacking any H-bonding group. Interestingly when the hydrazide group was replaced by amide, the amphiphile revealed cylindrical micellar structure which appears to endow even better multivalent effect for interaction with biological targets owing to more adaptable nature of cylindrical structure than vesicle. Highlights of these results will be described in the presentation.



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SPNA-07

A New Facile Synthesis of Tungsten Oxide from Tungsten Disulfide: Structure Dependent Supercapacitor and Negative Differential Resistance Properties

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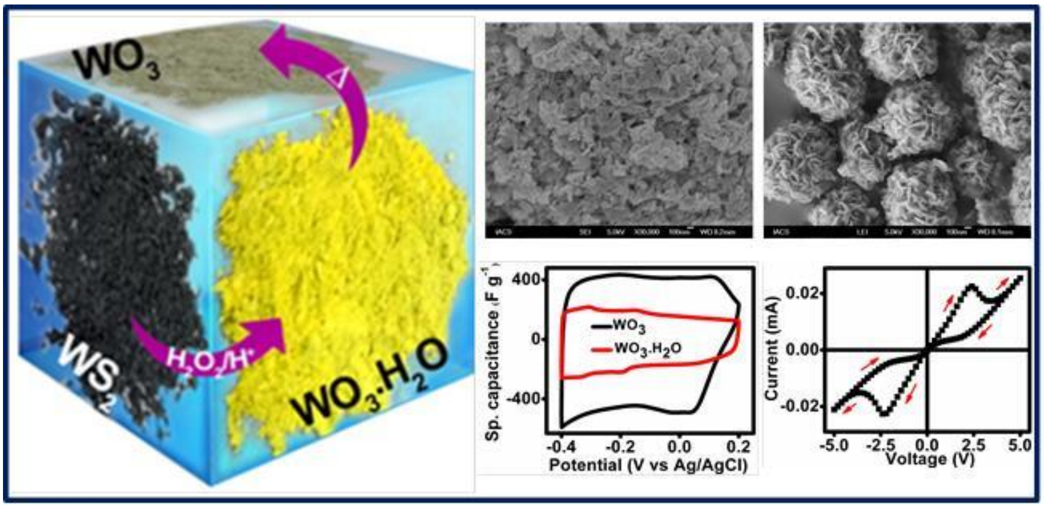
Abstract

Tungsten oxide (WO_3) is an emerging two-dimensional nanomaterial possessing unique physicochemical properties extending wide spectrum of novel applications which are limited for lack of efficient synthesis of high-quality WO_3. Here, a facile new method of synthesis of WO_3 from commercial WS_2 is reported. Microscopic, spectroscopic and X-ray studies corroborate formation of flower like aggregated nanosized cubic WO_3 through an intermediate orthorhombic $WO_3.H_2O$ phase. The charge storage ability of WO_3 is very high (508 F g^{-1} at 1 A g^{-1}) at negative potential region compare to intermediate tungstite ($WO_3.H_2O$; 194 F g^{-1} at 1 A g^{-1}) and other similar reported systems. Moreover, high capacity retention of 97% after 1000 cycles and capacitive charge storage nature of WO_3 electrode, suggest its supremacy to use as a negative electrode of supercapacitor. The asymmetric supercapacitor based on the synthesized WO_3 as negative electrode and mildly reduced graphene oxide as positive electrode manifests high energy density of 218.3 $mWhm^{-2}$ at power density 1750 mWm^{-2}, and exceptionally high power density of 17500 mWm^{-2} with energy density of 121.5 $mWhm^{-2}$. Furthermore, the negative differential resistance property of both WO_3 and $WO_3.H_2O$ are reported for first time and it is explained with density of state approach. Both electrochemical charge storage and NDR property involve the charge adsorption and desorption through the bridged oxygen atoms in both the crystal systems. This synthetic strategy can be further extended to develop new 2D materials for various electrochemical and electronic applications.



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SPNA-08

Supramolecular Assemblies of PS-*b*-P4VP(PBI-PDP)$_n$ probed in solution by NMR Spectroscopy

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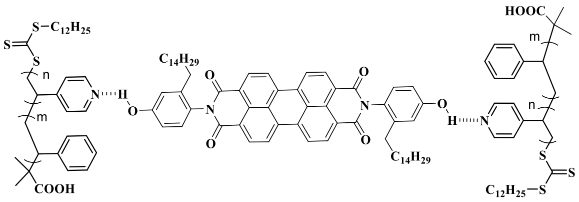
Abstract

Block copolymer is a copolymer consisting of two or more monomers where strong repulsion between monomers leads the sequences in block copolymer to segregate in microphase separated structure (10-100 nm length scale). Attaching small amphiphilic molecule to one block selectively by means of physical interactions results in another morphology (2-10 nm length scale) within the block copolymer ordering [1]. Amphiphilic block copolymers form micelles in solvents selective for one of the blocks which is very different from its bulk morphology.

Perylenebisimide derivatives are'n' type or electron poor materials with high thermal and photostability, molar extinction coefficient and broad absorption in the visible region. But this molecule is difficult to polymerise to high molecular weight. Self-assembly of unsymmetrically substituted perylenebisimide molecule with P4VP homopolymer by means of hydrogen bonding induces order to an otherwise completely disordered polymeric system, improving charge carrier mobility [2].

Here, we describe PS-b-P4VP with varying P4VP block lengths synthesised by RAFT polymerisation and its complex formation with a pentadecyl phenol substituted perylenebisimide molecule (PBI-PDP) through hydrogen bonding interaction. Self-assembly was studied in solid as well as solution state by means of IR, NMR, AFM, and DLS. PS-b-P4VP forms micelles in THF with P4VP core and PS corona. Attachment of PBI-PDP to 4VP block does not change the micellar structure of the assembly with PBI-PDP present in the core interacting with P4VP as studied by NMR spectroscopy. This is the first report in literature showing the interaction between 4VP and small molecule existing not only in solid state but it retained in solution state also.



Block copolymer-(PBI-PDP) complex

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SPNA-09

Molecular Interaction Guided Entropically Favourable Assembly of Engineered Macromolecules

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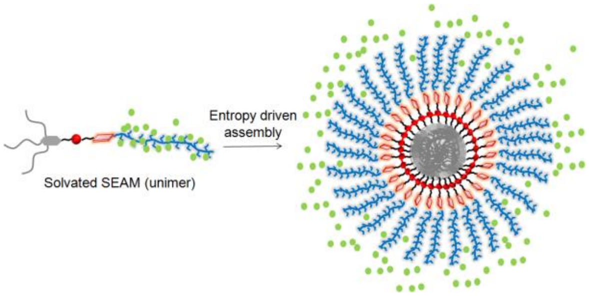
Abstract

Amphiphilic block copolymers self-assemble in water to produce various nano-structures such as spherical or cylindrical micelles, lamellar and polymersomes, depending on the packing parameter,[1] which does not offer molecular scale precision in governing structure formation. We have recently studied molecular interaction (H-bonding and π-π interaction) driven aqueous assembly of a series of Supramolecularly Engineered Amphiphilic Macromolecules (SEAMs) to predictable structure (cylindrical) by overcoming the rules of packing parameter.[2] All of these SEAMs contain a specific supramolecular structure directing unit (SSDU) attached with different water soluble polymers differing in hydrophilicity, backbone functionality and charge. Our studies show irrespective of the packing parameters, the self-assembly is fully governed by the molecular assembly motif of the SSDU which drives cylindrical micellar structure if the single H-bonding functional group present in the SSDU is amide while polymersome structure if it is hydrazide[3]. Combined results from variable temperature UV/Vis and ITC experiments reveal self-assembly of SEAMs is enthalpically disfavoured, but primarily driven by entropy factor in contrary to self-assembly of similar small molecular analogues. This can be attributed to the tightly packed J-aggregation of the NDI chromophore (SSDU) at the hydrophobic core that compels a close packing of the hydrophilic polymers in the corona, leading to the release of the surrounding water molecules causing enhancement of overall entropy.The presentation will highlight design, self-assembly and thermodynamic perspectives of these rather distinct class of macromolecules.



Scheme 1: Schematic representation of entropy-driven assembly of SEAMs by release of water molecules (represented by green dots).

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SPNA-10

SYNTHESIS AND CHARACTERIZATION OF POLYPSEUDOROTAXANE BASED ON HOST-GUEST COMPLEXATION OF PILLAR[5]ARENE WITH NEUTRAL GUEST

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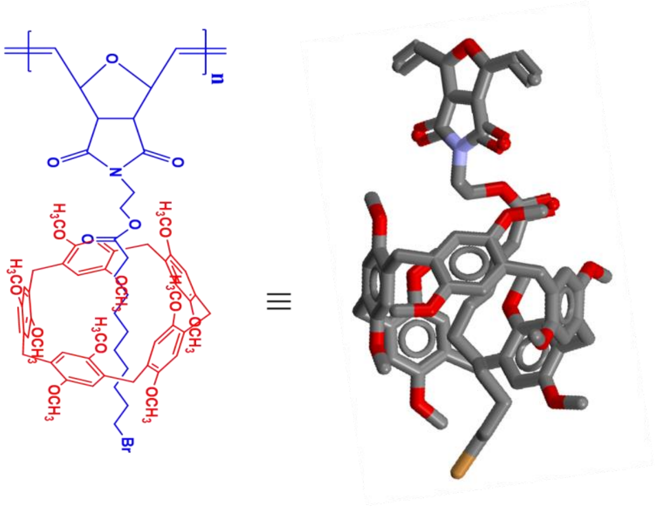
Abstract

Pillar[5]arene, P[5]A, is getting momentum as a versatile receptor in the field of host-guest chemistry since its first synthesis by Ogoshi et al. in 2008.[1] Pseudorotaxanes attracted much attention in recent years due to their versatile properties and applications.[2] One of the most important features of pseudorotaxanes is that the axle component can be dethreaded from the wheel. Herein we report the formation of Polypseudorotaxane based on molecular recognition of pillar[5]arene (**P[5]A**) host and bromoalkyl moieties in a side chain of a polymer as guest (**poly-G**). **P[5]A**was synthesized using literature procedure.[1] **Poly-G** hesized by ring-opening metathesis polymerization using Grubb's 1^{st} generation catalyst in good yield.The molecular recognition propensity of **P[5]A** with **poly-G** was confirmed by ^{1}H NMR titration experimentsin $CDCl_3$ at room temperature. Job's plot data confirmed the formation of 1:1 host-guest complexation. The nature of binding was also probed by 2D-NOESY NMR spectroscopic analysis which revealed the close proximity of **P[5]A** and bromoalkyl side chain of **poly-G**.



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SPNA-11

SYNTHESIS OF POLYPSEUDOROTAXANE BASED ON MOLECULAR RECOGNITION OF PILLAR[5]ARENE FUNCTIONALIZED TELECHELIC POLYMER

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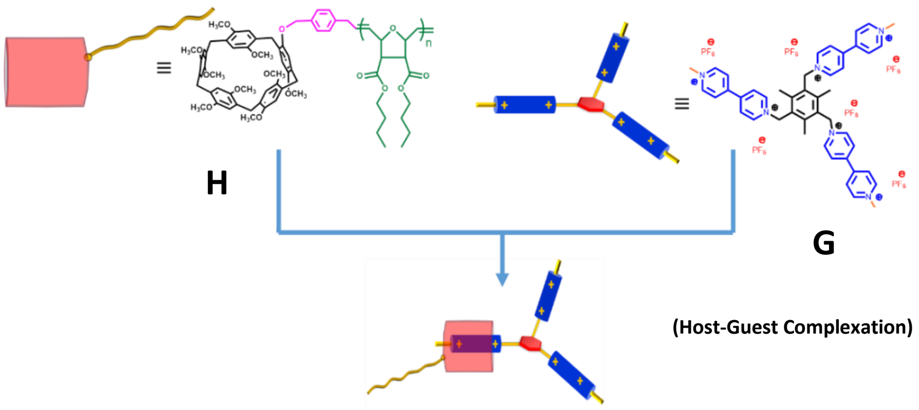
Abstract

Pillar[5]arene finds applications as good building blocks in the development of molecular sensors, vesicles, molecular machines, supramolecular polymers, etc.[1] Polypseudorotaxanes/polyrotaxanes are constructed simply by incorporating pseudorotaxane/rotaxane moieties into polymers.[2] Herein, we report the formation of polypseudorotaxane based on molecular recognition of pillar[5]arene functionalized telechelic polymer with tri-armed cationic guest. We have illustrated the new and efficient synthetic protocol to generate pillar[5]arene based telechelic polymer (**H**) by ring-opening metathesis polymerization using Grubb's 1st generation catalyst. Pillar[5]arene based Ring-Opening Metathesis(ROM) Polymer with Mw ~ 21 kDa was prepared by *insitu* functionalized Grubb's 1st generation catalyst. The Composition of telechelic polymer was confirmed based on end group analysis by ^{1}H NMR Spectroscopy and Gel Permeation Chromatography (GPC) techniques. Pillar[5]arene has high complementarity towards viologen derivatives.Tri-armed paraquat guest (**G**) was synthesized in high yield[3] and complexed with pillar[5]arene telechelic polymer (**H**). The Host-Guest complexation was probed by ^{1}H NMR titration experiments. Job's plot analysis of the ^{1}H-NMR titration experiments revealed the formation of polypseudorotaxane in **1:1** Host:Guest ratio rather than 1:3 as expected for the tri-armed guest. This might be due to the fact that upon polypseudorotaxane formation, the tri-armed guest is surrounded by the polymer chain that would have restricted the host-guest complexation of another pillar[5]arene telechelic polymer. We envisage that polypseudorotaxanes based on host-guest complexation of this kind could be used as self-healing polymers, drug-delivery vehicles, stimuli-responsive supramolecular materials etc.,



Scheme: Graphical representation showing Polypseudorotaxane formation

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SPNA-13

Fluorescent Polymer Nano-objects *via* Self-assembly of Block Copolymer/QDs Hybrids

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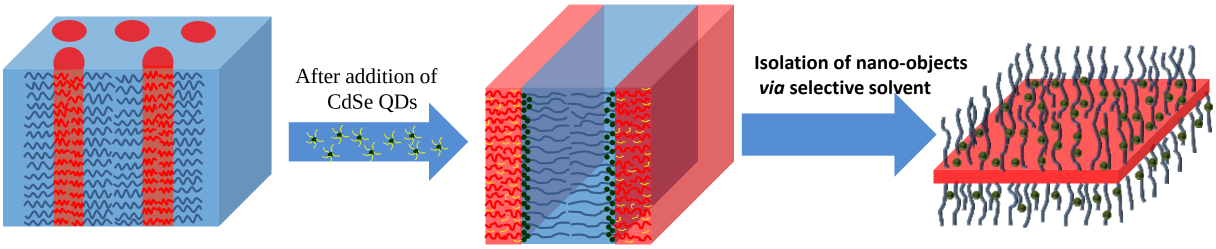
Abstract

Shaped nano-objects decorated with different functionalities has immense potential in a number of application like in sensors, drug-delivery, tissue engineering etc. However, the approaches for fabricating such nano-objects are few and most of them are tedious. Here, we present a simple approach for fabricating fluorescent polymer nano-objects which involves self-assembly of cylinder-forming polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) block copolymer (BCP) mixed with trioctylphosphine oxide (TOPO) capped cadmium selenide (CdSe) quantum dots (QDs). The QDs were found to be enthalpically compatible with the P4VP chains via ligand displacement of TOPO from the QD surface. Interestingly, a morphology transition was observed with increasing weight fraction of the QDs in the BCP/QD composite . Further, we demonstrate that these PS-b-P4VP/CdSe self-assembled hybrid materials could be used to obtain isolated core-shell nano-objects, such as nanofibers and nanosheets, containing CdSe QDs. The nano-objects so obtained exhibited photoluminescence properties typical of CdSe quantum dots. These photoluminescent polymer nano-objects could have potential application in biological targeting and fluorescence labeling.



Schematic illustration depicting the cylinder to lamellae transition on addition of TOPO coated CdSe quantum dots in BCP/CdSe QDs composites and isolation of fluorescent polymer nano-objects

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SPNA-14

Constructing Out-of-Equilibrium Molecular Assemblies

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Abstract

The supramolecular polymerization through non-covalent interactions is a promising approach to construct complex functional nanostructures. The creation of those architectures are well studied which are based on thermodynamic equilibrium states.[1] The understanding of the pathway and the rate to reach the equilibrium state are of great significance.[2] In this context, creation of out-of-equilibrium state are key to govern different spatiotemporal controlled assembly. To obtain such molecular assembly, several factors play crucial role, most importantly molecular functionalities, method of preparations, interactions with medium and external stimuli etc. Our previous report demonstrated the role of water to alter nature of aggregation of an amphiphilic molecule (OPE-Teg) with different fluorescence outcome.[3] Herein, through manipulation amphiphilicity from OPE-Teg to OPE-Meg, we are able to reach out-of-equilibrium assemby due to less interaction with surrounding molecules (water). This simple engineering to the molecule has huge impact on their molecular organisations. With course of time, molecular rearrangement occurs through optimization of interfacial surface energy between water and molecules. Because of the transformation, hypsochromic shift in absorbance as well as its fluorescence from cyan to blue with morphology changes from random to order fibers are observed. However, these time course transformations are absent in OPE-Teg. Best of our knowledge, this a unique example of achieving an out-of-equilibrium aqueous assembly from amphiphilic systems through modifying length of hydrophilic moieties.

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SPNA-15

Multi-stimuli Responsive Assembly of Amphiphilic Donor-Acceptor Alternating Supramolecular Copolymer

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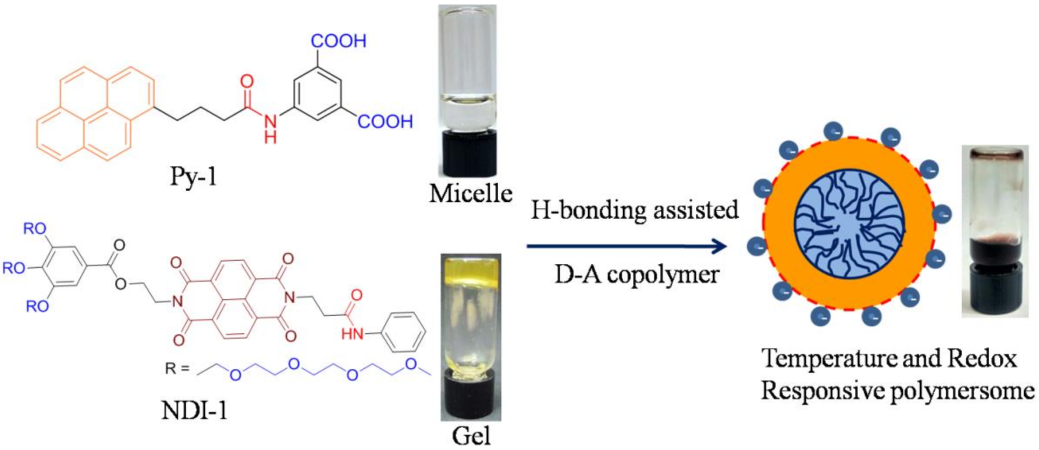
Abstract

Charge-transfer (CT)-interaction mediated alternating assembly between aromatic Donor(D) and Acceptor(A) π-chromophores although is well known, their weak binding affinity in majority examples prohibits hierarchical assembly. Recently we established alternating supramolecular copolymerization by H-bonding assisted D-A interaction.[1] This particular alternating copolymerization design has now been successfully extended to aqueous domain with newly synthesized water soluble D and A building blocks (Scheme 1). Py-1 and NDI-1 forms micelle and meta-stable fibrillar gel, respectively, while their 1:1 mixture exhibits highly stable alternating supramolecular copolymer and assembles to multi-stimuli responsive polymersome in water. Here, H-bonding driven alternating copolymer had distinct two faces; one displaying the carboxylic acid group in Py-1 and the other displaying the non-ionic wedge in NDI-1. In the resulting membrane, carboxylates were found to be displayed on the outer surface (confirmed by highly negative zeta potential in basic pH) which is attributed to (i) less electro-static repulsion and/ or (ii) directional H-bonding. It was reflected in very effective binding with an enzyme Chymotripsin and inhibition of its activity comparable to the best reported values in the literature. The polymersome showed lower critical solution temperature (LCST) due to the presence of the non-ionic wedge and the structure collapsed beyond LCST. Disassembly was also observed under reducing environment which generated the NDI radical anion and thereby destroyed the D-A interaction. The presentation will focus on design, structure and multi-stimuli responsiveness assembly of these alternating supramolecular copolymers.

Scheme 1. Structure of the donor-acceptor building blocks and their alternating copolymerization motif leading to formation of polymersome from (micelle + fiber)

References



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SPNA-16

Peptide based "in-field" detection of organic explosive

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Abstract

Nitro-aromatics are the principal ingredient of deadly explosives used in regular and other improvised explosive devices. Picric acid is a common constituent of many powerful explosives. It is also an environmental and biological pollutant. So the selective and sensitive detection of picric acid and discrimination from other are critical for practical applications. In this report, we have designed and synthesized a tripeptide, Boc-Trp-Tyr-Aib-OMe **1** containing electron rich aromatic amino acid i.e, L-Tryptophan (Trp) and L-Tyrosine (Tyr), and helicogenic 2-Aminoisobytyric acid (Aib). The tripeptide can detect picric acid in field in naked eyes almost immediately. A 1:1 host-guest charge transfer complex is formed between the tripeptide **1** and picric acid leads to fluorescence quenching. We have also checked with different nitro-aromatics and conclude that the designer tripeptide can recognize only picric acid. To study the structure-function relationship, we have also synthesized analogues Boc-Trp-Phe-Aib-OMe **2**, Boc-Phe-Tyr-Aib-OMe **3**, Boc-Trp-Aib-Tyr-OMe **4** and Boc-Phe-Phe-Aib-OMe **5** and summerized that peptide **1** can detect picric acid with LOD 6.60×10^{-7} (M) (150 ppb) with a binding constant $K_{SV}=6.3\times10^{4}$ M^{-1}. Steady-state and time-resolved spectroscopy show that the quenching process is static in nature. The detection of picric acid can be done in-field, solid state as well as vapour state also with a fast response time.

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SPNA-17

“Investigation of water absorption and moisture transmission behavior of carbon dots loaded chitosan nanocomposite thin film”

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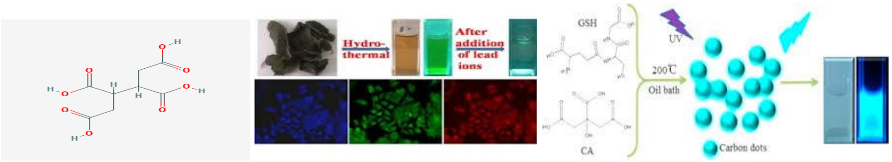
Abstract

Carbon dots have demonstrated great potential as lumniscent nanoparticles in biomedical applications. Although such nanoparticles appear to exhibit low toxicity .We know that toxicity of carbon dots strongly depends on the protocol of fabrication. In the present work, negatively charged carbon dots have been synthesized from butane tetra carboxylic acid (BTCA) via microwave exposure. The synthesized C-dots were firstly characterized by means of UV-VIS, fluoroscence various analytical techniques such as Fourier Transformation Infra-Red (FTIR) spectroscopy, X-ray diffraction (XRD), and X-ray photon spectroscopy (XPS). The size of the CDs was found to be in the range of 80 to 95 nm with almost spherical geometry. Their zeta potential was found to be -20.2 mV, thus indicating the presence of negative charges on their surface. It was found that , impregnation of C-dots into chitosan (biopolymer) film resulted in an almost seven fold decrease in the water absorption capacity of the film. The equilibrium moisture uptake (EMU) data of plain chitosan and CD-loaded chitosan films were interpreted by GAB isotherm and related parameters were also evaluated. Finally, the moisture permeation capacities of the plain Ch and carbon dots loaded sample Ch/CD was found to be 1758 and 956 g/m loaded sample Ch/CD was found to be 1758 and 956 g/m^2 /day.



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SPNA-19

"Microwave preparation of carbon dots: synthesis, characterization and preliminary in *vivo* application of fluorescent plant cells"

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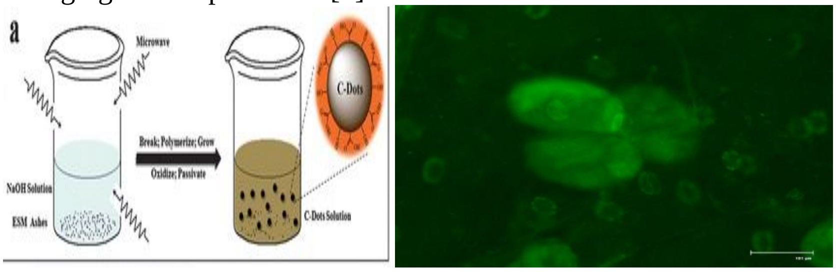
Abstract

Carbon quantum dots (CQDs, C-dots or CDs), which are generally small carbon nanoparticles (less than10 nm in size) with various unique properties. These CDs plays important roles in medicine, agriculture and electronics[1-3]. Nowadays, CDs have a wide use in nanotechnology. In the present work, A natural polysaccharides guar gum have been used as precursor to prepare carbon dots (CD) via microwave assisted synthesis.[4] The aqueous solution of Guar gum were synthesized and characterized by various analytical techniques such as Fourier Transformation Infra-Red (FTIR) spectroscopy, X-ray diffraction(XRD), Dynamic Light Scattering (DLS) analysis, UV-Vis spectroscopy, Transmission Electron Microscopy(TEM) and Fluorescent Microscopy(FM), The XRD indicates the crystalline and amorphous nature of the compound. SEM and TEM analysis the particle Size of carbon dot. The presence of CDs was also confirmed by DLS Pattern 28nm with an average diameter of 170nm. The carbon dots thus produced, showed the same green fluorescence when exposed to UV light. The U.V spectrum of a carbon dot synthesized compound showed a absorption peak about 240nm. While the results of fluorescence microscopy analysis indicated that the CDs had entered the plant tissue structure. It was observed that the carbon dots were used to image in the cells and fluorescence imaging will be performed[5].



Formation of Carbon dots, viewed through Fluorescent microscope.

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SPNA-20

Crystallization Behavior of Crystalline/Crystalline Polymer Mixtures under Confinement in Electrospun Nanofibers

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Abstract

The crystallization behaviour of polymers has been one of the most fascinating research area in polymer science for last several decades. With the advent of nanotechnology now focus has been shifting to understand the properties of materials in nano-dimensions and on crystallization study of polymers in nano-shaped materials. This is driven by the fact that any perturbation of crystallization behaviour in confinement may significantly alter the properties of the materials. Hence, an understanding of the polymer crystallization under nano-confinement is necessary for tailoring of the polymer properties when used in nanotechnology related applications. Study of polymer crystallization in electrospun nanofibers, in this respect, are interesting and provide knowledge about polymer crystallization in confined spaces. The electrospun nanofibers composed of an immiscible blend of an amorphous and a crystalline polymer, with the latter forming the dispersed phase in the fibers, could be used for studying the effect of confinement on the crystallization behavior. In this case, the limited radial dimension of the nanofibers may restrict the length scale of phase separation between the immiscible constituents, so as to generate the domains in nano-dimensions. In the present research, the crystallization behavior of polymers in polymer blend is systematically investigated by confining in electrospun nanofibers in order to gain vital fundamental understanding of confined crystallization in such materials. The effect of confinement on mixtures of crystalline/crystalline polymers is investigated which gives fundamental information on polymer crystallization behavior in confined conditions and structure-property relationship in electrospun nanofibers.

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SPNA-22

Self-healing Elastomers: Next Generation Elastomers for Advanced Tire Applications

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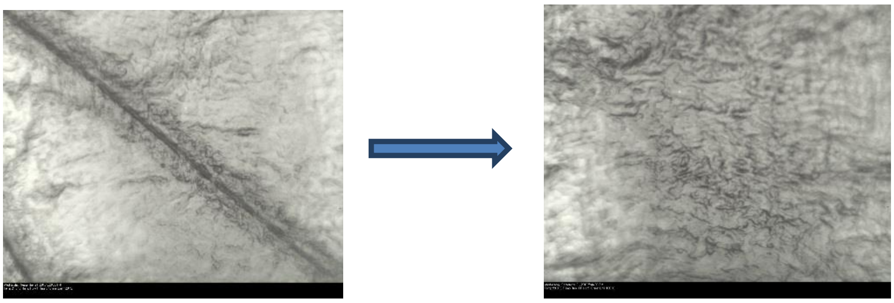
Abstract

A self-healing capability of injuries of biological system is truly remarkable phenomenon of nature. Challenge is to design smart elastomers which can mimic such behavior by not only sensing the defect, but also actively regain strength of damaged area. Self-healing elastomers are smart materials which can mend automatically or by assistance of external stimuli. Thermo-reversibility due to cooperative hydrogen bond dissociation / association is one of the viable approach among the various methodologies to achieve this phenomena. In the present work, we report for the first time that the cooperative hydrogen bonds were incorpoarted within chains of tire-grade polybutadiene rubber (BR) to produce modified BR. In this process, BR was grafted with anhydride compounds and then reacted with amine to create acid / amide-based cooperative hydrogen bonds by reactive mixing in melt mixing head of brabender plasticorder. Modified BR in gum state was found to be recyclable, moldable without any conventional vulcanizing agents. Once micro-cracks gets generated in the tire, it gets mended automatically in running a vehicle withut need for additional heat while using modified BR. Tire side wall formulations using modified BR showed superior performance with ease of processability, >30% improvement in dynamic properties without sacrificing mechanical properties compared to standard formulations. Modified BR may reduce tire-waste generation, improves tyre life cycle, safety and also find applications in non-tire sectors like conveyer belts, sealing joints, impact protection and many more.



Scheme 1: Thermo-reversibility of gum-modified BR observed under POM

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SPNA-29

Porous Complexes for the Structural Determination of Non-Crystalline Compounds

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Abstract

Metal-organic frameworks (MOFs) are a subclass of coordination polymers, containing metal cations centres linked by organic ligands. Traditionally, MOFs have been used for gas storage and separation, however, our group is focused on using MOFs for the structural determination of the non-crystalline materials. This is a new analytical technique known as 'crystalline sponge method' first reported by Fujita and co-workers in 2013.[1,2] In this regard, our group has studied a series of simple aromatic[3,4] guest molecules, such as benzene, and encapsulated them in the pores of $[\{(ZnI_2)_3(\text{tris(4-pyridyl)-1,3,5- triazine})_2\cdot x(\text{solvent})\}_n]$ MOF or 'crystalline sponge', shown in Figure 1. It was observed that π-π and CH-π interactions were responsible for the regular arrangement of the guests inside the pores enabling them to be subjected to X-ray analysis without having to be crystalline themselves.

We are expanding the technique and investigating the encapsulation of other species, such as isoprenes into the pores of the MOFs to realise the biomedical applications of the technique. Isoprenes such as Geraniol, Prenol and Farsenol have medicinal properties and function as metabolites in biosynthesis. The structural information of metabolites is key to understanding enigmatic cellular processes and for drug design. Since these are liquid compounds and their structural determination by the traditional X-ray analysis is not possible, the crystalline sponge method is expected to be useful under these circumstances. In this regard, we present the experimental method used to encapsulate these isoprenes followed by structural determination using XRD.

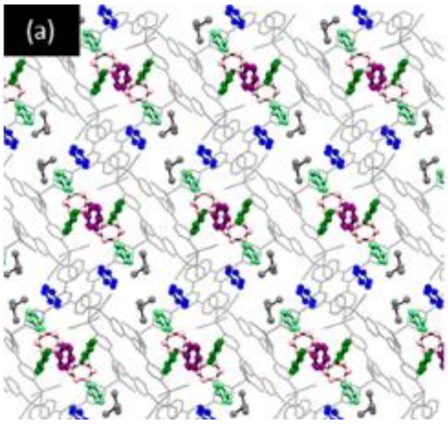

Figure 3. Unit Cell plots of the crystal structure encapsulated with benzene viewed down the b axis. The framework is shown as grey wire frame and benzene in colours.

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SPNA-30

Self-assembly of *i*-Indigo

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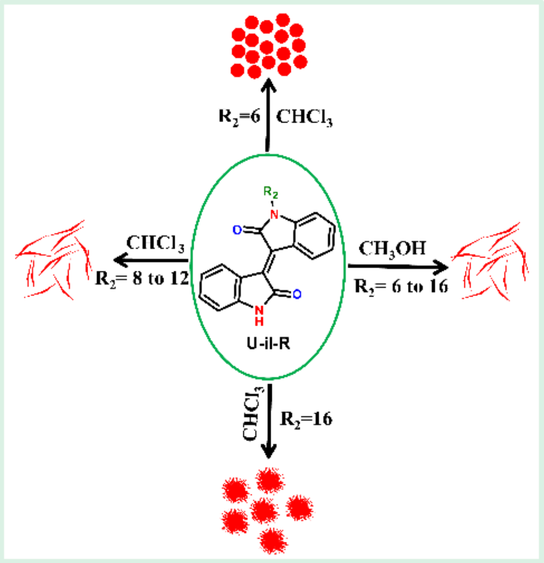
Abstract

Isoindigo (i-indigo) can be visualized as stilbene locked with lactam rings on either side of the vinyl moiety connecting the benzene rings. Thus, the molecule has been widely used as monomer to synthesize organic semiconductors. On the other hand, the conjugated backbone as well as the two –NH-CO-moieties in i-indigo are attractive for exploration in self-assembly. Lipophilic imbalance that is required to prepare self-assembly can easily be imparted to i-indigo. We have designed and synthesized a series of unsymmetrical i-indigo (U-iI-R) and studied their self-assembly properties. The U-iI-R has three interactions (i) π stacking, (ii) hydrogen bonding and (iii) interdigitation of alkyl chains. While all three interactions are in operation, the U-iI-R assembles into random structures. This is because the hydrogen bonding interaction between –NH-CO-moieties twists the conjugated backbone of the U-iI-R. By suppressing the hydrogen bonding, the twist was minimized and the U-iI-R self-assembled into long fibers. This inference lead to a question, is the hydrogen bonding essential for self-assembly of i-indigo? To answer this question, a series of symmetrical i-indigo was synthesized. They don't self-assemble into well-defined structures corroborating the need to have hydrogen bonding. We have identified and report interactions that are essential to self-assemble i-indigo, which has not been explored as a building block for self-assembled structures.



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SPNA-36

Organic Two Dimensional Sheets and Their Conversion to Curved Assemblies

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Abstract

Design and preparation of organic two dimensional (O2D) sheets and their conversion to curved nanostructures is in its infancy. To convert a flat structure to curved structure, the molecule must have multiple interaction possibilities and in-built twist. Conjugated small molecule iso-Indigo (*i*-Indigo) comprises two phenyl rings that is twisted (dihedral angle is 15°) at the junction. The *i*-Indigo has been connected with moieties that impart hydrogen bonding and ven Der Waals interactions. Due to the presence of π cloud in *i*-Indigo, π-π interaction is also present in the molecule. While all three interactions are in operation, rings and torroids are formed. Upon addition of hydrogen bonding competing solvents, the rings and torroids unravel to form O2D sheets. Control molecules that don't have hydrogen bonding moieties form random assemblies. Thus, curved assemblies such as rings and torroids and flat O2D sheets are formed in *i*-Indigo molecules, which comprise hydrogen bonding, van Der Waals interaction and π stacking. Please note that these assemblies are formed in single solvent by simple dissolution, unlike previous approaches that involve multiple steps and solvents.

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SPNA-38

Linear Organic Heterostructures via Multi-Component Supramolecular Co-polymerization

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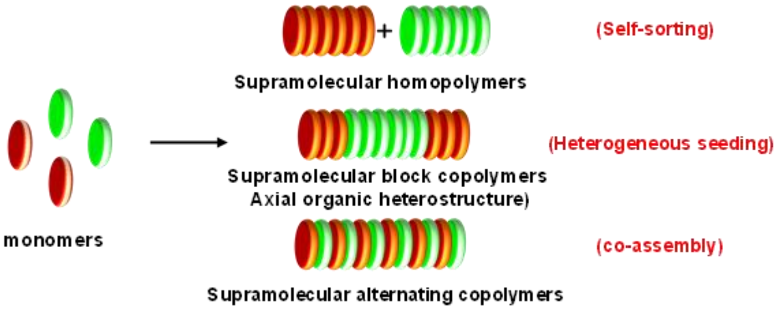
Abstract

Study of supramolecular polymers has entered an era that demands assemblies with more structural and dynamic control. With the emergence of better mechanistic understanding of supramolecular polymerization and recent breakthroughs in kinetically controlled supramolecular polymerization a firm control over dispersity and length of supramolecular polymerization has been realized. The next goal would be to use the increased mechanistic understanding and kinetically controlled growth to have a structural control over multicomponent supramolecular polymerization. Multi-component supramolecular co-polymerization with even two monomers can lead to various supramolecular structures based on structure and exchange dynamics of the monomers. The three possibilities could be either self-sorted homopolymers, alternating/random copolymer or a supramolecular block co-polymer. With the aid of various kinetic and thermodynamic pathways we have obtained a control over the sequences of two component supramolecular polymerization and this work addresses these aspects. These unique structures made from semiconducting monomers would be interesting materials to control exciton migration, axial p-n junctions and numerous exciting functional properties.



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SPNA-39

Supramolecular Graft Copolymer by Orthogonal Hydrogen and Halogen Bonding

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Abstract

Supramolecular polymers are non-covalent analogues of covalent polymers that are composed of repeating units connected together by non-covalent bonds. Due to their reversible nature, supramolecular polymers can adopt unique properties, such as adaptability, recyclability, and self-healing characteristics, which makes them interesting for various applications. Multi-component self-assembly, in which several distinct molecular motifs are associated together by specific non-covalent interactions offers a superior strategy for creating functional supramolecular polymers with higher degree of complexity and advanced properties. Such complex systems can be achieved by rationally employing multiple non-covalent interactions operating simultaneously and orthogonally i.e. without interfering with each other. Such strategies have been used with orthogonal hydrogen-bonding and pi-stacking, metal-ligand coordination and host-guest complexation etc. Halogen-bonding has recently emerged as a powerful tool for specific molecular interactions. It is known to be superior to extensively investigate hydrogen-bonding in terms of directionality. Orthogonal self-assembly of hydrogen- and halogen-bonding motifs is a unique and interesting combination for constructing functional supramolecular polymeric materials.

In the present work we demonstrate a novel design principle for creating stimuli-responsive supramolecular graft copolymers where the macromolecular backbone is constructed by hydrogen bonding discotic building blocks while orthogonal halogen bonding play a structural supporting role for grafting polymeric side chains to the backbone. Our preliminary results reveal that such orthogonal assembly not only contributes to the fabrication of the 2D architectures but also enhances the inherent stability of the copolymer in aqueous phase. Synthesis, self-assembly studies, stimuli-responsive behavior and future implications of this system will be the topic of this poster presentation.

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SPNA-40

Ag NPs Embedded Self-healable Inter Polyelectrolyte Complex based Injectable Hydrogel: It's Application in Wound Healing

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Abstract

This work demonstrates a precise preparation methodology of thermoresponsive and self-healable multi-layered micellar interpolyelectolyte complex (IPEC) hydrogel via interlocking of two oppositely charged block copolymers (BCPs). The polyelectrolyte BCPs were prepared via reversible addition fragmentation chain-transfer (RAFT) polymerization method. The inner block of the IPEC system consists of Ag NPs embedded thiolated poly(2-Hydroxyethyl methacrylate-b-2-(methacryloyloxy)ethyltrimethyl ammonium chloride) (PHEMA-*b*-PMTAC) (positively charged) whereas the outer segment of the IPEC consists of poly(N-Isopropylacrylamide-*b*-Sodium 4-vinylbenzenesulfonate) (PNIPAAm-*b*-PSS) (negatively charged) which provides the self-healing ability via ionic interaction. The morphology of the resulting IPEC particles was investigated by DLS, FESEM, AFM and HRTEM analyses. From the temperature variation DLS study it was found that the shell forming BCP (PNIPAAm-*b*-PSS) provides thermoresponsiveness to the IPEC system and showed a LCST value of 33°C. Upon application of this Ag NPs embedded IPEC in the wound site (*in-vitro* analysis) it immediately formed a physical gel at body temperature and facilitates the reepithelization process leading to wound healing. Along with this the gel showed a catastrophic effect over both Gram-positive and Gram-negative bacteria, confirmed through FESEM, live-dead assay (DAPI-PI assay) and flow cytometric analysis (FACS) . This type of IPEC hydrogel can be a promising material for wound dressing application.

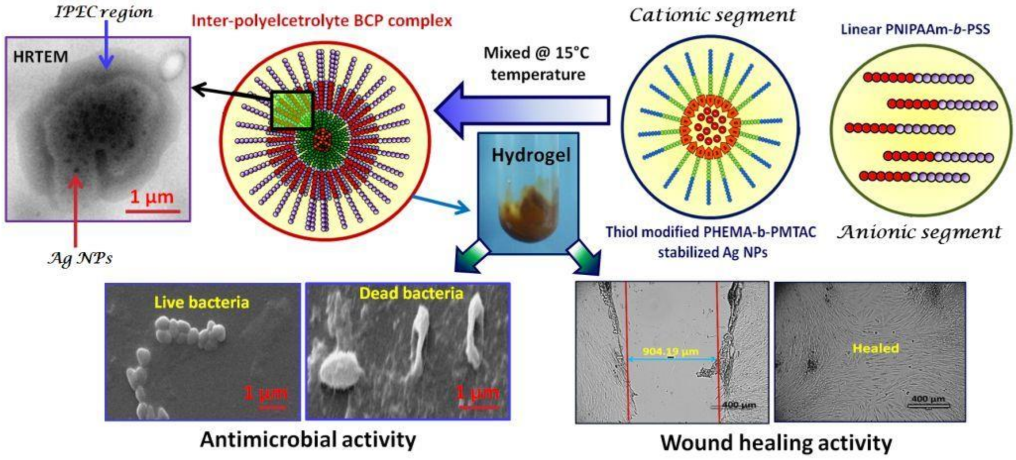

Figure: Schematic of the hydrogel synthesis route and their applications.

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SPNA-41

REDOX Responsive Fluorescent Active Glycopolymer Based Nanogel for Targeted Anticancer Drug Delivery

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Abstract

A well-defined glycopolymer based fluorescent active nanogel has been prepared via the combination of RAFT polymerization and Diels-Alder (DA) click chemistry. To prepare the nanogel, initially a functional block copolymer (BCP) poly(pentafluorophenyl acrylate)-*b*-poly(furfuryl methacrylate) (PPFPA-b-PFMA), having activated pentafluorophenyl ester group, has been synthesized via RAFT polymerization. The activated pentafluorophenyl functionality has been replaced by the amine functionality of glucosamine to introduce the amphiphilic BCP poly(Glyco)-*b*-poly(furfuryl methacrylate) (PGly-b-PFMA). Furthermore, the terminal acid (-COOH) functionality of the RAFT agent has been modified by gelatin QDs (GQDs) to generate fluorescent active glycopolymer. An anticancer drug Doxorubicin has been loaded in the micelle via successive addition of the drug molecule and crosslinking using dithio-bismaleimidoethane (DTME), a REDOX responsive crosslinker. The anticancer activity of the drug loaded micelle has been observed over MBA-MD-231, human breast cancer cell line, monitored via fluorescence spectroscopy and flow cytometric analyses (FACS). The cytotoxicity of the prepared glycopolymer based nanogel over the MBA-MD-231 cell line has been assessed via MTT assay test and it was observed that the synthesized nanogel was non-cytotoxic in nature.

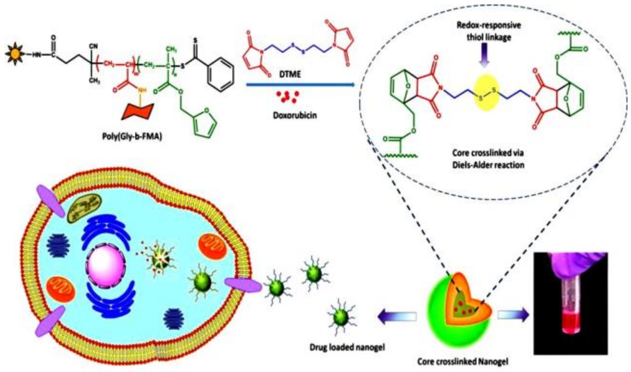

Figure: Schematic representation of the synthetic procedure of the nanogel and their working pathway of anticancer activity.

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SPNA-46

Synthesis of Magnetic - Cored Poly (Propylene Imine) Dendrimer

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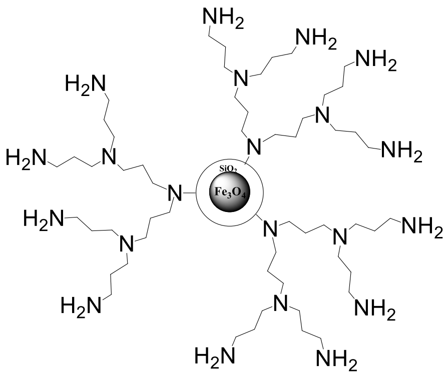
Abstract

In this work, we present the synthesis of poly (propylene imine) dendrimer with silica coated iron oxide nanoparticle core. It discusses the structural character of dendrimer via spectroscopy, microscopy, magnetometry, elemental analysis and conductometry methods. In actual practice, the well-versed cascade molecules are synthesized in homogeneous media with complicated purification procedures. Though it provides structural quality and purity, the method of synthesis is laborious, time consuming and costlier. Further, these kind of dendrimers are disposed after application to the desired task. To avoid these problems, we have synthesized and characterized iron oxide cored poly (propylene imine) dendrimer G_2 as semi-heterogeneous hybrid nanomaterials for catalysis.

The typical synthesis of magnetic-cored poly(propylene imine) dendrimer up to generation - 2 carries three sets of procedures as follows: i) Oleated superparamagnetic iron oxide (magnetite) nanoparticles are prepared by conventional co-precipitation method[1]; ii) silica shell is coated onto the magnetite via modified Stobber's methods[2] and iii) Poly (propylene imine) cascade structure has developed onto the silica coated magnetic core by sequential Michael addition of acrylonitrile followed by reduction of nitrile groups into amino groups[3]. The synthesized nanomaterials were characterized by using standard techniques and special attention has given to confirm the elemental nitrogen content by of the hybrid material by Lassigne's test (Prussian blue complex method) and conductometric titration method. Both methods provided the quantitative conformity for the stepwise formation (G_0, G_1 & G_2) of PPI dendrimer with slight defect in their structure.



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SPNA-47

Supramolecular hydrogel formation of sodium deoxycholate upon electrostatic interaction with a quaternary ammonium salt: its gelation mechanism

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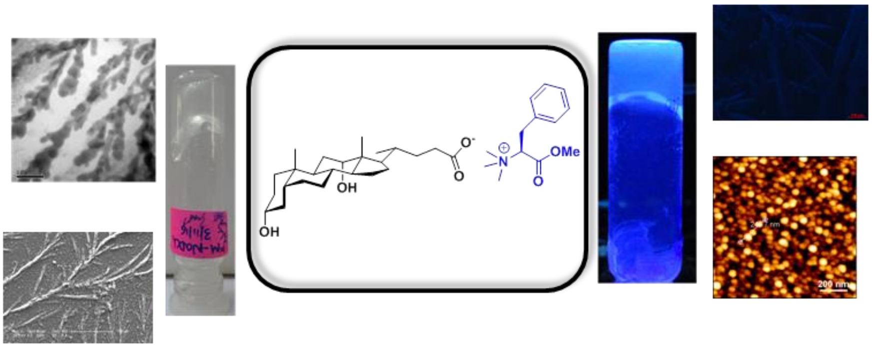
Abstract

Supramolecular gels derived from low molecular weight gelators (LMWGs) have gained much attention in recent times.[1] A class of gels belonging to this category are bile acid/salt based supramolecular gels. Bile salts, a class of well-known facially amphiphilic molecules, aggregate in a stepwise manner during the self-assembly process. Research on hydrogels of bile salts triggered by various types of metal ions (mono, di and trivalent) have been studied extensively.[2] However, reports on hydrogelation of bile salts induced by organic moieties are only a few.[3] We present the hydrogellation of sodium deoxycholate triggered by a positively charged quaternary ammonium salt. Negatively charged sodium deoxycholate interacts through electrostatic force with positively charged quaternary ammonium derivative of phenylalanine in aqueous medium to furnish a thermoreversible hydrogel. The hydrogel thus obtained showed dendritic and branched morphology. It is mechanically weak with thixotropic properties, and in addition, showed reversible thermoresponsive behavior. We have also successfully incorporated carbon quantum dots in the gel fibres and used it as a luminescent tool to visualize the self-assembled supramolecular fibre architecture. The details of the gelation mechanism, microscopic analysis and the nano-hybrid form of the gel will be discussed in the presentation.



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SPNA-48

APPLICATION OF LUMINESCENT LANTHANIDE HYDROGELS IN AMINE VAPOR SENSING

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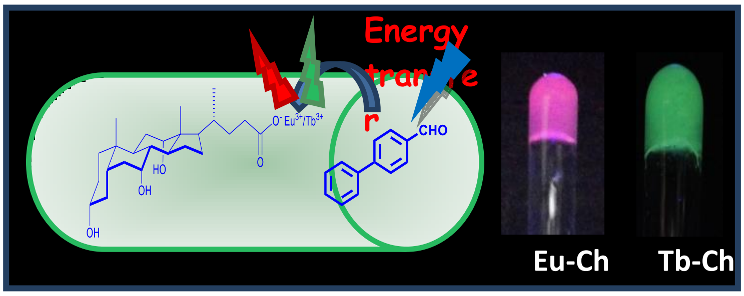
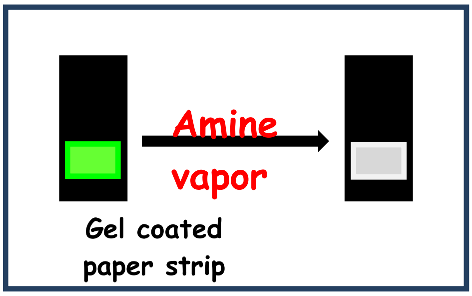
Abstract

"Luminescent" lanthanides have intrinsic low molar absorption coefficients, but this problem can be addressed by complexing the lanthanide ions with suitable chelating ligands which improve the luminescence properties drastically. A simpler way to sensitize lanthanides which avoids laborious synthetic steps was developed in our group. This involved the doping of 2,3-dihydroxynaphthalene (DHN) in terbium cholate, and pyrene in europium cholate hydrogel which resulted in significantly enhanced luminescence. Our recent studies revealed that several biphenyl derivatives could also sensitize Tb(III) in terbium cholate hydrogels. We have used such such as system for developing a luminescence *turn-off* response for detecting hazardous amine vapors. When terbium cholate gel doped with a biphenyl derivative was exposed to various amine vapors, luminescence quenching was observed. Interestingly, the quenching was selective to amine and nitro compounds only. Appreciable quenching was observed even at low ppm levels of the analyte. We have simplified this detection method by using a low-cost, user-friendly paper based approach for easy detection of the analytes.





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SPNA-49

Mesoporous MnO_2 Nanoflowers: facile Bile Salt-induced Synthesis and Preliminary Investigations of its Properties

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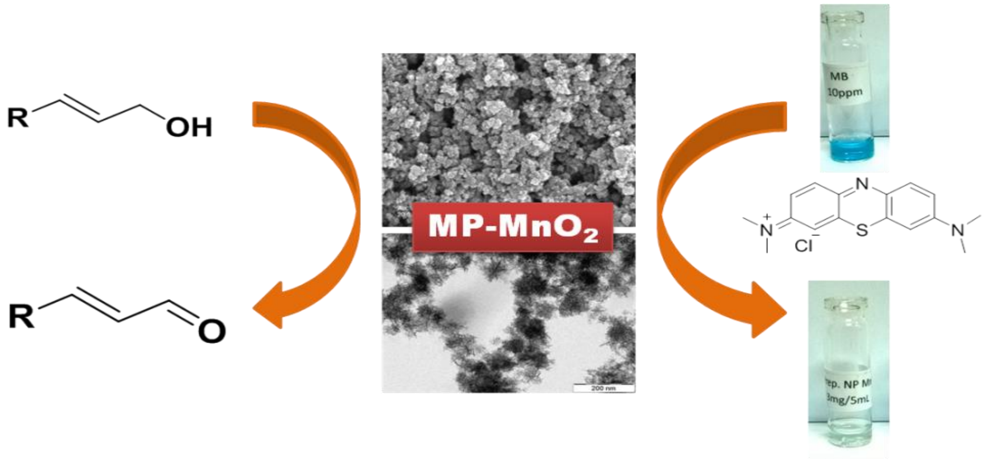
Abstract

MnO_2 is an important functional oxide with wide applications in organic synthesis such as the oxidation of benzylic and allylic alcohols. It is also used extensively as an electrode material for supercapacitors, and shows high adsorption capacity for cationic dyes. Herein, we demonstrate a simple, one-pot, bile-salt induced synthesis of mesoporous (MP) MnO_2 at neutral pH from potassium permanganate. X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscope (TEM), thermogravimetric analysis (TGA), elemental analysis, energy dispersive X-ray (EDX), and N_2 adsorption-desorption isotherms were done to characterize the synthesized MnO_2. This porous material was then used for the adsorption of methylene blue, an organic dye. Because of its exceptionally large surface area, this material was compared with commercial MnO_2 for standard oxidation reactions as well. Some of these studies will be presented in this poster.



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SPNA-50

Helical Self-Assembly of Amino-acid Based Polymerized Ionic Liquids

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Abstract

Naturally occuring chiral polymers like polysaccharides and proteins have been of great use owing to their chirality[1,2]. On the other hand, polymerized ionic liquids have opened a wide window of the possibility of a number of tailor made ionic polymers. Herein, we have synthesized amino acid based chiral PILs and studies their self-assebly along with photo-physical properties. Two different enantiomers of histidine, namely, D-histidinate (D-his) and L-histidinate (L-his) were employed as counter anions to the poyl(pyridinium) based cationic polymer backbone. Later, the self-assembly of these homopolymers were systematically studied. Dramatically, the self-assembly of these homo polymers resulted in generation of helical fibers of opposite handedness for D and L-his respectively. Aq. solution of these PILs were drop casted on glass slide with concentrations of 10^{-3} M to 10^{-6} M and relatively thick and thin fibers were obtained respectively. The obtained fibers were analyzed by polarized microscope, SEM and TEM respectively. In the case of polarization microscope, the birefringence could be clearly observed which can be attribute to the chiral nature of amino acids and helical assembly of fibers (**Figure 1**) which was further supported by circular dichroism measurements. Further, the photoluminescence of helical fibers of different thickness and aggregated states, was measured. Circularly Polarized Luminescence (CPL) was also measured for the isolated fibers.

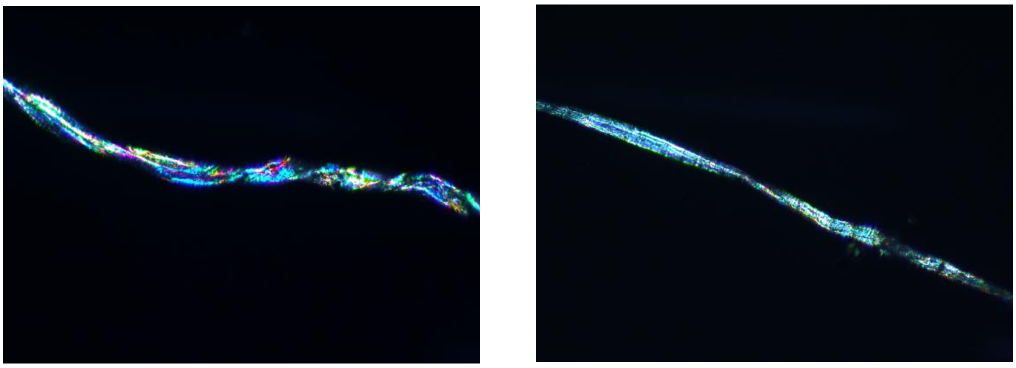

Figure 1: Polarized Optical micrograms of BuP4VP-L-His (left) and BuP4VP-D-his (right).

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SPNA-51

Polymer/Peptide Hydrogels for Biomedical Applications

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Abstract

Mankind has been trying to replace damaged or lost cells with new ones for centuries. Here, we propose the use of peptide hydrogels for cell therapy. Peptides are biocompatible, biodegradable and can produce suitable gelatinous environments for cell growth at extremely low concentrations (1% peptide)[1] . The tri-peptide Arginine-Glycine-Aspartic acid (RGD) is a well-studied cell binding motif for specific transmembrane proteins and is involved in cellular adhesion to the extracellular matrix[2] .There is continuous interest in the development of RGD-based therapeutics. Here, we use the phenylalanine (F) amino acid moiety to direct self-assembly[3]. These materials will supra-molecularly self-assemble to form nanoscale fibres, which entangle to form a 3-dimensional scaffold able to accommodate large volumes of water (known as a supramolecular hydrogel)[4-6]. Importantly, all components of the bio-hybrids are FDA approved. The synthesis and characterisation of RGD-based peptides and their gelation properties will be explored and discussed.The preparation, properties and applications of different bio and synthetic based polymer hydrogels will also be disscussed.

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SPNA-52

Understanding the Eletrospinnability of Polymer Supramolecular Complexes

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Abstract

Though, electrospinning is considered to be a straight forward technique to produce fibers from solutions of many polymers. There are still several challenges in the applicability of the technique, which are mainly related to the lack of electrospinnability of some of the polymer solutions. These include small molecules, rigid polymers, polyelectrolytes, some biomacromolecules and polymers with low molecular weight, which willingly do not entangle. In order to overcome the lack of electrospinnability of such polymer solutions using the strategy of supramolecular interactions is the main motivation of the current research work. Here, we are trying to understand the electrospinning of polymers complexed with the low molecular weight additives such as metal salts, surfactants and simple organic molecules through supramolecular interactions. The study is expected to have potential significance in designing functional polymer nanofibers involving an added functional additive.

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SPNA-53

Rational Design of Supramolecular Dynamic Protein Assemblies Using a Micelle-assisted Activity-based Protein Labeling Technology

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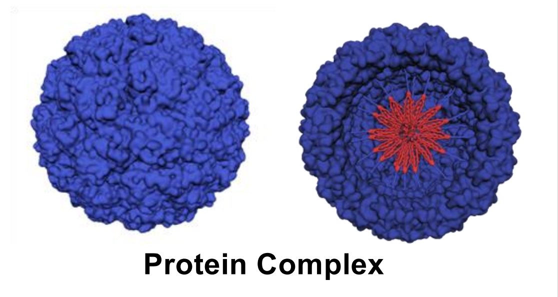
Abstract

Self-assembly of proteins into higher order super-structures is ubiquitous in biological systems. Genetic methods comprising both computational and rational design strategies are emerging as powerful methods for design of synthetic protein complexes with high accuracy and fidelity. Although useful, most of the reported protein complexes lack dynamic behavior that may limit their potential applications. On the contrary, protein engineering using chemical strategiesoffers excellent possibilities for the design of protein complexes with stimuli-responsive functions and adaptive behavior. However, designs based on chemical strategies are not accurate and therefore yield polydisperse samples that are difficult to characterize. Here, we describe simple design principles for the construction of protein complexes through supramolecular chemical strategy. Micelle-assisted activity-based protein labeling technology has been developed to synthesize library of facially amphiphilic synthetic proteins, which self-assemble to make protein complexes through hydrophobic interaction. The proposed methodology is amenable for the synthesis of protein complex libraries with molecular weights and dimensions comparable to naturally occurring protein cages. The designed protein complexes display very rich structural diversity, oligomeric states, sizes and surface charges that can be engineered through macromolecular design. The broad utility of this method is demonstrated by design of most sophisticated stimuli-responsive systems that can be programmed to assemble/disassemble in a reversible/irreversible fashion using pH or light as a trigger.[1]



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1 Sandanaraj, B., Reddy, M., Bhandari, P., Kumar, S. & Aswal, V. Rational Design of Supramolecular Dynamic Protein Assemblies Using a Micelle-Assisted Activity-based Protein Labeling Technology. *Chemistry–A European Journal* (2018).

SPNA-54

Self assembly of PMAA-triblock copolymers in solution

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Abstract

Macromolecular synthesis has changed quite a lot with the aid of techniques based on reversible deactivation radical polymerization (RDRP). This technique has made polymer syntheses very accurate in getting block copolymers with pre determined molecular weight with low PDI. These block copolymers show unique self assembly behavior in solvents and hence they can be tailor made according to application. Like other techniques, activators regenerated by electron transfer atom transfer radical polymerization (ARGET-ATRP) has also grown continually due to high catalyst efficiency compensated by added reducing agent (RA) that converts the deactivators into activators. Many RAs have been employed so far and alcohols have also made their place among them. Cyclodextrins being rich with hydroxyl functionalities have efficiently reduced Ag@Au and Au@Ag for the synthesis of core-shell nano-particles under aqueous medium and in our recent report we have showed how these hydroxyl functionalities could reduce Cu(II) to Cu(I) for synthesis of acrylate triblock copolymers via ARGET-ATRP in non-aqueous medium also. In the present work we utilized heterogeneous catalysis for synthesis of homo and block copolymers of acrylates using ARGET-ATRP which uses the □-cyclodextrin as RA. These block copolymers were then modified, their acrylates ends to convert to acids, using post-polymerization hydrolysis. The PMAA-PS-PMAA assembled in nano scale under the influence of the selective solvents confirmed using DLS and SEM. The resultant block copolymers were characterized by Gel Permeation Chromatography (GPC), H^1-NMR for the structural skeleton, Thermogravimetric analysis (TGA), Fourier Transform Infrared Spectroscopy (FT-IR), Differential Scanning Calorimeter (DSC). These results will be discussed in this presentation.

Figure 1. ^{1}H-NMR of PMAA-PS-PMAA

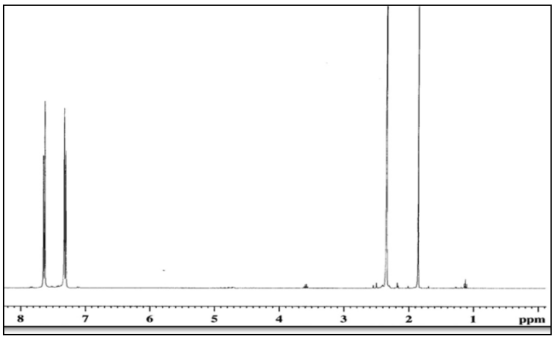
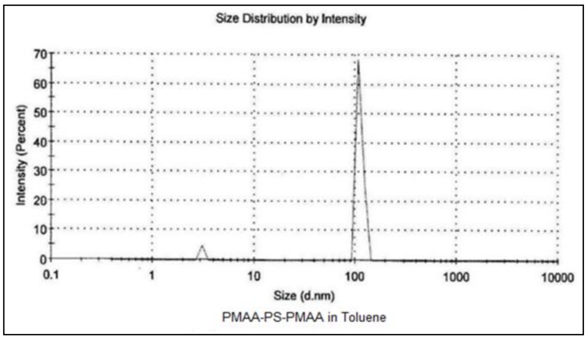


Figure 2.DLS of PMAA-PS-PMAA in toluene



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Theme –BIPDP

BIPDP-01

Imitating Articular Cartilage Using of Block-Copolymer-Brush of Acrylamide Derivatives

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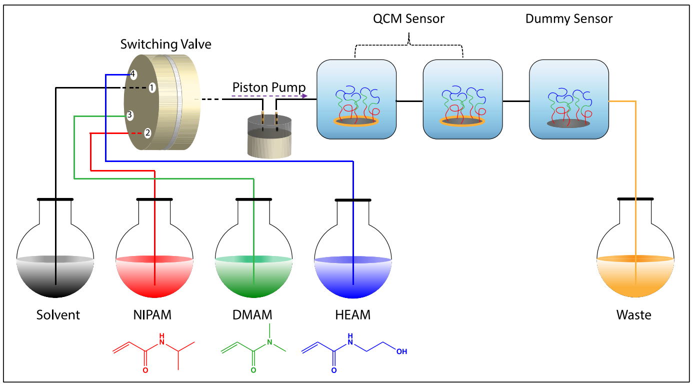
Abstract

Block copolymers are a fascinating class of materials because of their ability to form a variety of interesting nanoscale-ordered structures. This appeal of block copolymers is lost when either of the two ends is tethered to a surface because of the loss of a degree of freedom, but on the other hand, it provides a depth-dependent anisotropy, as is observed in the extracellular matrices of articular cartilage. Although interesting, growing water-soluble block copolymers from surfaces with precise block lengths has remained elusive because of the lack of control over the kinetics of surface-initiated atom transfer radical polymerization (SI-ATRP) when carried out in polar protic solvents.[1] Recently, we have demonstrated a very well controlled growth of poly (N-isopropylacrylamide), poly (N, N-dimethylacrylamide) and poly (*N*-hydroxyethyl acrylamide) brushes in ethanol/water mixture using SI-ATRP, where the brush-growth was monitored *in situ* using a quartz crystal microbalance with dissipation (QCM-D) and also by ellipsometry at different time intervals. Understanding the kinetics of SI-ATRP has helped in the design and synthesis of different types of surface-tethered block copolymer architectures under flow using a multi-position selection valve for a clean switching of monomers without affecting the flow rate. The growth of the block copolymers was monitored *in-situ* by QCM-D at each stage of the polymerization. Finally, a contact angle and XPS study of the dummy sensors (Si wafer cut into the shape and size of QCM sensors) taken out at each stage of polymerizations demonstrated the precision of the current flow-based synthesis of block copolymer brush architectures.



Reference

BIPDP-03

DEVELOPMENT AND CHARACTERISATION OF SILVER NANOPARTICLES CONTAINING BILAYER (KITCHEN WASTE-CORN STARCH/ CASEIN) FILM

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Abstract

Kitchen waste is defined as left-over organic material from restaurants, hotels, and households. Tons of kitchen waste gets wasted daily in highly populated areas. In the present world scenario, food security is the biggest challenge, so the proper utilization of food waste has become the necessity of the society. The present investigation was carried out to utilize kitchen wastes for the development of biodegradable antibacterial packaging material. Cooked rice and pulses were collected from a Boys' Hostel of Tezpur University campus and was sterilized, dried and converted to powder form for further development of a biodegradable film. The hydrolysis of starch during cooking was not sufficient alone to develop the film; hence combinations of kitchen waste- corn starch of different formulations were used for the development of a film. Film prepared with 70% corn starch and 30% kitchen waste was found to be effective to produce a film having good water barrier property, tensile strength and light barrier properties. To avoid any kind of contamination of packaged food through kitchen waste content of the film, silver nanoparticles were incorporated into the initial kitchen waste-corn starch single layer film. Casein was incorporated in the inner layer of that monolayer film to make it heat-sealable and improve its tensile strength; thus making it a bilayer film with casein (in contact of food) and kitchen waste-corn starch layer (in contact of the environment).

Keywords: Antimicrobial, Bilayer, Biodegradable film, Casein, Corn starch, Kitchen waste, Silver nanoparticles

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BIPDP-04

Synthesis of stimuli responsive and stretchable self-Healing Hydrogels of Chitosan formaldehyde in presence of CTAB Surfactants.

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Abstract

We report the synthesis of a hydrogel system by employing Chitosan (CS) and Formaldehyde (FD) as cross-linker. The modification of viscoelastic properties of the prepared hydrogel system was carried out by utilizing CTAB surfactant. These properties were studied under changing concentrations of CTAB and it was revealed that only at a particular CTAB concentration viscoelastic behavior of Chitosan-formaldehyde (CS-FD) hydrogels could be optimised.The hydrogels were characterized by Fourier Transform Spectroscopy (FTIR), Thermogravimetric (TGA), Scanning electron Microscopy (SEM). The structural properties were investigated by considering rheometric observations like viscosity measurements, oscillatory frequency sweep, oscillatory temperature sweep, and dynamic strain sweep , revealing that G' and G" values were found to be different than normal Chitosan-formaldehyde hydrogels dependent on the CTAB concentrations taken. The CS-FD+CTAB hydrogel were found to retain their elastic behavior at high frequency. The Hydrogels after exposing to some experimental concentrations of CTAB showed an abrupt change in the stretching behavior and the stretching properties could be seen 10-20 times than that of normal CS+FD hydrogel system and as such we have successfully achieved a hydrogel system with good stretching properties.

BIPDP-05

Bio-origin polybenzoxazines based on sustainable rigid diamines and phenols

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Abstract

Polybenzoxazines (PBz) are emerging class of polymers, obtained by initiator-free thermally mediated ring opening polymerization (ROP) of benzoxazine (Bz) monomers.(1) The properties exhibited by PBzs are more superior as compared to traditional commercial polymers epoxies, phenolics, bismaleimides.(2) The attractive thermo-physico-mechanical properties, near zero shrinkage upon polymerization, low water adsorption, high char yield and further molecular flexibility at structural level are additional attractive features.(3)Considering the sustainability perspective, replacement of raw materials with bio-based abundantly available feedstock is the need of hour.(4) For Bz monomer, the raw materials are phenol and amine which undergoes Mannich-like condensation reaction with formalin to form Bz monomer.(5) The natural origin of phenol is abundant while renewable amines are scarce in nature. In current work, alternative sustainable route of diamines based on polyols of carbohydrates origin is devised, synthesised and characterised. Fully biobased Bz monomers based on synthesised sugar diamines and renewable phenols such as cardanol, guaiacol, eugenol were synthesised. The monomers were structurally characterized using ^{1}H-, ^{13}C-, 1D NOE-, HSQC-NMR, and FTIR spectroscopy. The crystal structure was also determined by X-ray analysis. The temperature of ROP and thermal stability of PBzs was determined by DSC and TGA respectively. The adhesive property of resins was determined by lap-shear strength confirming their potential as solvent free green adhesives. Current work supports a further step towards substitution for petro-origin toxic chemicals like bisphenol-A (BPA) and diamines with environmental friendly sustainable materials.

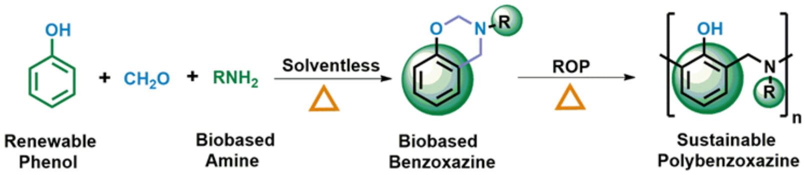

Figure: Generalized synthetic approach of sustainable Polybenzoxazine resin using renewable phenol and biobased amine.

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BIPDP-08

Stereocomplex Formation between Star-Shaped Enantiomeric Poly(lactide)s from the Amorphous Blends

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Abstract

Stereocomplex crystallites formed between enantiomeric poly(L-lactide) (PLLA) and poly(D-lactide) (PDLA) show a higher melting point by 50 °C than that of homocrystallites.[1] The peculiar interaction between L-lactide and D-lactide unit sequences favor the formation of stereocomplex crystallites between enantiomeric PLLA and PDLA and it could enhance the properties of PLA-based materials, such as thermal stability, thermal resistance, hydrolysis resistance, and mechanical performance.[2] In this work, we have attempted to understand the stereocomplex formation mechanism in the blends of star-shaped PLLA and PDLA using in situ wide-angle and small-angle X-ray scattering experiments, differential scanning calorimetry and FTIR spectroscopy. Star-shaped PLLA (SSPLLA) and star-shaped PDLA (SSPDLA)were prepared using dypiridamole as core molecules.[3] Our results revealed that the the crystallization of melt-quenched blend favored the stereocomplex formation irrespective of the crystallization temperature. It was also observed that the cooling rate from the melt significantly affects the sterecomplex formation in SSPLLA and SSPDLA blends.

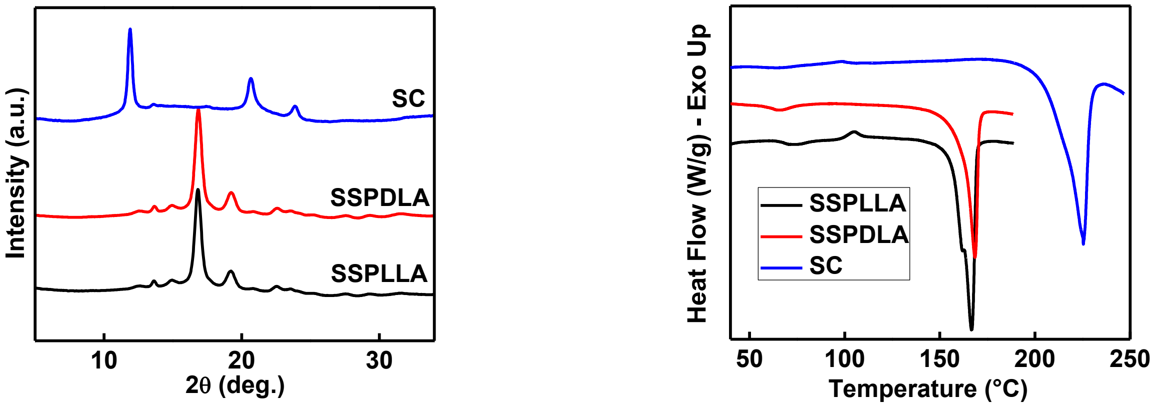

Figure 1.WAXS patterns and DSC thermograms of SSPLLA, SSPDLA and Stereocomplex (SC) of SSPLLA/SSPDLA.

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BIPDP-09

Blends of Chemically Modified Deproteinized Natural Rubber Latex and Pharmaceutical Polymers: Preparation, Characterization and Application

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Abstract

Novel membranes were prepared from physico-chemically modified deproteinized natural rubber latex (DNRL). Deproteinized NRL (DNRL) was initially prepared by incubating ammoniated NRL with urea and a polar organic solvent (acetone) in presence of a surfactant sodiumdodecylsulfate (SDS), followed by centrifugation. Chemical modification was done by grafting a hydrophilic polymer, poly(dimethylaminoethyl methacrylate) (PDMAEMA) onto the rubber particle surface using a redox initiator system cumene hydroperoxide / tetraethylenepentamine (CHP/TEPA). The chemically modified DNRL was then subsequently blended with two hydrophilic pharmaceutical polymers viz; hydroxypropylmethylcellulose (HPMC) and sodiumcarboxymethyl cellulose (SCMC). The compatibility between the components of the blend membranes has been confirmed by FTIR and TGA. Moisture uptake, swelling experiments and contact angle measurements indicated the enhancement in hydrophilicity after blending. Antibacterial properties of 15GDNRL have been found to be retained even after blending. The cell viability examination of DNRL and the blends using L-929 mouse fibroblast cells highlighted their biocompatibility after the appropriate physico-chemical modifications. The efficacy of membranes for drug release was analysed through permeation experiments using metformin hydrochloride (MET) as a model drug.

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BIPDP-10

Mechanistic Aspect of Fully Biobased Chitosan and Benzoxazine blends with Mutual Benefits of Low Curing Temperature and Improved Thermo-Mechanical Properties

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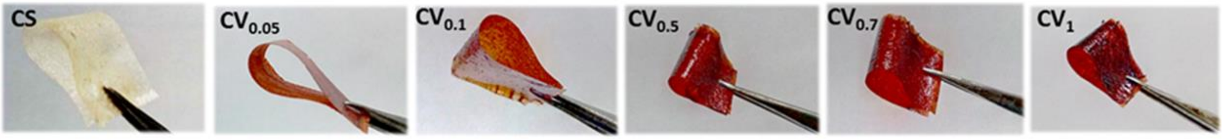
Abstract

Polybenzoxazines (PBzs) have come up as a superior class of thermoset polymers for variety of applications. However, their polymerization proceeds via ring opening reaction demanding high temperature which adversely affect their processability. On the other hand, biomacromolecule chitosan (Cs) is explored extensively, but their practical applications are limited due to poor thermo-mechanical properties. To circumvent these disadvantages, we developed a fully biobased reactive blend of vanillin benzoxazine (V-fa) monomer with Cs, which is effective in providing mutual benefits to the two along with benefits of sustainability. The resultant blends exhibited a higher potential in compatibility due to the development of physical and chemical crosslinks with effective lowering in ROP temperature of benzoxazine (by 109 °C) and an enhanced thermal stability of Cs. To understand this unusual lowering in ROP behaviour, we investigated structural interaction mechanism between solvated Cs and V-fa via *in situ* NMR studies. The benzoxazine molecules seep-within the inter-planar distance of Cs to provide characteristic interfaces as supported by powder X-ray diffraction (XRD) studies. The synergistic interactions were further supported by fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), scanning electron microscopy (SEM), thermogravimetry analysis (TGA) and tensile studies. This work represents preparation of Cs benzoxazine blends as a low-cost, efficient, and sustainable approach towards metal-free ROP reaction of Bz to afford both low curing temperature along with ease in processability. A new strategy is developed for the beneficial use of bio-sourced, Cs and PBz enhancing their scope in applications demanding thin and flexible films.



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BIPDP-11

Structural and thermal analysis of *Antheraea mylitta* silk fibroin/gelatin blend films

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Abstract

Blend films were prepared by mixing ionic liquid solution of *A. mylitta* silk fibroin (SF) and aqueous solution of gelatin in various blend ratios using solution casting method. Two different cross linkers namely glutaraldehyde and genipin were used and dextrose was added to enhance the film flexibility. The structural characteristics and thermal properties of blend films were examined through Fourier transform infrared spectroscopy (FTIR), thermo gravimetric analysis (TGA), differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). Swelling and water vapor transmission rate was also studied for optimized blend films. The FTIR spectra of methanol treated blend films showed β-sheet crystallinity. According to TGA data the blending of SF with gelatin, in presence of dextrose has enhanced the %water content of the films by ~36% and the degradation temperature of the cross-linked blend films has shifted as compared to pure gelatin and SF films. The DSC thermograms presented partial miscibility of the two components in blends. The data suggests that blending of SF with gelatin in presence of cross linkers and dextrose allows to tailor the physico-chemical properties of blends in order to obtain materials with extensive variety of possible applications.

BIPDP-13

Polyvinyl alcohol/carboxymethyl cellulose/ZSM-5 zeolite biocomposite membranes as efficient dye adsorbent with good recyclability

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Abstract

Biodegradable membranes were fabricated using polyvinyl alcohol (PVA)/carboxymethyl cellulose (CMC)/ZSM-5 zeolite systems. The membranes were characterised through FTIR, XRD, UTM, SEM, optical microscopy and thermogravimetry. The influence of various parameters viz., zeolite loading, initial dye concentration, temperature and contact time on the dye removal capability of the membranes was investigated. The results show that the adsorption capacity of the membranes increases with an increase in zeolite content and initial dye concentration, while an elevated temperature decreases the adsorption capacity. A high dye removal efficiency (97%) and high adsorption capacity (7.83) were observed for 5 wt% of zeolite loaded sample for an initial dye concentration of 10 ppm with a contact time of 10 h at 30 ^{o}C.The equilibrium adsorption data were analysed using Langmuir and Freundlich models. The regression results showed that the equilibrium adsorption data were more accurately described by the Freundlich model (R^2=0.998) rather than the Langmuir adsorption isotherm (R^2=0.961), suggesting heterogeneous adsorption. The adsorption kinetic results show that the pseudo-second order model (R^2= 0.996) is the suitable model to describe the kinetic behavior of MB onto PVA/CMC/ZSM-5 zeolite membranes.The present study suggests that the PVA/CMC/ZSM-5 zeolite membranes are suitable candidates for the efficient removal of methylene blue, from aqueous streams[1-3]

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BIPDP-14

Hydrophobically Modification of Psyllium seed husk for Advanced Applications

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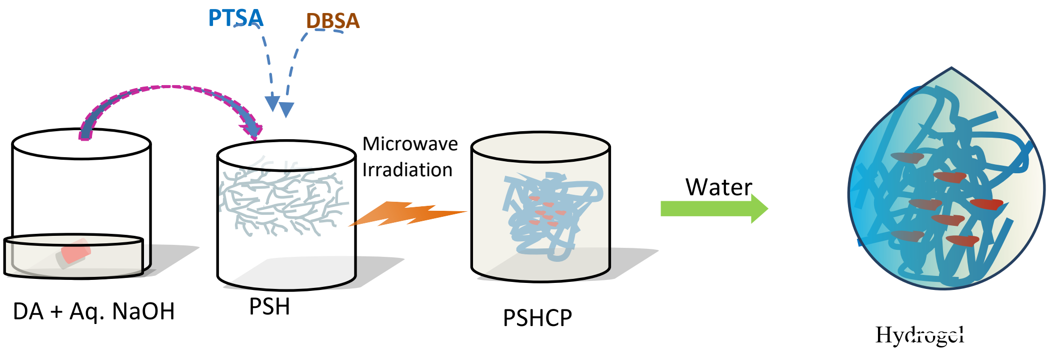
Abstract

The concern about environment has motivated to search renewable resources for diverse applications to replace the synthetic polymers, which are non-biodegradable. Natural polysaccharide-based hydrogels are suitable choice as they display unique properties, viz., biodegradability, biocompatibility, stimuli-responsive characteristics and biological functions. Psyllium seed husk (PSH) is a gel forming fraction of psyllium seed. PSH mainly contains arabinoxylan (AX), an anionic polysaccharide consisting of copolymer of arabinose and xylose. Glucose, galactose, mannose and uronic acid are also present in different concentration range. PSH is an abundant natural material, which is used extensively both in traditional herbal remedies and modern medicine. [1] Usually the formation of hydrogels involves the incorporation of chemical crosslinkers, which renders their biodegradability difficult. The present communication reports hydrophobic modification of (PSH) for formation of hydrogel. PSH was condensed with castor oil based dimer acid (DA) by microwave irradiation. The condensation product (PSHCP) was characterized by FTIR spectral analysis, X-ray diffraction measurements, SEM, particle size measurements. Swelling and de-swelling studies were performed in water and different solvents. Addition of PSHCP flocculated the copper salts from their aqueous solutions quickly. PSHCP was used to form hydogel by freeze thaw technique. The hydrogel showed 1000% swelling in water in a slow and steady manner. It can be a useful candidate for slow drug/ nutrient release formulations. The hydrogel disperses in acidic medium, stable in water and alkaline pH. It has shown antibacterial and antifungal properties against *Staphylococccus aureus, E.coli* and *Candida albicans* respectively. The hydrogel exhibited self adhesive nature and shape memory properties. It can be very useful for wound dressing applications. PSHCP undergoes biodegradation in moist garden soil in 40 days.



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BIPDP-15

Functionalization of Chitin for Pb(II) Ion Remediation

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Abstract

One of the serious consequences of the progress of is heavy metal ion pollution. Conventional processes for water treatment become inadequate and obsolete with the identification of progressively increasing contaminants in the water. Therefore, to overcome the challenges associated with traditional water treatment technologies green alternatives are being saught earnestly.Dithiocarbamates are very effective chelating agents towards a variety of heavy metal ions, however, their residual amount after water treatment may pose deleterious effect. Hence, we immobilized dithiocarbamate groups on chitin. Chitin is the second most abundant natural polymer after cellulose. It is a nitrogenous polysaccharide (polymer of an N-acetylglucosamine). Dithiocarbamylated chitin (CHDTC) was prepared by treating chitin with aqueous solution of sodium hydroxide and carbon disulphide. This was characterized by FTIR spectral analysis, X-ray diffraction measurements and scanning electron microscopy (SEM). CHDTC was used for extraction of Pb(II) ions from aqueous lead acetate solution by batch process at 18^{o}C, 28^{o}C and 38^{o}C. CHDTC was found to be a very good adsorbent for removal of Pb(II). Pb(II) ion concentration was measured by Atomic absorption spectrophotometer. Adsorption process was very fast and 84-93% removal of Pb(II) ions was observed in 1h. Results were somewhat inconsistent at lower temperature but the adsorption isotherm fitted well with the Langmuir model at 38^{o}C.The mechanism of adsorption by physical and chemical forces both, since the adsorbate was gradually released back, if the adsorbent was not removed from the solution. Chemisorption was evinced by the FTIR Spectral analysis. Metal ion could be recovered by extraction with dilute acetic acid. No turbidity was observed in the supernatant solution and nor any leachates released.

Table 1. Adsorption of Pb (II) by CHDTC

Initial concentration (mg/L)	**% Adsorption of Pb (II)**		
	Temperature (K)		
	291K	**301K**	**311K**
10	**84.7**	**84. 1**	**82.4**
20	**93.8**	**91.7**	**91.7**
30	**94.8**	**93.5**	**93.9**
40	**96.8**	**95.2**	**93.8**
50	**94.1**	**95.1**	**93.9**
60	**94.5**	**91.1**	**92.8**
70	**93.3**	**93.4**	**93.1**

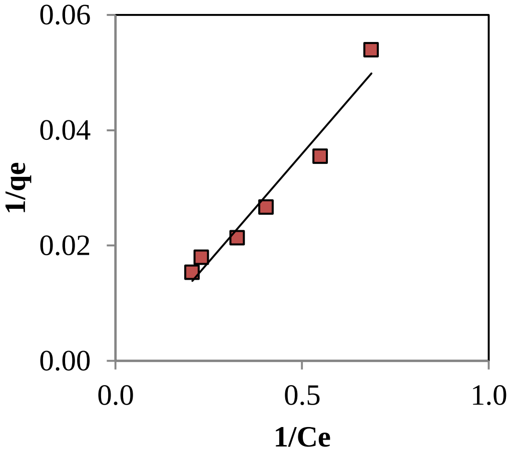

Figure 4.Langmur model of adsorption isotherm applied to the adsorption of Pb (II) ions on to CHDTC at 38 ºC

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BIPDP-16

GREEN AND METAL FREE CNF/PI COMPOSITE FOR THE DEGRADATION OF ORGANIC POLLUTANTS FROM WATER

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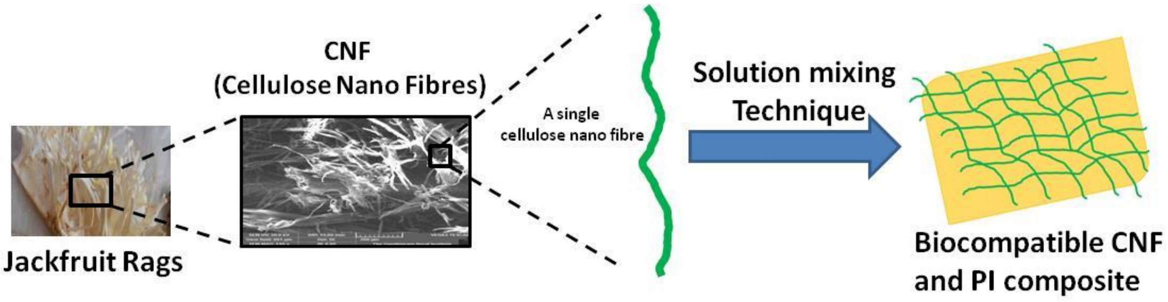
Abstract

A composite was prepared from biopolymer cellulose impregnated polyimide (PI) to be used as photocatalyst. Cellulose nano fibrils (CNF) are obtained from naturally occurring source. Owing to its mechanical, optical, chemical and rheological properties, CNF gained significance. Herein, rags of jackfruit were used as starting material for preparing nanocellulose via acid hydrolysis and ultrasonication technique [1]. Biocompatible CNF and PI were blended by following solution mixing techniques [2,3]. The CNF/PI composite was characterized using FTIR, SEM, EDAX and XRD. Further the swelling property of the composite was also analyzed. The efficiency of the composite was investigated for the degradation of Chlorpyrifos and Quinalphos pesticides.



A schematic representation for preparation of biocompatible composite

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BIPDP-18

Poly(hydroxyurethane)s from renewable diamines and dicyclocarbonate

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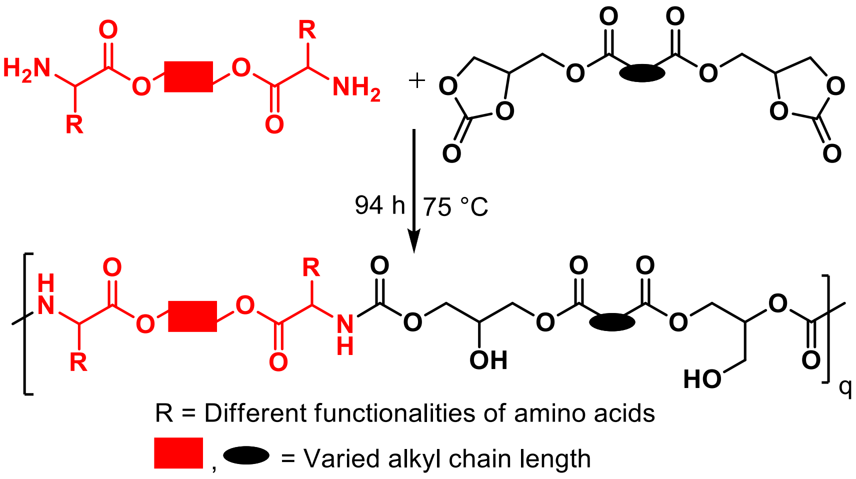
Abstract

Synthesis of polyurethanes (PUs) which are part of everydays' human life requires diisocyanates as one of the starting materials. Diisocyanate has very bad impact on the environment due to its toxic nature. Therefore, there is a growing demand for environment-friendly processes and products of this category. Several chemical processes has been developed in a view to avoid the issues related to isocyanate toxicity to prepare non-isocyanate based polyurethanes. One of the chemical processes is polyaddtion reaction between cyclic carbonates and diamines to prepare poly(hydroxyurethane)s (PHUs). PHUs contain additional hydroxyl groups adjacent to the urethane linkage which may enhance the chemical and hydrolytic stability of these materials compared to conventional PUs. In this work, we report the synthesis of PHUs by the reaction between renewable sebacic acid based bis cyclic carbonates and amino acid based diamines and structures are confirmed from the spectroscopic analysis. The prepared PHUs are thermally stable upto 200 °C. The molecular weights of these PHUs by SEC analysis are in the range of 6500-8500 Da.



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BIPDP-20

Synthesis characterization and application of edible polymer from agricultural waste (pineapple waste, sea weed)

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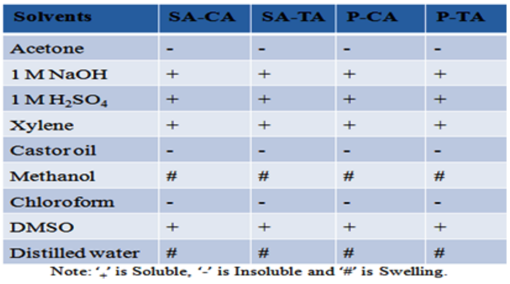
Abstract

Environmental concerns and sustainability of resources have triggered the need for alternative solutions. Consequently, a renewed interest has been carried out to develop and apply edible films and coatings made from a variety of agricultural and/ or food industries wastes. These films have the potential to replace conventional packaging in some applications. In the present study, cross-linked polymers are obtained by pectin/ sodium alginate cross-linked with bio-based acids such as citric acid and tartaric acid respectively. Pectin used here is extracted from waste pineapple shell. The use of alginates as films in food applications has increased in the recent years due to their swelling capacity and overall functionality. Overall, alginate-based films are a good candidate to obtain tailor-made edible films for food applications. Glycerol was added as plasticizer and films were evaluated using different techniques, and structure was confirmed by FTIR and ^{1}H NMR. Thermal properties were measured by thermogram, surface morphology through SEM micrograph. Edible films and coating are used in many food industries. So it is necessary to study their biological properties like cytocompatibility, antimicrobial activity etc. in order to these we have studied some biological properties such as *in-vivo* study on mice, cytocompatibility, antimicrobial and they showed a good results. Intended for future applications, we have studied seed germination and biodegradation of crosslinked films and they showed satisfactory results.

Figure: Edible film from a) pectin, b) alginate.

Table: Chemical resistivity test of edible films.



Solvents	SA-CA	SA-TA	P-CA	P-TA
Acetone	-	-	-	-
1 M NaOH	+	+	+	+
1 M H_2SO_4	+	+	+	+
Xylene	+	+	+	+
Castor oil	-	-	-	-
Methanol	#	#	#	#
Chloroform	-	-	-	-
DMSO	+	+	+	+
Distilled water	#	#	#	#

Note: '+' is Soluble, '-' is Insoluble and '#' is Swelling.

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BIPDP-24

Synthesis and evaluation of different Biopolymers-Acrylamide Hydrogel Networks

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Abstract

Hydrogels are hydrophilic organic crosslinked polymers that form three-dimensional structures and show the ability to swell and hold large amounts of water while maintaining their chemical structure and integrity.

Polyacrylamide based hydrogels have been extensively studied for a different purposes such as ophthalmic operations, drug treatment and purification. Also, biomass derived polymers such as gelatin, chitosan and sericin are known for their excellent biocompatibility, biodegradability and availability. This study attempts to link these two and quantitatively study them.

In this study, semi-interpenetrating networks of polyacrylamide and various biopolymers were prepared by free radical polymerisation, then physically dried and crushed, and finally subjected to experimentation. They were investigated for swelling kinetics in distilled water at room temperature. This was followed by quantifying their release kinetics at constant temperature of 38℃. These two sets of data were used for comparative analysis of hydrogels.

After this, the chemical structure of polyacrylamide-sericin hydrogel was characterized through FTIR. The performance of this hydrogel was investigated by varying different parameters such as surface to volume ratio, pH, nature and concentration of the medium. All these parameters can potentially aid in optimizing the behavior of hydrogels.

Quantitative analysis of the swelling mechanism in hydrogel was attempted, understanding the underlying reasons for the non-fickian behavior of diffusion in the present polymer system. Finally, a potential application of this hydrogel in agriculture for controlled irrigation systems was studied by studying release kinetics in locally procured soil medium. Swelling kinetics in natural fertilizer was also performed for possible use as fertilizer systems.

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BIPDP-25

Synthesis and Evaluation of Different Biopolymer-Acrylamide Hydrogels

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Abstract

Hydrogels are hydrophilic organic crosslinked polymers that form three-dimensional structures and show the ability to swell and hold large amounts of water while maintaining their chemical structure and integrity.

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BIPDP-26

pH-Responsive Autofluorescent Amphiphilic Brush Copolymer for Efficient Delivery of Nonfluorescent Chemotherapeutic Agents

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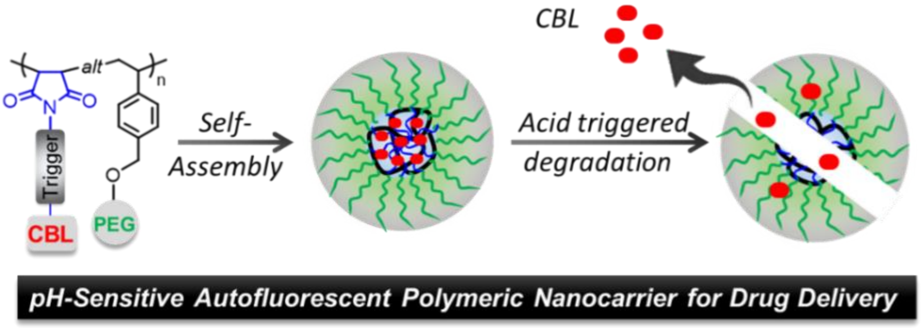
Abstract

Nowadays, delivery of clinically approved nonfluorescent drugs is facing lot of challenges because it is difficult to monitor the intracellular drug delivery without having any integrated fluorescent moiety into the drug delivery vehicle. Nonfluorescent drug such as, chlorambucil (CBL), an aromatic nitrogen mustard has been emerged as a suitable candidate for cancer therapy owing to their ability to alkylate deoxyribonucleic acid (DNA) *via* the construction of aziridinium ring as an intermediate. Herein, we have strategically developed an autofluorescent acid-disintegrable polymeric nanocarrier based on poly(maleimide-*alt*-styrene) skeleton by virtue of the sequence-specific copolymerization of two rationally designed monomers, PEG bearing styrene and CBL conjugated *N*-substituted maleimide *via* reversible addition-fragmentation chain transfer (RAFT) polymerization. The as-synthesized amphiphilic brush copolymers could self-assemble into 100-150 nm diameter nanoparticles depending on the copolymer compositions in water. *In vitro* release studies revealed that about 70% drug was retained under physiological conditions at pH 7.4. Notably, at endolysosomal pH 5.0, 90% of the CBL was released by the pH-induced cleavage of the aliphatic ester linkages connecting CBL to the maleimide unit. Cytotoxic analysis implies the superior cell killing property of the nanocarrier towards cervical cancer (HeLa) cell lines compared to the normal cell lines. The copolymers can exhibit photoluminescence under UV light irradiation although it doesn't contain any conventional fluorophore unit into it. This facet assists us to track the CBL conjugated autofluorescent nanocarriers intracellularly through fluorescence microscope imaging technique. Ultimately, 4-(4-nitrobenzyl)pyridine (NBP) colorimetric assay was executed to evaluate the ability of CBL-based polymeric nanocarriers towards DNA alkylation.



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BIPDP-27

Color Tunable Materials Prepared from Monodispersed Core-Shell Microspheres

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Abstract

Structural colors due to ordered photonic crystals are widely used as an effective platform for manipulating the propagation of light. Currently, there exists a strong demand for color shifting photonic crystals that can be tuned by external stimuli. These responsive photonic crystals (RPCs) have important applications in areas such as color displays, sensing of biological and chemical substances. In this study, we synthesized monodispersed core-shell microspheres having polystyrene as core and polyacrylate derivatives as shell by adopting surfactant free emulsion polymerization. Further, these microspheres were self-assembled to obtain well-ordered colloidal photonic crystals. The diameter of core-shell microspheres was engineered to obtain photonic crystals having brilliant structural colors and thus as-prepared color tunable materials were demonstrated as a sensing platform for the detection of volatile organic compounds.

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BIPDP-28

Orthogonal Self-assembly of Triazine based p97 Inhibitor and 5-Fluoro Uracil Induce Cancer Cell Death through ER Stress & Nucleus Damage.

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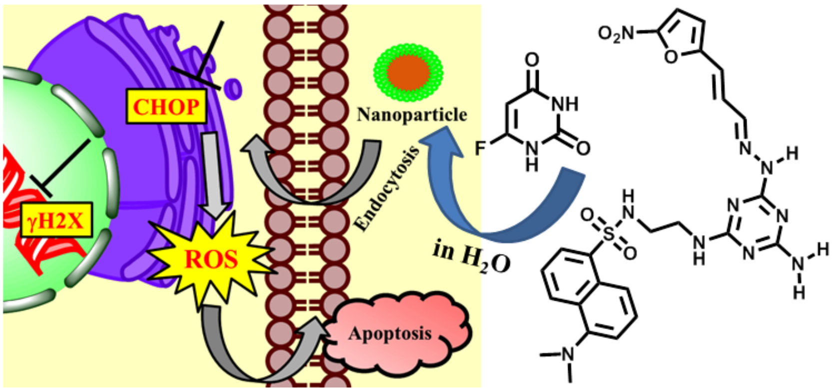
Abstract

The Endoplasmic Reticulum (ER) plays a critical role in processing of secreted and transmembrane protein. Selective delivery of small molecule into specific organelle is a challenging task. To deliver small molecule into ER, we synthesized triazine based ER specific small molecule which can induce ER stress through p97 inhibition. This modified triazine molecule target selectively ER and designed such a way that it can form spherical self-assembled nanoparticles with nucleus damaging drug 5-fluoro uracil. These unique self-assembled nanoparticles accumulate selectively in ER and by passing other organelle such as lysosome and Mitochondria. Interestingly these Triazine-5FUnps are inducing apoptosis through ER stress and nucleus damage which are confirmed by over expression of CHOP/GADD153 and □H2X respectively. Moreover, nanoparticles are able to generate ROS this leads to the severe stress inside the cells; subsequently cells undergo programmed cell death. This orthogonal self-assembled nanodrug can be used for future treatment in cancer therapy.



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BIPDP-30

Ring Opening Polymerization of L-Lactide using Biocompatible Salen complexes

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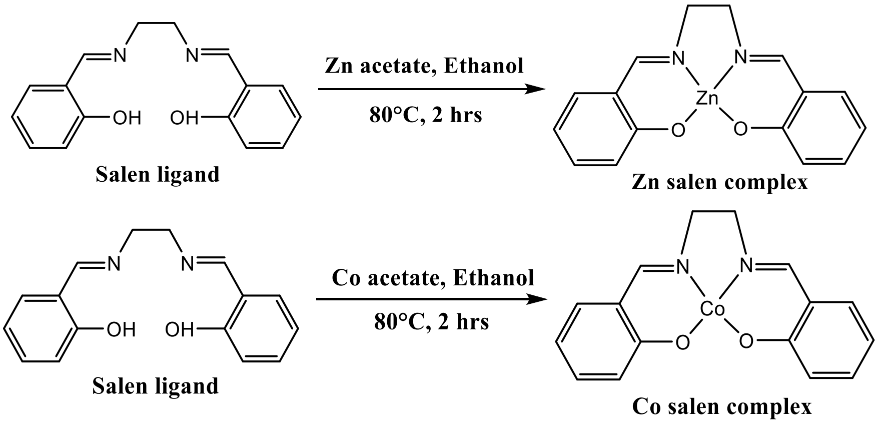
Abstract

Polylactide (PLLA) is one of the biodegradable, biocompatible polymers for the use in the biomedical applications. The commercially available PLLA is homochiral in nature because L-lactic acid with high optical purity can only be obtained by the fermentation process of carbohydrate. PLLA is mostly synthesized by the ring-opening polymerization (ROP) of L-lactide using various catalysts and initiators. Most recently, there is a scientific challenge for developing new catalysts that will be biocompatible and nontoxic to use in the biomedical applications. Schiff bases are of interest, because of their antibacterial, antifungal, anticancer activity. In the present research, Schiff base metal complexes were synthesized using salen ligand and metal acetates (Zn(II)acetate and Co(II) acetate). The synthesized complexes were characterized by FTIR, NMR, UV-Vis, Mass spectra and Thermogravimetric Analyzer. These salen complexes were used as a catalyst in the bulk solvent-free ring-opening polymerization (ROP) of L-lactide and high molecular weight(>100,000 Da) with narrow molecular weight distribution were obtained. The PLLA was characterized using Nuclear Magnetic Resonance spectroscopy, Fourier Transform Infrared Spectroscopy, Gel Permeation Chromatography, Thermogravimetric analyzer, Differential Scanning Calorimeter, X-ray powder diffraction, and Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF). The antibacterial activities of salen complexes against the bacteria *Staphylococcus aureus*, *Escherichia coli* were studied and showed promising results.



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BIPDP-31

Polyesters for Sustainable Packaging

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Abstract

The polymers used for packaging applications are more than one third of globally produced plastics each year. The big chunk of this are single use plastics which mostly ends up in landfills and oceans creating serious environmental pollution. To overcome this issue polyesters are the promising materials with ester linkages that have potential to hydrolysis in certain ambient conditions. However, choice of raw materials and polymer microstructure is the determining factor to make a polyester eventually biodegradable. For example, aliphatic polyesters and their combination with aromatic moieties in a random fashion are suitable for this purpose along with high amorphous content and functional moieties. The present work deals with a random and block copolyesters based on natural and fossil resources. The composites of synthesized polyesters are prepared with inorganic fillers. The polymer has been characterized and have potential application in packaging sector.

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BIPDP-32

Characterisation of Chitosan Molecular weight distribution by Multi-Detection Field-Flow Fractionation and SEC-MALS

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Abstract

Molecular weight determination of chitosan is commonly conducted using intrinsic viscosity measurements, light scattering and/or size exclusion chromatography (GPC/SEC)[1]. All of these techniques require complete dissolution of the polymer to avoid inaccurate estimation of molecular weight (MW) due to the presence of intermolecular aggregates[2]. Recent studies have reported the use of asymmetric flow field flow fractionation (AF4) to characterise the MW distribution of chitosan[3-5]. However, the full experimental conditions used have been vaguely reported, making the methods difficult to reproduce. We present here a method for determination of the MW of chitosans by AF4 coupled with MALS and DRI detectors. The method allows the separation of the dissolved polymer from the aggregate fraction, making possible the accurate determination of molecular weight distribution. We also evaluated the effect of different experimental conditions on the results obtained and compared them with results from SEC-MALS-DRI under identical solvent conditions. We analysed a set of chitosan samples from different sources (crustaceans, squid and fungi) and of varying degree of acetylation (DA ~1 to ~50%). AF4-MALS-DRI results revealed that although aggregates are significantly minimised when using a good solvent, some still remain, and are only eliminated by filtration through small pore sizes (~0.2 µm). This represents a limitation for chitosan, as filtration can lead to high amount of the material being retained in the filter. The method described here has the advantage of allowing us to identify and separate the aggregates and to accurately determine the MW distribution for a wide range of chitosan types.

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BIPDP-33

Self-assembly and Thermoresponsive Behaviours of Polypeptide-Polyoxazoline Graft/Block Copolymers

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Abstract

Polypeptides are bio-inspired materials with good self-assembling capability. However, their hydrophobicity restricts their use in biomedical applications such as drug/gene delivery, tissue engineering. Pseudopeptidic poly(2-oxazoline)s are also bio-inspired, water-soluble polymers with potential for biomedical applications. Thus, the combination of polypeptide and poly(2-oxazoline) may lead to amphiphilic polymers with high propensity to self-assemble into various nanostructures, which can be used for various potential applications. This report describes a convenient approach to functionalize hydrophobic polypeptide with a hydrophilic polymer to make the final molecule water soluble. Here, 'grafting onto' technique is utilized to prepare water-soluble amphiphilic polypeptide-*graft*-poly(2-isopropyl-2-oxazoline) (PCys-*g*-P*i*pOx) copolymer. The process involves the synthesis of propargyl functionalized polycysteine (PCys-S-Pr) via ring-opening polymerization of the corresponding *N*-carboxyanhydride (NCA) and azide functionalized poly(2-isopropyl-2-oxazoline) (P*i*pOx-N_3) via cationic ring-opening polymerisation. The Cu(I)-catalysed alkyne-azide "click" reaction of the PCys-S-Pr and P*i*pOx-N_3 of different molecular weights, finally produces PCys-*g*-P*i*pOx copolymers. The attachment of P*i*pOx-N_3 block introduces thermoresponsiveness into the copolymer exhibiting LCST-type transition in water. The cloud point of copolymer thus can be tuned by varying chain lengths of the pendent poly(2-isopropyl-2-oxazoline) moiety and copolymer concentration. This amphiphilic copolymers self-aggregates into various nanostructures in aqueous/nonaqueous media. An attempt is also been made to synthesize block copolymers (PCys-*b*-P*i*pOx) from corresponding functionalized polycysteine and poly(2-isopropyl-2-oxazoline). This followed by the study of their self-aggregation behaviour in DMF/DMSO solvents as they are not soluble in water.

BIPDP-34

Amphiphilic Glycopolypeptide-based Cross-linked Nanostructures for Dual Stimuli-Responsive Drug Delivery

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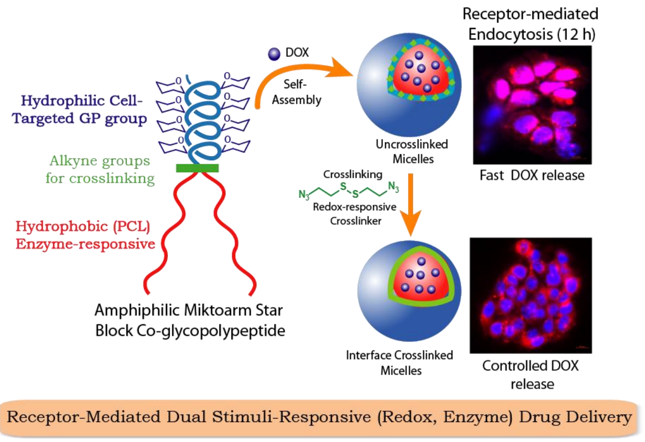
Abstract

Glycopolypeptides as a mimic of natural glycoprotein's involved in regulation of cellular processes through polyvalent interaction with cell surface carbohydrate-binding receptor.[1]As several carbohydrate based nanocarriers (micelles, vesicles, etc.) are being currently explored for the biological applications. Out of which, micelles have been extensively used because they can increase drug solubility, reduce early degradation.[2] Only drawback of micelles is their dynamic dissociation upon dilution in the circulation system *in vivo* which cause the premature drug release and low drug targetability at the affected area.[3] One effective approach to solve this problem is to stabilize micelles by cross-linking.[4] Thus, Herein, we designed a glycopolypeptide based dual stimuli-responsive (redox and enzyme) crosslinked micellar system which exhibits both specific cell-targeting ability and controlled drug release property. An amphiphilic miktoarm star copolymer $[(\text{PCL}_{50})_2\text{-}b\text{-Pr-gly}_6\text{-}b\text{-GP}_{40}]$ which comprises two hydrophobic poly(ε-caprolactone) blocks, a short poly(propargylglycine) middle block and the hydrophilic glycopolypeptide block were designed and synthesized. The block copolymer initially self-assembled into uncrosslinked (UCL) micelles. Further, free alkyne groups of the middle block (core-shell interface) of the UCL micelles was crosslinked by using bis-(azidoethyl) disulfide as redox-responsive crosslinker *via* click chemistry to form interface crosslinked (ICL) micelles. Hydrophobic Poly(ε-caprolactone) was chosen as the degradable enzyme-responsive block. The synergistic effect of dual stimuli (redox and enzyme) on release behavior of DOX as a model drug was studied by applying dual stimuli sequentially or reversely. Biological studies of micelles have been done to check their ability to target specific cancer cells and release the drugs in a time-dependent manner.



Receptor-Mediated Dual Stimuli-Responsive (Redox, Enzyme) Drug Delivery

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BIPDP-35

Modification of a commercial polyurethane imparts anti-biofilm activity to combat catheter associated infections

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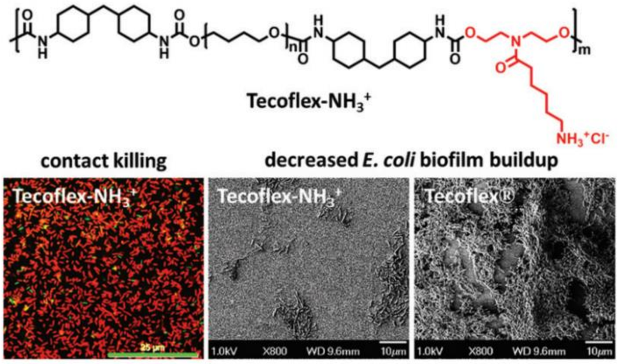
Abstract

Infections associated with urinary and intravascular catheters are one of the most common nosocomial acquired infections, primarily caused by build-up of bacterial biofilms on the catheter surface[1]. Biofilms are extracellular polysaccharide enclosed microbial communities, generally characterized by increased resistance to antibiotics and host responses.[2] We aim to modify commercially available thermoplastic polyurethanes like Tecoflex®, used extensively in manufacturing of medical devices and catheters, utilizing our library of pendant cationic functional groups to impart antimicrobial characteristics and reduce the accumulation of biofilm on the material surface. The pendant cationic functional groups were incorporated into the polyurethane in a manner similar to the synthesis of Tecoflex® by copolymerizing the amine functionalized N-substituted diol to give a compositional variant of the commercial polyurethane. As a proof of concept, we studied the antimicrobial properties of the modified Tecoflex® against a Gram-negative bacterium *Escherichia coli*, a common cause of urinary tract infections associated with catheters. As confirmed by microscopic studies and bactericidal assays, the cationic polyurethanes exhibited contact killing mechanism and significantly slowed down the accumulation of biofilm compared to Tecoflex®, even after 5 days of incubation, while having minimal toxicity towards mammalian cells, evidenced by negligible cytotoxicity and hemolysis[3]. These cationic variants of commercial polyurethanes, as catheter materials, have potential to combat nosocomial infections.

References



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BIPDP-36

NANO COMPOSITES OF BIO POLYMERIC CHITOSAN AS A PEROXIDASE NANOZYMES

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Abstract

Artificial enzymes or nanozymes are the nanomaterial's, possess the natural enzyme like activity and coherently overcomes the major drawbacks of natural enzymes i.e. thermal stability, storage, yield and production cost. Fullerene C60, Graphene oxide (GO), Selenium doped GO, carbon quantum dots were reported good peroxidase activity.

Chitosan is a biopolymer synthesized from chitin. It is long chain polysaccharide composed of random distribution of deacylated D-glucosamine and N-acetylated of D-glucosamine. It has diverse applications in the development of edible nanomaterials and bio-adhesives.

In present work, we are proposing transition metal nanoparticle(TMnps) functionalized chitosan as nanozyme with peroxidase activity. Au, Fe, Cu, Ti and Ag transition metal naoparticles were synthesized using green approach. Nanoparticles were characterized by surface Plasmon resonance, IR spectroscopy, powder X-ray Diffraction and TEM analysis. All these characterized TMnps were loaded on biocompatible supports chitosan using sonocation method and tested for peroxidase activity. All the TMnps composite materials formed were tested for anticancer activity using HeLa cell lines. From these TMnps, Ag chitosan nano composite showed enhanced peroxidase activity compared with other nano composites.

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BIPDP-38

Biocompatible, dual responsive biopolymeric hydrogel as potential carrier for colon targeted drug delivery

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Abstract

Herein, we report the development of a stimuli responsive hydrogel (cl-Gly/pNIPAm) based on glycogen, *N*-isopropylacrylamide (NIPAm) and ethylene glycol dimethacrylate (EGDMA) using free radical polymerization.[1] The hydrogel demonstrates excellent pH and thermo responsive behavior. The LCST of the developed hydrogel has been found to be ~32.5–34 °C. The hydrogel demonstrates good compatibility towards human mesenchymal stem cells (hMSCs). The hydrogel has been observed to be biodegradable towards hen egg lysozyme. The hydrogel is capable to load colonic drugs 5-amino salicylic acid (5-ASA) and ornidazole efficiently and released in sustained manner. Moreover, the release pattern of both the colonic drugs from the gel surface has been observed to be almost similar for a prolonged period of 2 months, which has been confirmed from stability study.

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BIPDP-39

Self Cleanable and Self healable Superhydrophobic Print of Water Soluble Agent

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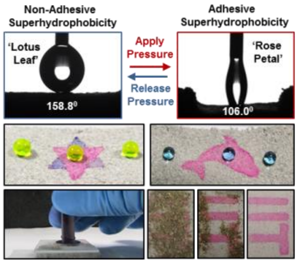
Abstract

Lotus leaf[1] is a well known example of bio-inspired non-adhesive superhydrophobicity because of its ability to repel water extremely (advancing contact angle ≥150°) with a very low roll-off angle (≤10). The low-energy surface coated hierarchical and rough topography plays a important role in achieving superhydrophobicity. Any kind of physical damage to the hierarchical features may result in loss of anti-wettability. Therefore, self-healing ability is essential for the utility of this property in practical circumstances. However, the attempts to develop such material are rare in the literature. Very few materials have been recently introduced that are capable of recovering their micro/nano features, but only after application of appropriate external stimuli.[2] In this work, we have reported a superhydrophobic material which is highly durable and can completely able to restore the lost non-adhesive property without application of any external stimuli.[3] This synthesized material exhibited simple, unique and reversible switching property between two bio-inspired special wettabilities—that are a) non-adhesive (lotus leaf) and b) adhesive (rose petal) superhydrophobicity. It was further strategically exploited in developing rewritable aqueous patterns on the extremely water-repellent polymeric coating. This synthesized material was capable of impregnating hydrophilic agents, directly from aqueous phase without sacrificing the embedded antifouling property of the polymeric coating, and which is of potential interest in many fundamental and applied contexts, including synthesis of smart drug delivery systems, catalysis, self-assembly of colloids, cell culture chip, robust open microfluidic system, reusable chemical sensing etc.



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BIPDP-40

Ultrasound Enhanced Radical Graft Polymerization of Butyl Acrylate onto Ethyl Cellulose

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Abstract

The graft polymerization reactions of butyl acrylate onto ethyl cellulose were performed with and without ultrasound irradiation. The ultrasound probe of frequency 20 kHz was used to perform the reactions to enhance graft polymerization process. Two different initiators, potassium persulfate and ammonium persulfate, were used as radical initiators in the present work and their efficiencies were compared. The effects of reaction time, temperature, initiator and amount of monomer in feed on graft ratio, graft efficiency and monomer conversion were studied. The graft polymers were also characterized by other sophisticated techniques such as FT-IR, TGA, and SEM. The results obtained revealed that the ultra-sonication has effectively enhanced and influenced the composition of graft polymer. Compared to the conventional graft polymerization i.e. without ultrasound, the graft ratio, graft efficiency and monomer conversion increased significantly in ultrasound assisted reactions. The two initiators used in present work showed different behavior with reference to graft ratio, graft efficiency and monomer conversion under the same reaction conditions.

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BIPDP-42

Green polymeric adhesives from castor oil- synthesis and properties

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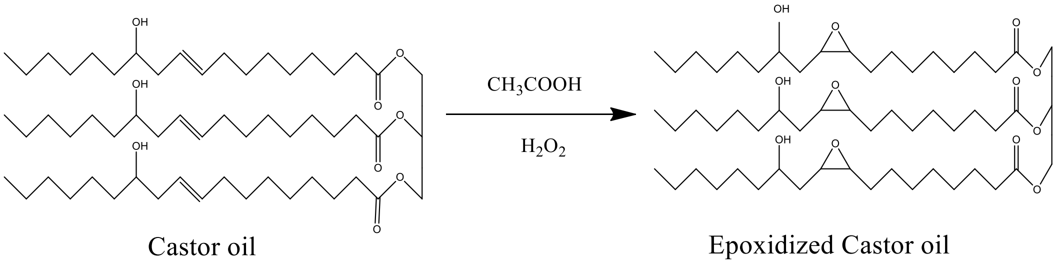
Abstract

In view of the alarming rate at which the petroleum is getting depleted, there is an increased drive for developing resources based on renewable resources that are easily convertble to useful industrial raw materials.[1] In this perspective, we have explored the possibility of deriving value added precursors for deriving polymeric adhesives from castor oil.[2] The rich chemistry of the castor oil (CO) makes it a good starting material for a wide range of application.[3] In this work we are reporting the conversion of the double bond C=C present in raw castor oil to oxirane groups by epoxidation of CO by insitu generated performic acid.[4] This is characterized through NMR and IR spectroscopic analysis. The epoxidised castor oil is cured using Maleated castor oil and Jeffamine . The cured systems are evaluated for mechanical, adhesive and thermal characteristics. The so formed polymer shows good PEEL adhesion properties. The mechanical strength of the developed adhesive polymer is also good.. The epoxidation of castor oil is done through the reaction as shown below.



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BIPDP-44

Biotin-Tagged and GSH-Responsive Polysaccharide Nanovesicle for Drug Delivery

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Abstract

Development of polysaccharide based drug delivery systems are emerging as important class of vectors in recent past. These polysaccharides are biocompatible in nature and presence of multiple functional groups makes them ideal candidates for anticancer drug delivery application. In the present work, biotin-conjugated multi-stimuli-responsive polysaccharide vesicular nanocarriers are designed and developed, for the first time, to accomplish receptor-mediated endocytosis in cancer cells and to deliver anticancer drugs at the intracellular compartments. For this purpose, a new renewable hydrophobic unit was custom designed with redox-degradable disulphide and enzyme-biodegradable aliphatic ester chemical linkages and it was conjugated along with biotin on the dextran backbone. The dextran derivative self-assembled into nanovesicles of < 200 nm in size which were characterized by dynamic and static light scattering, electron and atomic force microscopes.Redox-degradation by glutathione (GSH) showed 60 % drug release whereas lysosomal esterase enzyme enabled > 98 % drug release in 12 h. Confocal microscope and flow cytometry assisted time-dependent cellular uptake studies revealed that the biotin-receptor over expressed cervical cancer cells (HeLa) exhibited larger drug accumulation through receptor-assisted endocytosis process. This process enabled the delivery of higher amount of DOX and significantly enhanced the killing in cancer cells (HeLa) compared to wild-type mouse embryonic fibroblast cells (WT-MEF, normal cells)[1]. Further the attempt was also made to modify the polysaccharide backbone with vesicular director hydrophobic tail along with several acid finctional group via redox responsive disulfide linkages. This design was also decorated with biotin ligand to achive the site specific delivery of the drugs at tumor tissues. These redox responsive acid functionalised dextran derovatives were used for cisplatin conjugation and their subsequent targted delivery in human breast cancer MCF 7 cells. This report presents synthetic strategy for polysacchride backbone modification using different stimuli which are susceptible to cleave at tumor micrenvironment.

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BIPDP-46

Fabrication of new benign nanobiocomposite based scaffolds for Bone Tissue Engineering by *in situ* mineralization of Hydroxyapatite on Graphene oxide loaded Curcumin

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Abstract

With the growing bone defects arising from trauma and bone diseases, orthopedic surgoens have faced severe challenges in identifying alternate bone substitutes. The biomaterial to be employed as bone substitute should be osteoinductive, biocompatible, biodegradable and non-immunogenic. In this context, Graphene oxide (GO) has attracted much attention in bone regenerative medicine owing to its osteoinductive behaviour and biomimic with natural ECM [1]. In view of such remarkable properties of GO, in this study, we have attempted fabrication of new, benign nanobiocomposite based scaffolds for bone tissue regeneration using GO, hydroxyapatitie (HAP) and Curcumin. The synthesis involved two steps: initially the hydroxyapatite was mineralised on graphene oxide sheets through in situ co-precipitation method. The oxygen enriched groups present in GO provides effective nucleation site for hydroxyapatite crystal growth & synthesis and produced HAP mineralised GO nanobiocomposite (GO-HAP). The nanobiocomposite was thoroughly characterised by FT-IR, XRD, HR-SEM, and EDAX analyses. The XRD results prove the nano crystalline size and decreased crystallinity of hydroxyapatite in GO-HAP compared to pure hydroxyapatite. In the second step, curcumin was loaded on nanobiocomposite to further enhance its osteogenic potential. The enriched hydrophobic polyphenol in curcumin provides a positive effect on bone health [2]. The quantum of curcumin loaded on GO-HAP and pure HAP was equal to 93 and 22% respectively.The anti-oxidant activity of curcumin loaded scaffolds was studies by DPPH assay and observed stronger anti-oxidant activity for GO-HAP loaded curcumin (26.74%) than pure HAP loaded curcumin (3.55%). Hence, GO-HAP loaded curcumin can be a potential scaffold for bone tissue regeneration.

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BIPDP-48

Biodegradation and morphological study of PLA based biocomposites under composting conditions

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Abstract

The use of conventional plastic products leads to problems associated with landfills and littering during improper waste disposal. On the other hand, biodegradable plastics have significant potential to replace the conventional plastics. These plastics mainly include poly(lactic acid [PLA], polycaprolactone [PCL], polyhydroxybuterate [PHB], etc[1-3].This study demonstrates the biodegradation behavior of melt extruded PLA based biocomposites films under composting condition by monitoring online CO_2 evolution using gas chromatography. The aerobic biodegradation under controlled composting conditions is monitored according to ASTM standard. Aerobic composting tests were conducted under laboratory conditions at 58 ± 2 °C and 60% RH. PLA/Chitosan samples evolved 70% of CO_2 during first 100 days, followed by NPLA, PLA/CNC-SO_4 (~1%) and PLA/Gum Arabic 5% in ascending the number of days. Further, PLA/Chitosan 5% biodegraded ~97% in 113 days, which is followed by NPLA> PLA/CNC-(SO4) (~1%) > PLA/Gum Arabic 5% taking 136, 138 and 146 days, respectively. Some of the samples were observed for morphological changes under Field Emission Scanning Electron Microscope (FESEM). Results showed that due to biodegradation samples got disintegrated under composting condition, which confirms molecular chain scission of the biopolymers, which facilitates microbial assimilation. From GPC analysis, reduction in number average molecular weight confirms biodegradation. Molecular weight kinetics data also confirms biodegradation due to chain scission of the biopolymers. Colony formation in the test samples incubated at 55 ºC for 72 h further confirms that degradation in molecular weight was due to microbial presence and chemical hydrolysis.

Keywords: Biodegradation, poly(lactic acid)(PLA), biocomposites, assimilation, colony formation

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BIPDP-49

An environment friendly route to synthesize vegetable oil based nonisocyanate polyurethanes

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Abstract

Polyurethanes, a substantial class of multi-specialty polymers, is most widely used polymer globally. Polyurethanes(PUs) are mainly synthesized by the polyaddition between a polyol and a polyisocyanate, obtained from petroleum resources. However, keeping in view to the dramatic health issues caused by the prolonged exposure to isocyanate in concomitance with the environmental regulations limiting the use of isocyanates, greener and safer routes to produce a new class of materials named NIPUs (non-isocyanate PUs) has acquired overwhelming recognition over the last decade because of their abundance and environment-friendly nature. Non-isocyanate polyurethanes (NIPUs) is a novel class of polyurethane formed by the reaction of carbonates and amines eliminating the use of toxic isocyanates. NIPU has captivated booming attention because of its enhancement in porosity, water uptake, and chemical resistance in comparison to conventional polyurethanes. In this study, sustainable Bio-based Non-Isocyanate Polyurethanes were synthesized by polyaddition of a naturally-occurring amine with Carbonated Soybean oil(CSBO). Carbonated Soybean Oil was obtained by a mixture reaction of CO_2 with epoxidized soybean oil and characterized by FTIR, ^{1}H NMR, and ^{13}C NMR spectroscopy. NIPUs based on non-isocyanate route showed improved properties such as higher water uptake, thermal stability, and chemical resistance. Fourier transform infrared spectroscopy (FTIR) analysis confirmed the typical linkages of polyurethane and Swelling test justified the enhanced resistance to organic solvents. Furthermore, the synthesized NIPUs is also moisture insensitive in the neighboring environment. These properties enable NIPUs with diverse probable applications in the field of chemical-resistant coating and sealant.

***Keywords**: non-isocyanate; water uptake; moisture insensitive; sustainable.*

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BIPDP-50

Effect of Coconut oil on Contact Angle of Biodegradable PLA Films

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Abstract

Controlling wettability by varying surface chemistry and roughness or by applying external stimuli is of interest for a wide range of applications including self-cleaning, water harvesting, smart packaging etc. The surface wettabilities of Poly (lactic acid) (PLA) and Coconut oil (CO) blend at different concentration were studied with three different food simulants (distilled water, Ethanol and Acetic acid). The static contact angle of these simulants were measured at different temperature conditions viz., 15°C, 25°C and 40 °C, on the surface of PLA coconut oil blend films. The wetting behaviour of the PLA films shows significant changes with increasing coconut oil concentration. Additionally the wetting behaviour is controlled by varying the temperature of the surrounding atmosphere. As the temperature of the surrounding decreases the contact angle tends to increase this may be due to the solidification of coconut oil present in the films which make the surface more smoother and on the contrary increasing the temperature have reduced the contact angle. The collaborative effect of coconut oil and temperature shows interesting results. This temperature depedent wetting behaviour can have a significant effect on the water permiability of the films and has potential to be used as a smart packaging material delivering preservatives to the food in contact.

KEY WORDS: PLA, Coconut Oil, Wettability, Temperature controlled

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BIPDP-51

Modification of bacterial cellulose surface by "click" polymerization

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Abstract

Bacterial cellulose (BC) is an organic compound which formed by different bacteria. It has attracted significant attention in recent years because of their applications in biomedicines, and electronics. Particularly, surface modifications of BC are important for improving their bio-compatibility and other properties. In most of the cases, BC-modified materials have been prepared by simple blending and doping technique which causes an incompatibility between BC and polymeric materials. In this context, chemical modification/functionalization of bacterial cellulose offers the dimensional stability to the bacterial cellulose. We have chosen click chemistry approach to functionalize the BC surfaces that has been proven effective and versatile tool for preparing new class of functional materials for different applications.

In this presentation, we will discuss about our recent results on polymerization on surface of BC with different aryl monomers by using "click" reaction conditions. The synthetic methodology for the preparation of precursor organic molecules and functionalization of BC will be described. The characterization of the BC materials using solid state NMR, AT-IR, SEM, and AFM techniques will also be discussed. Finally, the wettability behavior of the modified-BC surface will also be discussed.

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BIPDP-52

Hypocholesterolemic effect of dietary chitosan biopolymer extracted from carapace of freshwater edible crab *Sartoriana spinigera* on albino rats

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Abstract

Presently,hypercholesterolemia is a serious health issue caused due to obesity and increased body weight.In order to cure these problems, the society demands for medicines that are of natural origin.Chitosan is one such natural origin zootherapeutic biopolymer which is found in the exoskeleton of arthropods and crustaceans.*Sartoriana spinigera* is a freshwater crab of Jharkhand ,India which has great ethnobiological significance.The purpose of this study was to investigate hypolipidemic effect of chitosan extracted from carapace of freshwater crab *Sartoriana spinigera* on body weight ,blood cholesterol and triglyceride level in hypercholesterolemia induced albino rats. Chitosan was extracted and characterized by FTIR . DD% was found to be 78.53%. Experiment was conducted on 20 albino rats divided into 4 groups with different experimental diets. Group A(control)-basal diet, Group B-high fat diet, Group C-high fat diet +5% chitosan, Group D-high fat diet+5% hypolipidemic drug 'Ezetimibe'. Initial and final body weight gain, blood cholesterol and triglyceride were noted on 1st and 30th day respectively. Findings:After 30 day experiment,statistical analysis by Student's t test showed that in group C ,body weight significantly decreased at 1% level than group B advocating that chitosan has hypolipidemic effect and inhibits obesity. Statistical analysis also showed that blood cholesterol and triglyceride were significantly decreased in group C fed with chitosan than group B at 0.1% level. These findings advocate that chitosan from carapace of freshwater edible crab *Sartoriana spinigera* has hypocholesterolemic effect as chitosan is cationic in nature and binds to anionic fatty acids and remove them out of the body.

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BIPDP-53

Lignin & Lignin oligomers based Polyurethane synthesis and characterization

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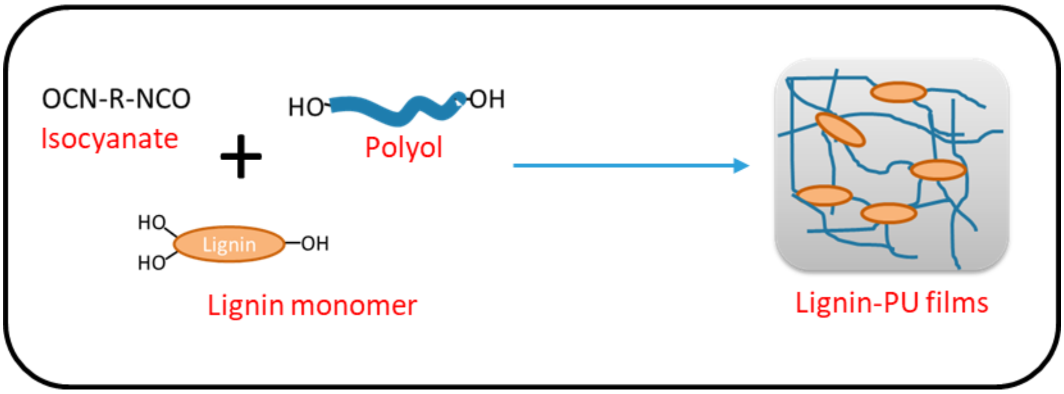
Abstract

Lignin being one of the most produced biorenewable materials, it is highly desirable to valorize it to create high value products and applications. Valorizing lignin is a big challenge due to its irregular structure and high polydispersity. Here we report the results from our efforts to create lignin and its oligomers based polyurethane (PU) synthesis as well as characterization. We show that Kraft lignin and base catalyzed depolymerized (BCD) lignin was covalently incorporated into crosslinked PU films. Methylene diphenyl diisocyanate (MDI) reacts with polyols such as polyethylene glycol, polypropylene glycol and poly(THF) along-with 10-30 w% lignin fraction formed mechanically robust films. These films were further analyzed for thermal, mechanical and swelling behavior. Future directions for the project is intended to create lignin based PU coatings and investigate them.



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BIPDP-54

Synthesis of Furyl-Containing Bisphenol Based on Chemicals Derived from Lignocellulose and its Utilization for Preparation of Clickable (Co) Ploy(ether sulfone)s

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Abstract

Lignocellulose-derived chemicals such as furfural, syringol, guaiacol, etc are highly attractive as sustainable alternatives to petrochemicals for the synthesis of monomers and have attracted great attention of polymer community. We wish to report herein the facile synthesis of fully bio-based bisphenol containing pendant furyl group by base-catalyzed condensation of furfural with guaiacol- both of which are derived from lignocellulose. Bisphenol possessing pendant furyl group represent valuable monomer for the synthesis of a range of polymers which include epoxy resins, polyesters, polycarbonates, poly (aryl ether)s, etc. New (co)poly(ether sulfone)s were prepared by polycondensation of 4, 4'-(furan-2-ylmethylene)bis(2-methoxyphenol) or a mixture of 4, 4'-(furan-2-ylmethylene)bis(2-methoxyphenol) and bisphenol-A with 4, 4'-(fluorodiphenyl sulfone) in N N-dimethylacetamide as a solvent. (Co)poly(ether sulfone)s showed inherent viscosities in the range 0.92-1.47 dL/g and number average molecular weights ($\overline{M_n}$), obtained from gel permeation chromatography (GPC, PS standard), were in the range 91,300-1,31,000 g/mol. (Co)poly(ether sulfone)s could be cast into tough, transparent and flexible films from chloroform solutions. X-Ray diffraction studies indicated amorphous nature of (co)poly(ether sulfone)s. (Co)poly(ether sulfone)s showed T_g values in the range 179-190 ^oC. Most interestingly, the pendant furyl groups in (co)poly(ether sulfone)s provide reactive sites for click modification and cross-linking *via* Diels-Alder reaction with maleimides and bismaleimides, respectively. Cross-linked (co)poly(ether sulfone)s were prepared by the Diels-Alder reaction of furyl containing (co)poly(ether sulfone)s with bismaleimide at 60 ^oC and the cross-linked polymers underwent retro Diels-Alder reactions at 120 ^oC. These (co)poly(ether sulfone)s containing pendant furyl groups are potentially useful as mendable materials.

Theme- PHCMD

PHCMD-01

Development of polymeric track detectors for Neutron dosimetry

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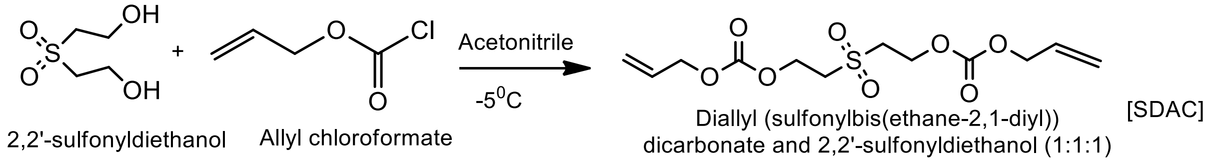
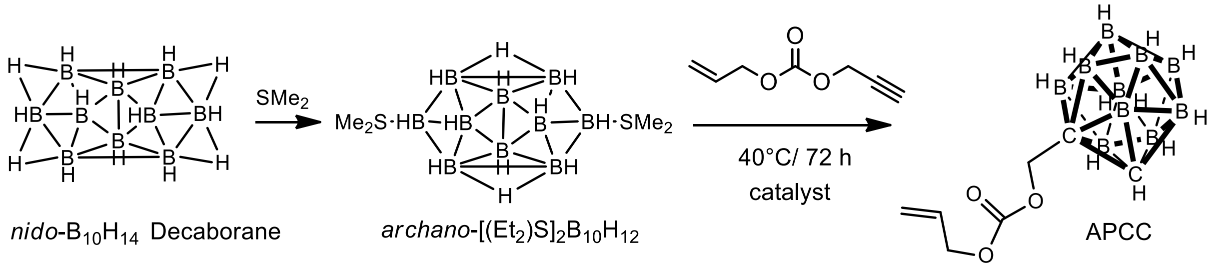
Abstract

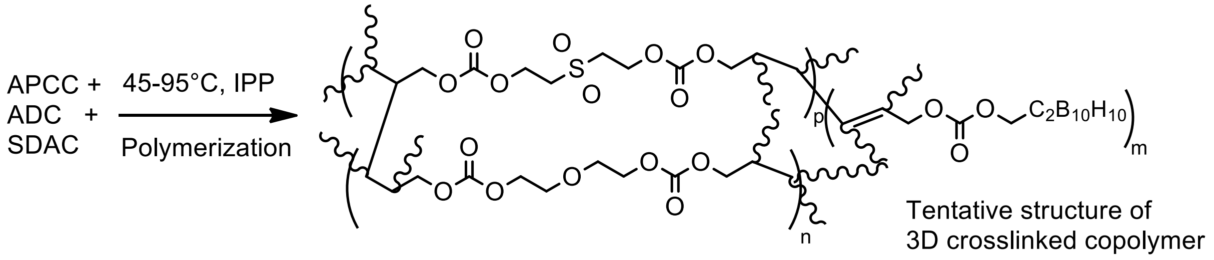
$^{10}B(n, \alpha)$ reaction is most popular to detect thermal neutrons because of higher cross section for the $^{10}B(n, \alpha)$ reaction (3840 barns) and isotopic abundance of ^{10}B nucleus is 19.8 % which makes it easily available[1]. Allyl propargyl carbonate carborane (APCC) copolymerized with allyl diglycol carbonate (ADC) was found to be a promisimg material for neutron dosimetry[2]and 2,2'-sulfonyldiethanol bis(allyl carbonate)(SDAC) based polycarbonate were found to provide a way for swift detection of alpha particles[3,4]. Based on these observations, we have developed a new polymer called poly (APCC-*co*-ADC-*co*-SDAC) for swift detection of thermal neutrons. Synthesis chain of monomer and polymer is schematically shown below.



Scheme 1: Synthesis of SDAC monomer



Scheme 2: Synthesis of APCC monomer



Scheme 3: Synthesis of copolymerpoly (APCC-*co*-ADC-*co*-SDAC)

The polymer films with concentration of boron in the range 1-5% were prepared. The films were exposed to thermalised ^{241}Am-Be neutron to recive a ambient dose equivalent of 1 mSv. The films were etched with 2N NaOH at 50^{0}C. Preliminary observations regarding neutron dosimetry using the copolymer are described.

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PHCMD-02

Investigation of Morphology, Mechanical and Biological Properties of Poly Lactic Acid (PLA) and Thermoplastic Poly Urethane (TPU) Elastomer Blends for Biomedical Application

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Abstract

Poly lactic acid (PLA) and thermoplastic polyurethane elastomer (TPU) both are biocompatible and biodegradable materials. PLA being internally brittle, to enhance its toughness and impact strength it was melt blended with TPU.[1,2] The phase morphology, mechanical properties, permeability, toughening mechanism and biological evaluation of the TPU/PLA blends were investigated. The blends were prepared using poly lactic acid with 10%, 20%, 30%, 40 % and 50% thermoplastic polyurethane elastomer and vice versa. The characterization of morphological properties were obtained using Scanning Electron Microscopy (SEM) indicates that the spherical PLA particles dispersed in the TPU matrix when PLA concentration was low and for higher PLA concentrations, TPU particles were dispersed in PLA. Co-continuous morphology was observed in samples with 30 and 70 wt % PLA. Thus the dispersed phase i.e. the hard segment and soft segment based on the inherent property of the materials leads to decrease in Tensile Properties but increase in elongation. It was observed in DSC results that increasing TPU concentration in the blends lowered the glass transition and melting point of PLA indicating that the components were compatible and partially miscible. Thus there is no much change in stability of blends by incorporation of PLA. Finally leaching tests show that there was no effect of the solvents on the blends making them suitable for biomedical applications.

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PHCMD-03

Synthesis of Biodegradable/Cytocompatible Amphiphilic Co-network Injectable hydrogels for Biomedical Application

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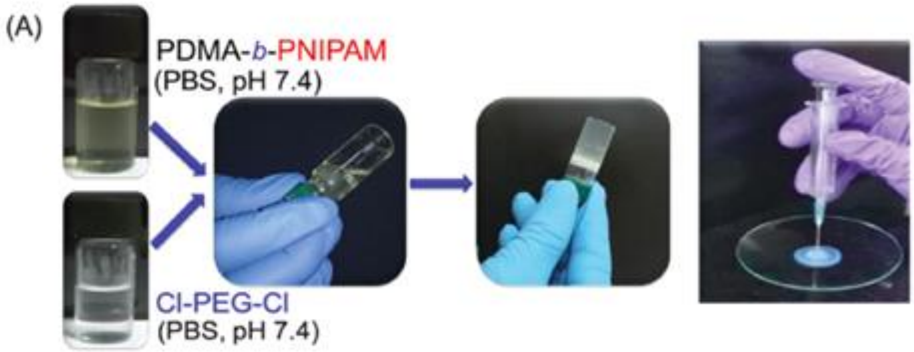
Abstract

We have developed an advance hydrogel system which exhibited rapid gelation, encapsulation of hydrophobic as well as hydrophilic therapeutics, biocompatibility, biodegradability, low heat generation, and high mucoadhesive stress. We have prepared a series of dually crosslinked injectable hydrogels of halide terminated PEG and poly[2- (dimethylamino)ethyl methacrylate]-*b*-poly(N-isopropyl acrylamide) or long-chain alkylated poly[2-(dimethylamino)ethyl methacrylate][1] through extremely simple chemistry. The sequential nucleophilic substitution reaction between PEG containing reactive termini and the copolymer provided chemically crosslinked hydrogels with a gel fraction as high as 96–99% and gelation time of 1–4 min under physiological conditions. The gelation occurred with ca. 1 °C rise in temperature per gram of the injectable solution, avoids formation of by-products and can be performed in the temperature range of 20–37 °C. The hydrogels undergo hardening at a physiological temperature as confirmed by rheological experiments. The mucoadhesion, gelation time, water swelling, mechanical properties and degradability of the hydrogels depend on the PEG to copolymer ratio in the injectable prepolymer solution. The rheological behaviour of the fully hydrated hydrogels showed storage modulus of 10 kPa, suitable for soft tissue regeneration. The hydrogels exhibited blood compatibility and retained the viability of HepG2 cells with time. Platelet adhesion and aggregation followed by fibrinogen adsorption ability makes these hydrogels suitable for hydrophobic drug delivery, and wound healing applications [2].



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PHCMD-04

Synthesis of Multi-Responsive Self-Assembly of Cationic Multiblock Copolymers for Targeted Drug Delivery Application

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Abstract

We have synthesised multi-responsive self-assembly of cationic multiblock copolymers through combined of individual dissimilar blocks to obtain well-defined AnBn and (A-B-A)n types of cationic amphiphilic multiblock copolymers (MBCs) via mild sequential nucleophilic substitution reaction without formation of by-products. MBCs were synthesized by reacting activated halide end-functionalised polymer blocks of poly(caprolactone) (PCL), poly(ethylene glycol) (PEG), and PCL-*b*-PEG-b-PCL with tertiary diamine.[1] For selective degradation, acid and base labile ester as well as reducible disulphide groups were introduced as linkers between the blocks. The micellar self-assemblies of these MBCs showed exceptional stability at normal physiological conditions with the negligible release of the guest molecules. Selectively targeted disassembly under a mildly acidic condition, such as in tumour cells or in the presence of the reducing agent caused triggered release of the guest molecules. Our strategy is versatile and opens an opportunity to obtain verities of tailor-made MBCs for the targeted and triggered release of therapeutics which minimize side effects of the drug, nonspecific drug binding and decrease of the dose of the drugs.

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PHCMD-05

Camptothecin loaded Electrospun Poly [N-(2-hydroxy propyl) methacrylamide] based nanofibers for anticancer treatment

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Abstract

Electrospinning is a resourceful technique to produce polymer fibers in nanoscale diameter. The aim of the present study is to produce fibrous scaffolds of Poly [N-(2-hydroxy propyl) methacrylamide] (pHPMA) / Polyethylene oxide (PEO) blend and evaluate its suitability as drug carrier. Poly [N-(2-hydroxy propyl) methacrylamide] (pHPMA) is a linear, water soluble, inert, non-immunogenic and biocompatible polymer. The optimised concentration for electrospinning is pHPMA:PEO (10:10) w/v % solution in water and the optimised processing parameters were 25 kV, 15 cm distance between tip and collector and 1.5 ml/h flow rate. The average diameter of the nanofibers was found to be 400 - 800 nm. Camptothecin is a prominent anticancer drug with good activity against wide range of cancer cells. However, poor aqueous solubility and pH dependency of camptothecin limits its usage. Camptothecin was incorporated in pHPMA / PEO blend and electrospun into fibers. Thermal stability, functional group analysis and surface morphology were studied using DSC, FT-IR, SEM for both drug incorporated and free pHPMA / PEO fibers. Cell viability using MTT assay were analysed for both drug incorporated and free pHPMA / PEO fibers on MCF7 and VERO cell lines respectively. Cell viability of MCF7 cell lines was found to be 7.8% and that of VERO cell lines was found to be 96.8%. Drug delivery of camptothecin incorporated fibers in phosphate buffered saline solution were analysed using UV-Vis spectrometer at a λ_{max} of 360 nm. The cumulative drug release was 79.6%. Kinetic studies of the drug release were also studied.

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PHCMD-06

Designing of Polymeric Electrospun Absorbent pads for Adhesive Bandages

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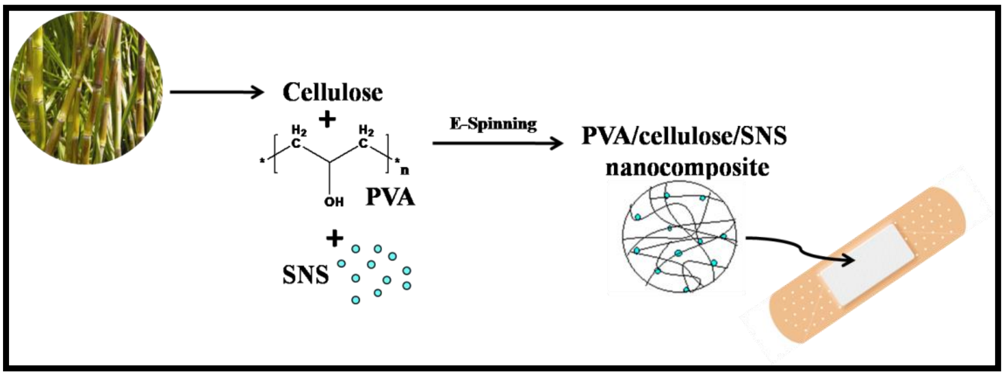
Abstract

The purpose of utilising adhesive bandage attached with adsorbent medicated pads for dressing wounds of various types is to basically protect the part of the wound area from infection and moisture through external sources and to heal the injured part with the growth of new cells. Hence the medically proven antiseptic and quick healing action are obtained by the secure way of using adhesive bandages.The main objective of the proposed work is to fabricate a bio-compatible and bio-degradable nanofibrous absorbent pad material for adhesive bandages. Nanofibers are obtained by Electrospinning technique, an efficient and cost effective way to develop well-interconnected porous structure possessing very high surface area. In the current work, Polyvinyl alcohol (PVA)/ cellulose composite containing the silver nanospheres (SNS) were produced for wound dressing application. Here, the PVA/cellulose composite and SNS acts as the base polymeric matrix and the active healing agent respectively in the absorbent pad of the adhesive bandage. PVA, the synthetic hydrogel demonstrates good biocompatibility hence preferred in advanced wound dressing and as drug carrier systems. The hydrophilic character of PVA restricts its use as wound dressing material. Therefore, to decrease hydrophilicity, increase mechanical strength and biodegradability, PVA is blended with the cellulose extracted from sugarcane bagasse. The synthesised silver nanospheres exhibiting high resistance to bacteria and low toxicity to human cells were incorporated into the polymeric composite which imparts the antibacterial property to the absorbent pad. The composite material was characterised using various analytical techniques such as FT-IR, SEM, and antibacterial studies against both gram positive and gram negative stains. Thus the developed composite containing silver nanoparticles are expected to serve as a potential adsorbent pad in adhesive bandage.



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PHCMD-07

Self-Assembly and Antimicrobial Activity of Cationic Polyurethanes

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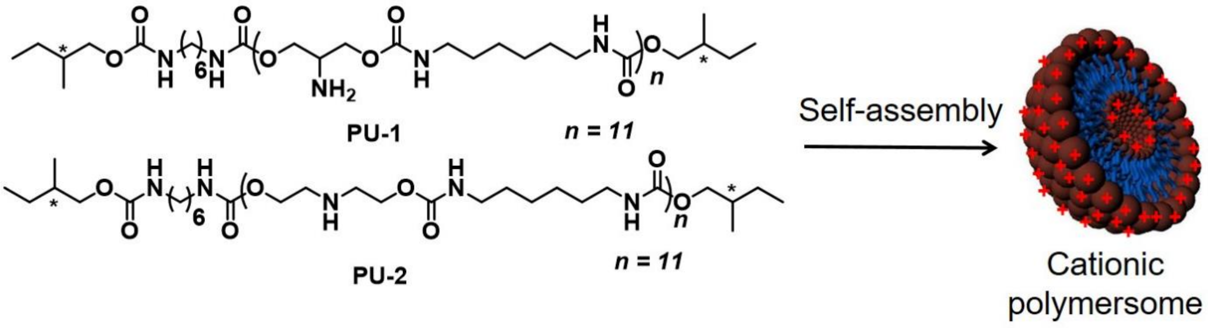
Abstract

Growing microbial resistance to conventional antibiotics has presented a threat to global health. Therefore, new antibiotics are urgently needed to tackle these drug resistance bacteria with new class of antimicrobial compounds as alternative to antibiotics.[1-3] To overcome these antimicrobial resistance, researchers have introduced/developed antimicrobial polymers and polymer-based antimicrobial hydrogels.[4] The key motivation is to design such antimicrobial polymers displaying cationic functional groups (such as hydrophilic and hydrophobic amines *etc*.) to selectively kill the microbes using multivalent effect.

Here we have discussed the synthesis of two cationic amphiphilic polyurethanes (PU-1 and PU-2) which can self-assemble utilizing intra chain H-bonding[5] to form polymersome assembly (size ~ 100-200 nm) in acidic pH. The formation of polymersome has been probed by DLS, TEM, SANS and hydrophilic dye encapsulation experiments. As expected the zeta potential measurements showed a positively charged surface which are known to interact with negatively charged bacterial membrane *via* a direct-contact mechanism. Interestingly, PU-1 and PU-2 exhibit potential antimicrobial activity against Gram-negative bacteria (*E. coli*) selectively over Gram-positive bacteria (*S. aureus*). Furthermore, both the polymers showed very low minimum inhibitory concentrations (~ 10 – 30 µg/ml) towards *E. coli*. On the other hand, these polymers were non-toxic towards mouse RAW264.7 macrophages (~ 50 µg/ml) and showed very good HC_{50} values in the range of 250 µg/ml. Thus, we have shown a design of stable cationic polymersomes using a biocompatible polyurethanes backbone which hold promise for future biomedical applications.



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PHCMD-10

Novel Gelatin based Electrospun Trilayered Vascular Graft for Small Diameter Blood Vessel Regeneration

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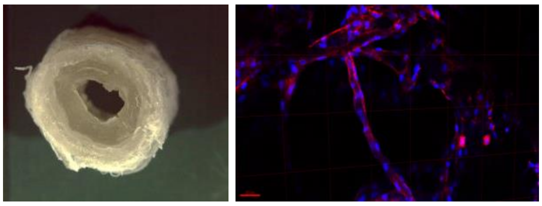
Abstract

An attempt to mimic the native extracellular matrix of blood vessel using electrospun gelatin, protein based vascular grafts can improve the biocompatibility of the grafts compared to the clinically available inert grafts based on e-PTFE and Dacron. Hence, a novel approach in the development of hybrid tri-layered electrospun vascular scaffold based on gelatin hydrogels for blood vessel reconstruction has been proposed. While the electrospun randomly arranged gelatin fibres; mimic the morphology of the native extracellular matrix, the trilayerd tubular structure would help in mimicking the architecture of the blood vessel. Similar to the native vessel, the three layers of the scaffold have been designed with different gelatin based blends. The composition of the gelatin blends from the innermost layer to the outermost layer consists of gelatin-oxidized carboxymethyl cellulose, gelatin-polytrimethylene carbonate and gelatin- polycaprolactone respecively, which were optimized in accordance to resemble the properties of each layer of the native blood vessel.



Electrospun tubular trilayered graft based on gelatin hydrogels and cell growth along the fibres

The hybrid morphology from nanofibrous in the innermost layer to microfibrous structure in the middle and the outermost layer was observed. Confluency was observed with endothelial and fibroblast cells within 3 weeks. The cells were seen to spread and proliferate along the length of the fibres. Neo blood vessel formation and patency was observed within 3 months of arterial implantation as a graft and as a patch. Thereby, this graft may be used as a biodegradble and biocompatible off-shelf coronary by-pass graft a much required aspect in the field of cardiovascular tissue engineering.

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PHCMD-11

Synthesis of folate conjugated nanoceria: A nanotheranostic intervention towards cancer therapy

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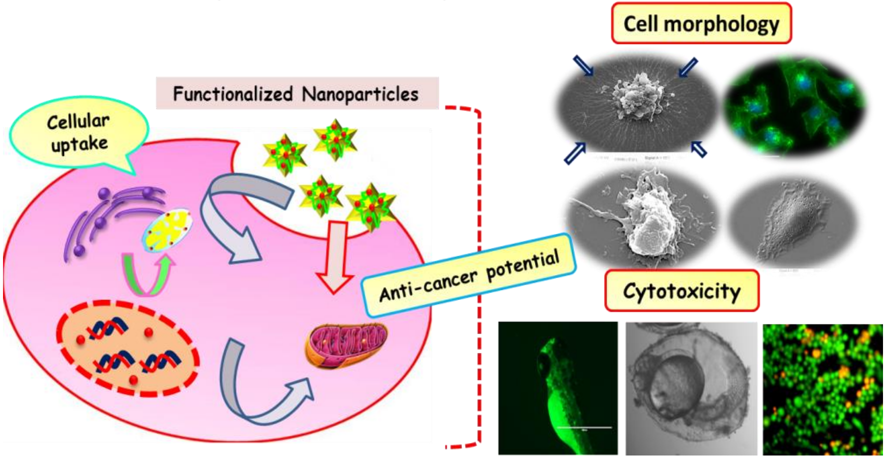
Abstract

The enormous exploration of nanoscience and nanotechnology endeavors new avenues for the advancement of novel materials in the nanoscale range. Multifunctional nanoparticles are now becoming extensively explored and establishing their versatility as drug delivery vehicles in cancer chemotherapeutics. Herein in this proposed work folic acid (FA) functionalized rare earth metal oxide has been utilized as nanotherapeutics in cancer therapy and diagnostic field. Functionalization of FA onto cerium oxide (CeO_2) enables enhanced cellular uptake in breast cancer cells confirmed from JC1 micrographs. The cytomorphological arrangement of the cancer cells has also been monitored using scanning electron microscopic images. The cell migration assays was also scrutinized implying the inhibition of cancerous cells migration upon treatment. Cellular uptake studies revealed that FA-CeO_2 could specifically internalize within a cancerous cell. Further the nanotherapeutic modality of these nanoparticles was evaluated by utilizing neuronal cells imparting the anticancer efficacy of the nanoparticles. Additionally the toxicity profile of the synthesized nanoparticles was screened in zebra-fish model which shows no such significant morphological deformities in the embryonic phase.



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PHCMD-12

Bio-derived cellulose nanofibril reinforced poly(N-isopropylacrylamide)-g-guar gum nanocomposite: An avant-garde biomaterial as a transdermal membrane

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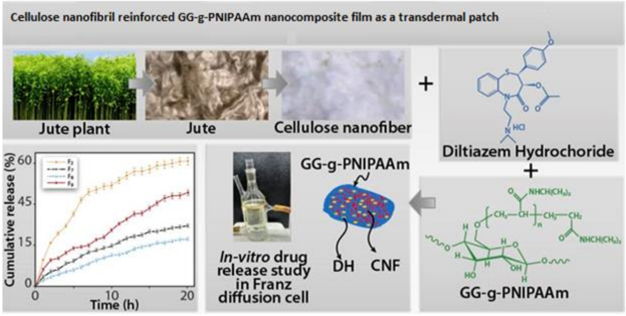
Abstract

The delivery of diltiazem hydrochloride in therapeutical doses has attracted an immense research interest. However, its slower penetration through the transdermal route has stipulated to develop a competent transdermal membrane. Therefore, a nanocomposite based patch was formulated by exploring co-polymer and jute derived nano-cellulose. Poly(N-isopropylacrylamide) was grafted into guar gum (GG-g-PNIPAAm) with different feeding ratios. The co-polymer formation was authenticated by FTIR and ^{13}C NMR spectra. The nanocomposite were prepared by incorporating nanofibre (0.5-2 wt%) into GG-g-PNIPAAm. The structural and morphological studies supported good interactions and presence of nano-cellulose on co-polymer. GG-g-PNIPAAm has showed higher thermostability than guar gum. Moreover, the addition of CNF has improved the thermo-mechanical and barrier properties of the nanocomposite. The nanocomposite containing 1 wt% CNF was found to be best performing. The patch showed in-vitro cyto-compatibility and non-irritant behaviour. The in-vitro release study of best nanocomposite revealed controlled drug release capability with 7.78 and 22.9% after 5 and 20 h, respectively.



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PHCMD-14

Development of Polymeric Scaffold for Facilitating Cellular Repairment and Regeneration by employing Tenet of Tissue Engineering

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Abstract

There is a paradigm shift towards the development of injectable tissue scaffolds from the previously well established pre-formed scaffold. This shift is quite obvious choice as injectable scaffolds embed many advantages over the preformed one in terms of introduction into a patient without surgery and patient compliance. But, it is practically difficult to exactly presume the stability of the injectable formulation as they are administered and if it delayed to crosslink/gel or get diluted by body fluid once injected, then its transformation into solid phase is difficult to attain. Moreover, though the implantation of preformed scaffold is a difficult task, but it ensures stability within the host and it could be predicted that it would not disintegrate immediately and therby support the cellular growth atleast for the initial hours. Therefore an inevitable debate persists in the scientific community to choose an appropriate system for their potential applicability in tissue engineering. In this context, we aimed to synthesize different type of scaffold like pre-formed and injectable by exploring the potentiality of in-situ forming hydrogel, biodegradable polyurethane and its nanocomposites. The physico-chemical and bio-interfacial prospective of the developed scaffold material were performed to qualify them as scaffold. Mechanically strong hyperbranched polyurethane based scaffold was prepared and the properties of the optimized composition were improvised by the incorporation of nanomaterials like CNT and iron oxide nanomaterials.

In another front, the in-situ hydrogel were prepared exploring thermosensitive methylcellusose and the effect of the size/ concentration of additives or biocompatible viscosity enhancer were comprehensively studied.

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PHCMD-15

Colored Polymeric Nano-carrier for the Efficient Delivery of Colorless Drugs for Cancer Therapy

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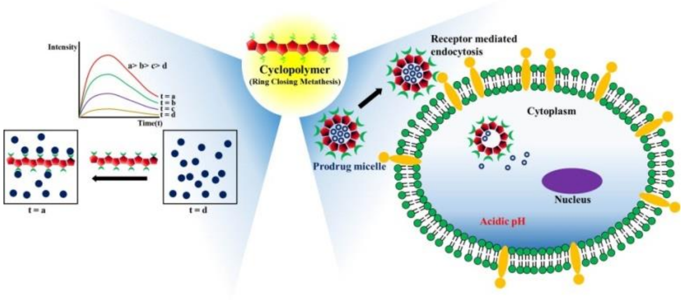
Abstract

The need for efficient non-fluorescent anti-cancer drug delivery with polymeric system is always a challenge. Motivated with this challanges, we have developed a newly tumour targeting polymeric nonocarrier which has been developed by cyclopolymerization of 1,6-heptadiynes using Hoveyda-Grubbs' second generation catalyst. We have developed novel polymeric nanocarrier to encapsulate chlorambucil, a non-fluorescent anticancer drug. The continuous conjugation in the cyclopolymer backbone gives intense red-orange colour i.e. highly active in UV region, which has helped to track non-fluorescent anticancer drug, chlorambucil. Polyethyleneglycol monomethyl ether is used for water solubility to synthesize **mPEG-RCP** copolymer. Further, mannose moiety has been introduced for the site specificity and water solubility in the **RCM-Man** polymer. All the monomer and polymer are characterized carefully with standard analytical techniques. Self-assembly of the polymer has been studied by dynamic light scattering, scanning electron microsope and Ttransmission electron microscope. Cell viability of cyclopolymer is observed to 500 µg/ml. Chlorambucil and Nile Red have been encapsulated and the release. Studies are done at different pH which shows good efficiency at higher concentration. For the site specificity of **RCM-Man** polymer, interaction of Concovalin A and **RCM-Man** polymer have been studied by fluorescence spectroscopy. Gradual increase in the fluorescence intensity while increase in Concovalin A confirms the formation of aggregate networks. We are hopeful that developed polymeric nanocarrier could open a new avenue in cancer therapy, due its unique design and its biocompatibility.



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PHCMD-16

Silk fibroin composite microparticles with bioactive ceramics towards development of biological scaffolds with enhanced osteoregenerative properties

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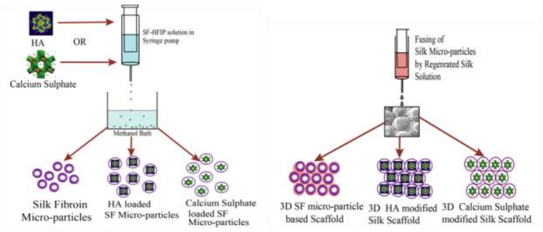
Abstract

Advanced strategies for bone tissue engineering today involve growing cells, in 3D scaffolds containing bioactive factors. In this work, we demonstrate 3D scaffold of silk fibroin microparticles loaded with hydroxyapatite nanoparticles - an essential element of natural bone or calcium sulphate. The physico-chemical and mechanical characterization of these scaffolds show that ~30% loading of the filler particle can be consistently obtained. These modified microparticles filled 3D scaffolds also demonstrate optimum porosity, pore size and excellent pore interconnectivity which results in enhanced load bearing capacity. This overcomes the brittleness and difficulties in the processing of bioactive ceramics while retaining their inherent osteoconductive properties. *In-vitro* data shows that these scaffolds exhibit significantly improved osteoinductive behaviour when seeded with hBMSCs resulting in better cell proliferation and further differentiation into the osteogenic linage. These unique newly modified 3D microparticles based silk fibroin scaffolds having great potential for the long bone defect caused due to trauma or infection.



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PHCMD-17

Crosslinking of Polyether block amide (PEBA) with Mercaptoethanol (ME) to obtain Mechanically Strong Breathable Membrane for Antimicrobial Applications

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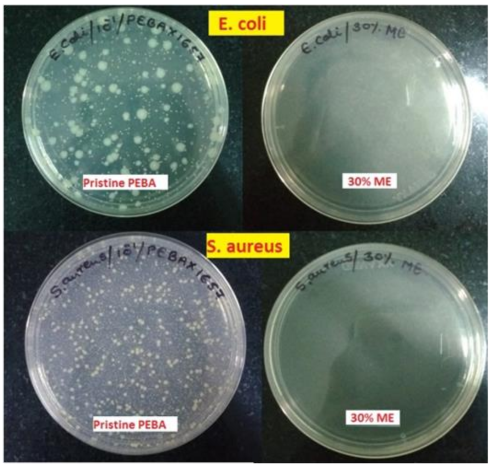
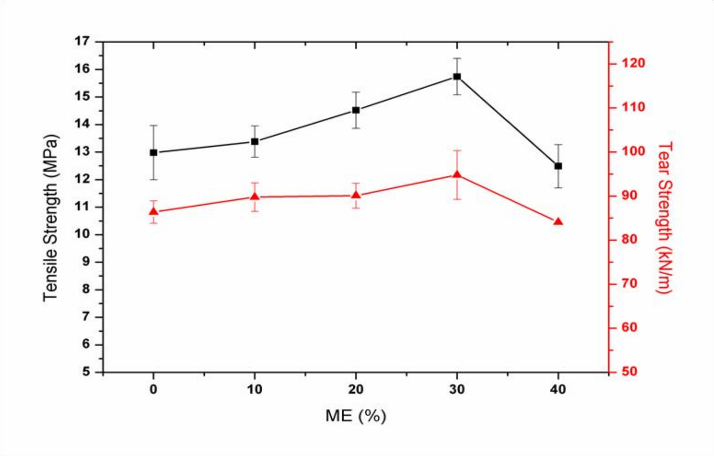
Abstract

Polyether block amide (PEBA MH 1657) was cast polymerized with Mercaptoethanol (ME) to enhance the antimicrobial properties. Non-porous breathable membranes with properties of permeability, tensile strength, tear strength, antibacterial and antifungal properties were studied for the membranes. Analytical techniques such as FTIR-ATR, SEM, AFM, DSC, TGA and DTG were used to characterize the membranes. Different amount of ME (10 to 40% w/w) was added to PEBA, and 30% ME was found to be most effective in increasing the mechanical properties (Tensile strength from 12.98 MPa to 15.74 MPa & Tear strength from 86.4 kN/m to 94.8 kN/m). Sulfhydryl group of ME introduces crosslinks between PEBA segments (determined through Soxhlet extraction) and enhance mechanical strength of the membranes. PEBA-ME membranes possess 99.99% antibacterial activity membrane (against S. aureus & E. coli) which was only 16-28 % for pristine PEBA. The membranes showed excellent antifungal properties against *Asperglus niger*, *Penicillium pinophilum*, *Aureobasidium pullulans*, *Chaetomium globosum* and *Trichoderma virens.* Antimicrobial behavior of the membranes is due to the presence of sulfur moiety since various sulfur containing compounds are known for their antimicrobial activity [1]. PEBA-ME based non porous breathable membrane with excellent mechanical strength is a novel material that can be used for various biomedical applications.





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PHCMD-19

Crosslinked alginate-gelatin polymeric coatings for titanium-based bone implants

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Abstract

Metallic implants fabricated from titanium and stainless steel are widely used in orthopedic field to support/replace damaged bone parts. The implants are mostly inert towards tissue surfaces, thus leading to poor integration with the tissue surfaces and formation of fibrous capsule around the implant. It may result in loosening of implants, requiring surgical intervention. Surface properties, like topography, roughness, chemical modification, and electrochemical treatment, have been modified to achieve osseointegration, but only moderate success could be achieved[1]. Consequently, several proteins, peptides, and other biomolecules have been immobilized on implants via physical/chemical methods but these suffers from uncontrolled desorption or loss of bioactivity of biomolecules. Owing to their extracellular matrix (ECM)-mimicking characteristics, polymeric coatings have emerged as attractive alternative to modulate cell activities on these implants[2]. In this context, we fabricated and characterized gelatin-alginate polymeric coatings on the titanium surfaces, to create ECM-mimicking environment for promoting cell activities and osseointigration. Ti discs were functionalized with amine groups for covalent grafting of alginate layer on metal surfaces. Maleimide groups were incorporated onto the alginate layer for fabrication of thiol-maleimide crosslinked alginate-gelatin layers, using thiolated gelatin. Each step was characterized using ATR-FTIR spectroscopy and UV-Vis assays. Gelatin is a protein having cell binding sequences and alginate is a polysaccharide with promising biocompatibily and degradation profiles. The combination of these polymers have shown promise in cartilage regeneration applications but rarely evaluated as coating on the titanium implant surfaces[3]. These coatings are being evaluated for cell activities and local release of active moieties.

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PHCMD-20

Malonic Acid Based Site Specific Chemotherapeutic Polymeric Nanocarrier

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Abstract

Incidence and progression of cancer is increasing worldwide and it is estimated to become the first cause of disease related mortality leaving behind cardiovascular disease. In lab to clinic transition, targeted molecular systems remains to be the last standing hope.[1] Herein, we have designed and successfully synthesized a site specific chemotherapeutic polymeric nano-system, where ring opening polymerization has been employed to get dipropergyl malonate functionalized poly caprolactone. Azide derivatives of doxorubicin and PEG folate moiety are anchored to the system by well-known azide-alkyne click reaction in presence of copper sulfate and sodium ascorbate. All the synthesized monomers and polymers are thoroughly characterized standard analytical and spectroscopic techniques. Folate moiety helps to reach the macromolecular nano-system to cancerous-site specifically and the presence of hydrazone bond between polymeric system and doxorubicin makes it capable of acid triggered drug release at cancerous environment.[2] This newly developed therapeutic system has showed very effective drug release in acidic medium as well as it has showed a great potential *in vitro* biology studies.

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PHCMD-23

Prevention of protein aggregation in neuronal cells using antiamyloidogenic molecule-based polymeric nanoparticles

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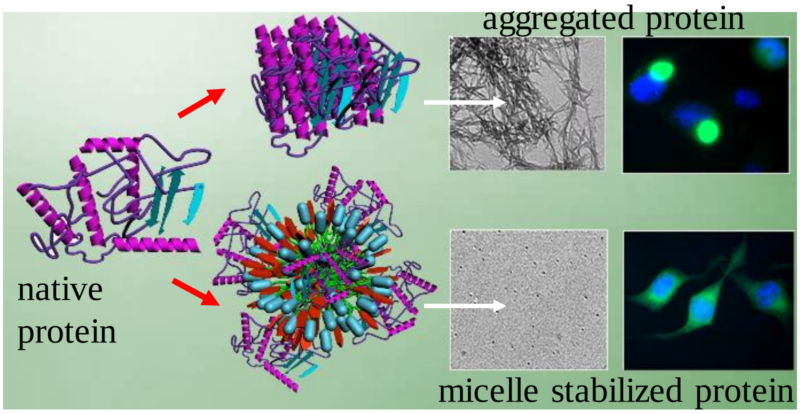
Abstract

Protein aggregation is linked to a variety of neurodegenerative disorders and other diseases (Alzheimer's disease, Huntington's disease). Current research involves understanding the mechanism of protein aggregation, inhibiting protein aggregation under intra/extracellular space, lowering toxicity arising due to soluble oligomers, and augmenting the clearance of protein aggregates from the cell/brain.[1] Toward this direction, different types of antiamyloidogenic small molecules, macromolecules, and nanomaterials are identified that can inhibit protein aggregation, and extensive progress has been made for their effective utilization.[2-4] We work on designing functional nanoparticles,[2] polymer micelles[4,5] to target neuronal cells and to prevent protein aggregation intracellularly. In this presentation, I will demonstrate how polymeric nanoparticles stabilizes protein's folding state and will display our effort in designing biocompatible, biodegradable, self-assembled polymer nanoparticles to prevent protein aggregation inside Huntington model neuronal cells (HD150Q).[5] We have designed self-assembled micelles with trehalose/EGCG/dopamine/arginine functionalization, that enter into neuronal cells efficiently and reduce protein aggregation ~10^2-10^5 folds more than respective antiamyloidogenic molecules. This approach is further extending to clear aggregates from cell/brain to cure neurodegenerative disorders. Thus *In-vitro* results strongly encourage that this kind of biodegradable polymeric nanoparticle systems has bright prospect to cross Blood-Brain Barrier to prevent protein aggregation in the brain.



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PHCMD-24

Iron(III) based polymeric nano-theranostic system for effective T_1 weighted magnetic resonance imaging and cancer therapy

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Abstract

Recently, polymeric theranostic nano-medicine showing a huge response in cancer treatment due to the combined effect of therapy and diagnosis.[1] Herein two different polynorbornene based polymeric nano-carrriers were utilized to deliver chemotherapeutic agents like doxorubicin and camptothecin. These drugs were covalently linked with respective macromolecular systems through pH responsive hydrazon and ester bond. To make both the systems cancerous-site specific, folic acid was conjugated in addition with hydrophilic poly ethylele glycol moiety. Nephrotoxicity of post transition metal based MRI contrast agents were abandoned by utilizing terpyridine and diethylenetriaminepentaacetic acid chelated iron based strong paramagnetic complexes.[2] Relaxivity and 1D MRI studies proved the potentiality as T_1 positive contrast agent. All these molecular property were combined together into a single macromolecular system through ring opening metathesis polymerization. Drug release studies and *in vitro* biological studies were supported the effectiveness of these macromolecular systems for effective cancer treatment.

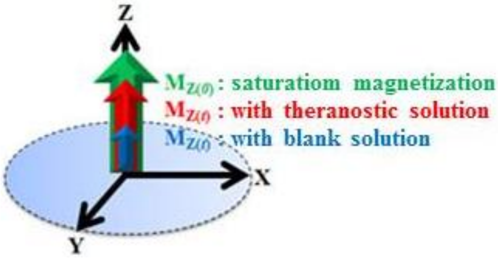

Figure: Cartoon representation of longitudinal magnetization (M_z) recovery.

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PHCMD-26

Polymer based nanoparticles for the delivery of cardiolipin to the mitochondria for barth syndrome

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Abstract

Barth Syndrome (BTHS) is an X-linked recessive genetic disorder characterized by cardiomyopathy, skeletal myopathy, left ventricular non-compaction, abnormal fatigability, and neutropenia [1]. BTHS is primarily caused by alteration of cardiolipin (CL) remodeling from tafazzin (TAZ) mutation. CL is an anionic phospholipid situated mainly in the inner mitochondrial membrane. CL plays important roles in mitochondrial functions such as mitochondrial protein import, structure integrity, super-complex construction, optimal mitochondrial enzymes activities, and apoptosis. The deficiency of CL leads to a series of mitochondria associated dysfunctions [2]. In the current study, we are using FDA approved poly(lactic-*co*-glycolic) acid (PLGA) and CL to create a mitochondrion targeted biodegradable CL-based nanoparticle (NP) to increase CL and decrease oxidative stress in BTHS population for overall therapeutic outcome. We are conducting these studies in two induced pluripotent stem cell (iPSC) cell lines; one with the wild type TAZ gene, and the other with a deletion in the TAZ gene sequence, mimicking the effects of BTHS. This finding will open up the true therapeutic window of BTHS.

Acknowledgment: This work is supported by Barth Syndrome Foundation, Sylvester Comprehensive Cancer Center, and Bankhead-Coley Cancer Research Program.

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PHCMD-30

Fabrication of Curcumin embedded Chitosan Nanoparticles in L-Lactic acid to Combat Breast Cancer

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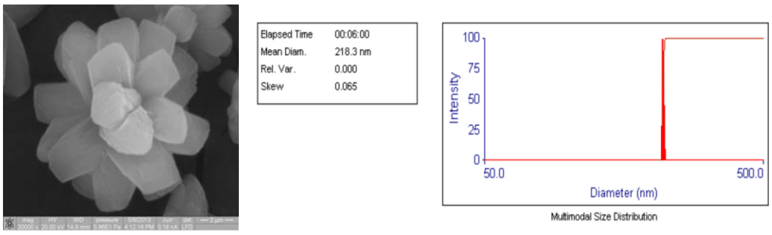
Abstract

Curcumin ((1E,6E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione) is majorly used as a chemotherapeutic agent with anticancer, antioxidant, anti-inflammatory, antiproliferative and antibacterial effects. However, the biomedical application is limited due to its hydrophobicity and poor bioavailability. Chitosan (CS) is non-toxic, biocompatible and biodegradable biopolymer and has been used in drug delivery, gene therapy, and tissue engineering. In this work, we prepared a formulation of Curcumin with chitosan in presence of L-Lactic acid, which are chemopreventive and chemotherapeutic nanoparticles. The solubility in aqueous medium was increased. These nanoparticles were characterized using DLS, AFM, SEM, FTIR, and XRD. DLS studies revealed nanoparticles with a mean diameter of 218±0.3 nm and polydispersity index is 0.091. AFM and SEM confirmed that the particles have a new flower-like morphology. The entrapment efficiency was 65%. The *in-vitro* release of curcumin nanoparticles was studied at different pH (5.8, 6.8 and 7.4) at 37 °C for different incubation periods. The cell viability of nanoparticles was confirmed by cell viability assay using HUVEC cell line, and the anticancer activity of nanoparticles was studied by MTT assay using a breast cancer cell line (MCF-7) and leukaemia cancer cell line (K562). Therefore, it was found that the curcumin-loaded in chitosan nanoparticles showed significant anticancer activity towards cancer cells and nontoxic toward normal cells. Formulation of Chitosan in L-lactic acid will be an efficient nanocarrier for delivering Curcumin to cancer cells.

Keywords

Chitosan, Curcumin, Nanoformulation, Cytotoxicity, Cancer drug delivery.



ESEM image and DLS graph of Curcumin loaded Chitosan Nanoparticles

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PHCMD-33

Synthesis and characterization of poly(vinylalcohol) modified gelatin (Gel-PVA) nanoparticels for controlled release of ciprofloxacin

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Abstract

Gelatin, abiocompatible, biodegradable,easy availableand multifunctional biopolymer has been investigated extensively as a drug carrier, due to its properties and history of safe use in wide range of medical application. The flexibility of gelatin structure has evoked great interest in chemical modifications of gelatin to amend the drug release kinetics and to design targeted drug delivery carriers. Ciprofloxacin is a broad -spectrum antibiotic having poor solubilityand low dissolution rate in gastro-intestinal fluids which limits its bioavailability. In this current work an attempt was made to synthesize ciprofloxacin loaded gelatin polyvinylalcohol (Gel-PVA) nanoparticles using two step desolvation method and were characterized by FTIR, DLS and SEM. The IR spectra shows the grafting of Gel-PVA. DLS and SEM reveals the formation of Gel-PVA nanoparticles.The drug entrappment efficiency and drug release pattern were studied. The drug entrappmnet efficency in phosphate saline buffer was 87.7 % and the drug release pattern under different pH revealed the biphasic and controlled release. The maximum cumulative release of ciprofloxacin was observed in pH 1.2 followed by 6.8 and pH 7.4.

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PHCMD-35

Mannose-6-Phosphate Modified Peptide and Lipid Based Nanocarriers for Lysosomal Delivery of Macromolecules

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Abstract

Lysosomal Storage Disease (LSDs) describes a class of over 40 genetic disorders each resulting from a deficiency of a particular lysosomal enzyme. Treatments of LSDs involve enzyme replacement therapy using modification of enzyme with mannose-6-phosphate (M6P). The development of nanocarriers that is surface modified by an "in-house" developed mannose-6-phosphate (M6P) based polymer/lipid that can efficiently encapsulate and deliver lysosomal enzymes directly into the lysosome of the diseased cell is reported. We have synthesized biocompatible amphiphilic M6P functionalized polypeptide and M6P functionalized lipids in our efforts to develop nanocarriers. The amphiphilic glycopolypeptide and lipids were self-assembled in water into morphologies such as micelles and liposomes. These nanostructures were characterized in detail using a variety of techniques such as TEM, AFM, cryogenic electron microscopy and dye encapsulation techniques. We show that it is possible to sequester both hydrophobic as well as hydrophilic dyes within the nanostructures. *In-vitro* studies show that these non-cytotoxic M6P functionalized micelles were selectively and efficiently up-taken by L-929 cells and MCF-7 breast cancer cells demonstrating their potential as nanocarriers for small hydrophobic drug molecules.

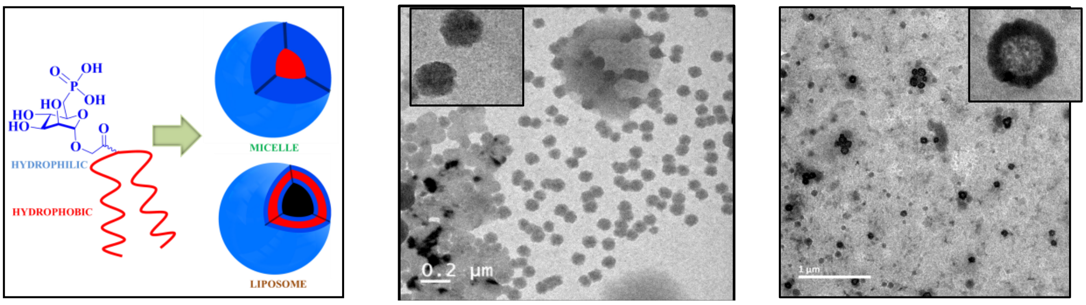

Figure: Nanocarrier Formation, TEM Image of Liposome and Micelle

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PHCMD-37

β- Cyclodextrin based pH and thermo-responsive crosslinked gel as Ofloxacin carrier

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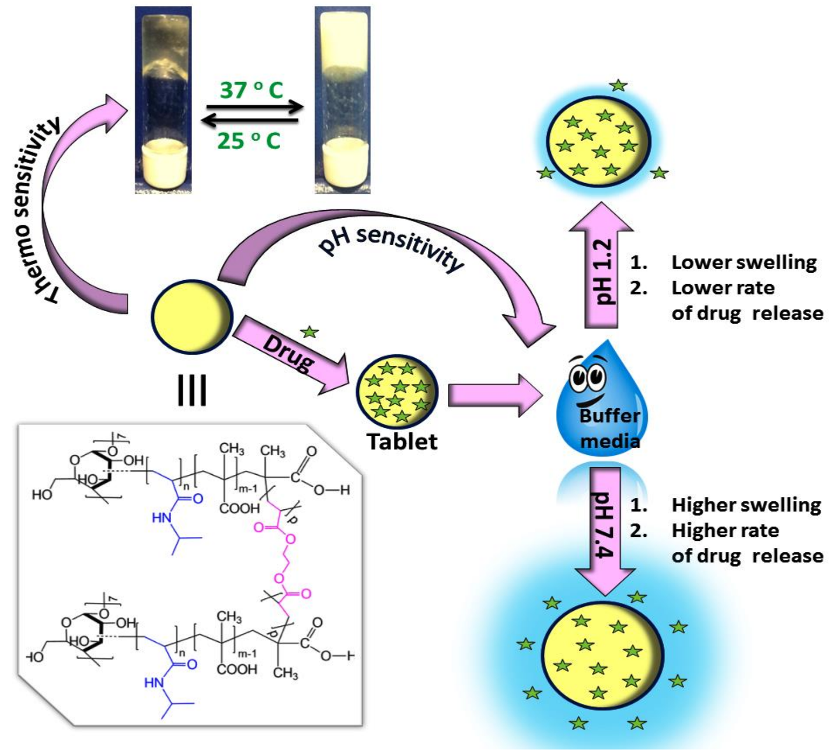
Abstract

Here, a chemically crosslinked, biocompatible, pH and thermo responsive polymeric gel has been synthesized using β-cyclodextrin, *N*-isopropyl acrylamide, methacrylic acid and diethylene glycol dimethacrylate. The biopolymeric gel has been fabricated here to investigate its suitability as carrier for controlled release of colonic drug ofloxacin. β-CD-cl-(PNIPAm-co-PMAc) hydrogel has been characterized in details with several characterization techniques. The developed gel reveals excellent pH and temperature responsive behaviour. Gel properties of the synthesized material have been established by measurement of rheological parameters. The hydrogel network displays nontoxic nature towards MG-63 cell lines. The *in vitro* release of ofloxacin from the gel endorses that it released the colonic drug at preferred pH (colonic pH 7.4) at a desired rate.



PHCMD-38

Non-Ionic Cellulose Nanofibers: An effective wound dressing material

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Abstract

Nanofibers obtained from electrospinning technique provide outstanding properties such as high elasticity, strength, porosity and surface-area-to-volume ratio. They find wide range of applications in filtration, tissue engineering, scaffolds, wound dressings, catalysts and enzyme carriers, protective clothing, sensors, drug delivery, and cosmetics etc.

In the present work, we report on the nanofibers consisting of ethyl hydroxy ethyl cellulose (EHEC) and Poly vinyl alcohol (PVA) with the incorporation of silver nanoparticles (AgNPs). The presence of AgNPs was confirmed by UV spectroscopy. The SEM and TEM images revealed the diameter of the nanofibers in the range of 300-350 nm and the size of the silver nanoparticles was in the range of 20-30 nm. The nanofiber mats exibhited very good tensile strength in the range of 8 to 11 MPa.The antibacterial studies on the nanofiber mats were performed using *S.aureus* and *E.coli* bacteria.The zone of inhibition increased with increase in AgNPs. The release of AgNPs was studied in the phosphate buffer. These nanofibers show great promise in wound healing applications.

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PHCMD-39

Poly (caprolactone) Based Nanofiber Scaffolds for Drug Delivery and Tissue Engineering Applications

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Abstract

To overcome the present challenges in drug delivery and tissue engineering different classes of biomaterials have been developed. In recent years, the use of electrospun nanofibrous nonwoven scaffolds has gained a significant momentum in the field of biomedical tissue engineering. In this presentation, we will be discussing the poly (caprolactone) (PCL) based electrospun composite nanofiber scaffolds for drug delivery and tissue engineering applications. The antibacterial drug, chloramphenicol loaded nanofiber scaffolds shows the sustained release up to 20 days in phosphate buffers saline at the pH of 7.4. These nanofibers also showed good biocompatibility for human epithelial cells (HCT-116 WT). As the PCL nanofibers have less wettability, we are successful in enhancing hydrophilic property by adding poly (ethylene glycol) (PEG) in specific concentration, as wettability is an important factor during the cellular attachment and proliferation. In in-vitro experiments these scaffolds showed slow drug release and excellent biocompatibility. Hence, these scaffolds can be used for antibacterial wound healing applications.

We will be also talk on PCL-PLCG-PEG composite nanofiberous scaffolds for soft and hard tissue engineering and natural *Emblica officinalis* derived composite nanofiber scaffolds for anti-proliferative applications, tested in-vitro against MCF-7, a breast cancer cell line. The scaffolds also show good antibacterial activity against gram positive and gram negative bacterial strains.

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PHCMD-42

Evaluation of cytotoxic effect of Curcumin loaded Pluronic-EDTA based microgels against breast cancer cell line

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Abstract

Micro-organism has tendency to change their conformation and composition in the surface protein depending upon change in environment such as pH. So to mimic these kind of change in the biological behaviour many stimuli responsive polymeric systems such as microgels and nanogels have been developed. The work focuses on synthesis of curcumin loaded microgels based on Pluronic F127 against breast cancer cell line that involves chemical modification of the polymer. The generation of Pluronic-EDTA microgels proceeded by emulsion polymerization using EDC coupling reaction between amine modified pluronic and EDTA. Further loading of curcumin in synthesized microgel. The study also includes drug loading and the release phenomenon of these microgels under different pH and temperature conditions. These curcumin loaded Pluronic-EDTA microgels were characterized using different techniques. *In vitro* studies of the Pluronic –EDTA microgels carried out on MDA-MB-231 cell line of breast cancer, such as flow cytometry,cell viability and cellular uptake demonstrated improved anticancer acitivity.

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PHCMD-44

Synthesis of biodegradable polymers from natural extracts and fabrication as non-woven nanofiber mats for tissue regeneration

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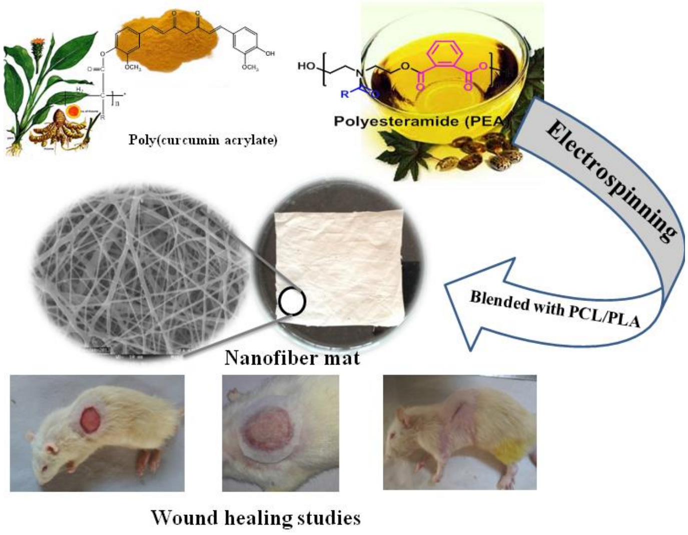
Abstract

Naturally originated biodegradable polymers are having good scope in wide range of applications, mainly in biomedical field, because they are biocompatible, biodegradable in physiological condition and also non-toxic to the live cells. To developing biomaterials, different materials like inorganic (metal oxides, cage molecules and etc) and polymeric (polysaccharides, polyesters, polycarbonates and etc) materials are being used in the form of bulk and nano-materials. Nano-materials (nanoparticles, nanofibers, nanogels, dendrimers and etc) are more efficient than bulk materials (films, gels, patches and etc) for biomedical applications because nano-materials have the high surface area, good stability, more interaction with cells and high permeability. However, in view of environmental concerns, it is always recommended to use polymers of natural origin for biomedical applications.

Here, we developed biodegradable polymers namely, poly (curcumin acrylate) and polyesteramides from natural extracts, curcumin and vegetable oils respectively. The synthesized polymers were fabricated as non-woven nanofiber mats with blend of poly (L-lactide), polycaprolactone and albumin by electrospinning method. The morphology of the nanofibers was studied by scanning electron microscope and transmission electron microscope. The diameter of the nanofibers was ranging from 300 to 450 nm. Mechanical and thermal studies were performed by DMA, TGA and DSC. Further we studied antibacterial, cytotoxic, *in vitro* drug release studies to confirm the developed material suitability for biomedical applications. Moreover, *in vivo* wound healing studies of the nano-materials by rat model shows good healing properties as compared to the commercial wound healing material. Hence these nano-materials may be considered as potential scaffolds for tissue regeneration applications.



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PHCMD-45

Development of L-Lysine Based Biodegradable Polyurethanes for Drug Delivery to Cancer Cells

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Abstract

Amino acids are biologically active molecules and play a vital role in many biological processes.[1] The present investigation reports the first example of L-lysine amino acid based thermo and enzyme dual responsive polyurethanes. These polyurethanes were developed by solvent free melt polycondensation approach[2-3] and their aqueous self-assembled nanostructures were employed for anticancer drug delivery. L-Lysine amino acid was tailor made in to di-urethane monomer having the acid group anchored with PEG-350 to bring the appropriate amphiphilicity. The diurethane monomer was polycondensed with 1,12 dodecane diol to get amphipilic polyurethanes.[4] These polyurethanes were self-assembled in to 180±10 nm nanoparticles in the aqueous medium. Interestingly the polymer solution is transparent at ambient temperature whereas upon increasing the temperature from 38-50 °C the solution becoming completely turbid and the polymer are precipitating out from the aqueous medium (LCST behaviour). This temperature responsive phase transition of the polyurethanes was extensively investigated by transmittance and dynamic light scattering techniques (DLS). The self-assembled polymer nanoparticles are capable of encapsulating anti cancer drugs such as doxorubicin (DOX). *In vitro* drug release studies revealed that the polymer nanoparticles are very stable at physiological conditions and undergo burst release at temperature near to cancer tissue temperature. Since the polymer backbone has made with urethane linkage these polymer nanoparticles are undergoing disassembly in the presence of lysosomal esterase enzyme and releasing the loaded drugs in a controlled manner. Cytotoxic effects of these polyurethanes were investigated in human breast cancer MCF 7 cells, cervical cancer heLa cells and normal cell lines (WT-MEFs) which show the biocompatible nature of the polymers. From the cytotoxicity studies it is confirmed that these drug loaded polymer nanoparticles are selective in killing the tumor cells over the normal cell lines. Confocal and live cell images show the cellular internalization of the drug loaded nanoparticles and flow cytometry data has revealed that the DOX loaded polymer nanoparticles were taken up better than the free DOX.

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PHCMD-46

Soy protein/polyacrylamide nanohydrogel for oral delivery of ciprofloxacin

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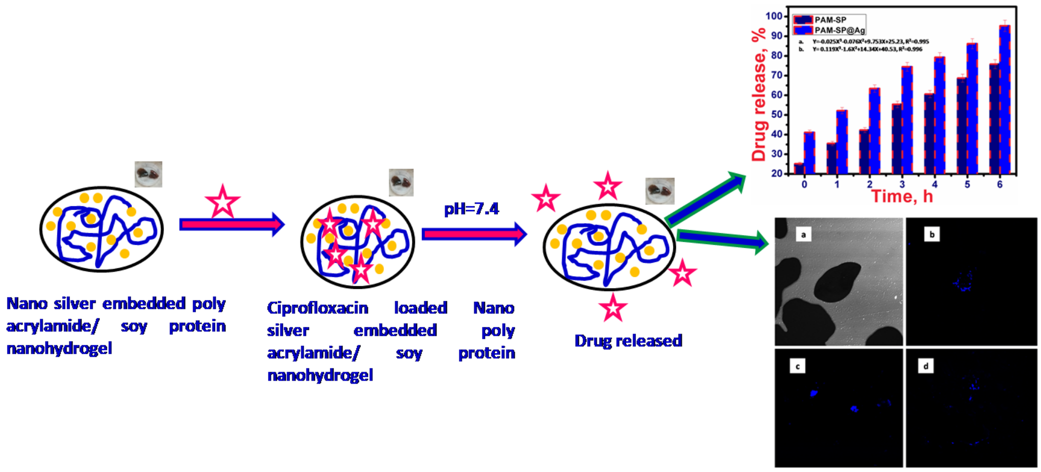
Abstract

Recently, silver nanoparticles (AgNps) have attracted considerable attention in various biomedical applications like drug delivery, photo thermal ablation of cancer and imaging agent for cancer diagnosis. The nanoparticles are used as carrier vehicle for drugs and bioactive molecules with an aim of enhancing the therapeutic effect and to decrease their side effects. The present work is demonstrated on the nano silver embedded soy protein polyacrylamide (PAM-SP@Ag) nanohydrogel which is synthesized by *in situ* polymerization process for the release of ciprofloxacin drugs. The structure and morphology of the nanohydrogels have been explored using FTIR, XRD, XPS, and FESEM analysis. It is found that, the average size of AgNps is 50 nm whereas; size distributions of AgNps are studied from DLS study. The investigation of the release rate of ciprofloxacin drugs carried out by measuring water retention and swelling properties of nanohydrogels. The *in vitro* ciprofloxacin drug release rate is noticed to be 95.3% in a time period of 6hr. The investigation of cytotoxicity tests and antibacterial behaviour alongwith negative and positive action of nanohydrogels are studied. The gelling actions of prepared nanohydrogels are given by the rheological study. The cytotoxicity behaviour of PAM-SP@Ag nanohydrogels along with improved swellings and rheological properties are enabling the material as suitable vehicle for safe release of ciprofloxacin drug.



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PHCMD-47

Fluorescence Resonance Energy Transfer Based Wash-Free Bacterial Imaging and Antibacterial Application Using Cationic Conjugated Polyelectrolyte

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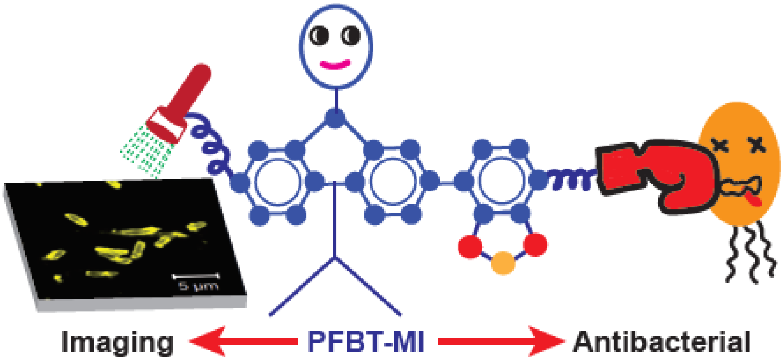
Abstract

Bacterial Infection is one of the global health issue that should be addressed immediately. The detection of bacteria at early stage plays an important role in prevention of upsurge of epidemic diseases. Herein, we report a fluorescence resonance energy transfer (FRET) based probe for the wash-free imaging of Staphylococcus aureus (Gram-positive) and Escherichia coli (Gram-negative) bacteria and their killing. The conjugated polyelectrolyte (CPE) [9,9-bis(6′-methylimidazoliumbromide)hexyl-fluorene-co-4,7-(2,1,3-benzothiadiazole)] (PFBT-MI)) has cationic imidazolium group that makes the CPE water soluble as well as act as a binding site for the negatively charged bacterial membrane. The presence of bacteria in aqueous media could be easily envisaged under UV lamp as the CPE undergo change in fluorescence color from blue to yellow, due to electrostatic interaction with negatively charged bacterial membrane. Furthermore, the PFBT-MI shows excellent antibacterial property against both *S. aureus* and *E. coli* with a minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) value of (30 μM or 23.7 μg/mL) and (60 μM or 47.7 μg/mL) for *S. aureus* and for *E. coli* (60 μM or 47.7 μg/mL) and (100 μM or 79 μg/mL), respectively.The antibacterial action of PFBT-MI is due to the amphiphilic nature that results in the intercalation and disintegration of the bacterial cell membrane and thus bacterial cell death. Besides, antibacterial activity the PFBT-MI shows less cytotoxicity against mammalian cells and thus it can be applied for biomedical application.



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PHCMD-48

Biodegradable polymeric multi-layered microparticles for food packaging applications

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Abstract

Biodegradable Poly (lactic-co-glycolic acid)/Poly(lactic acid) microparticles with loaded actives were successfully fabricated for packaging applications. The microaprticles were well designed with specific layered compositions having respective actives. The outermost layer consists of more hydrophilic polymer (PLGA: Poly(*dl*-lactic-co-glycolic acid, 50:50) with antibacterial (benzoic acid) encapsulated in it and the inner core contains hydrophobic polymer (PLLA: Poly(*l*-lactic acid) with antioxidant (tocopherol) localized in it. The morphological as well as layer compositions of microparticles were characterized by SEM and Raman analysis respectively. To know the effect of these microparticles against different microbes (*Escherichia coli* and *Staphylococcus aureus*), the controlled release behavior of loaded actives were carried out. This study involves how multilayered microparticles can tune the release profiles of multiple actives for a longer period of time and can increase the shelf-life of food materials.

Keywords: multi-layer microparticles, controlled release, active packaging.

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PHCMD-49

Cationic PCL Homo- and Block Copolymers for Antibacterial Applications

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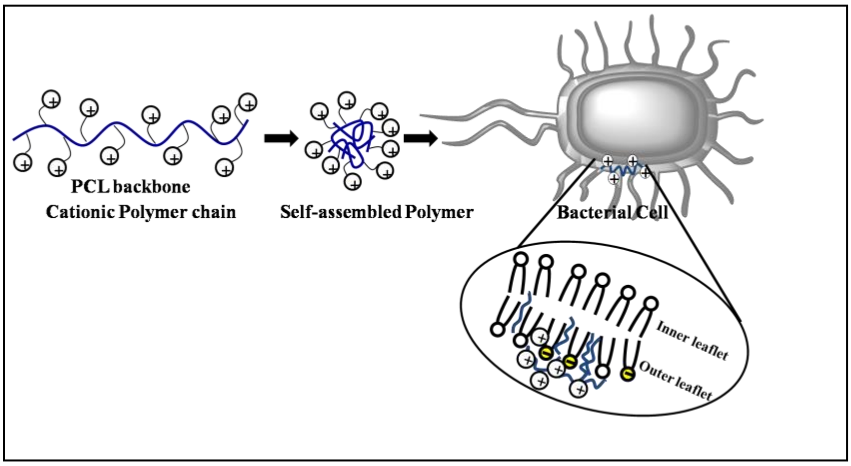
Abstract

Antimicrobial resistance (AMR) is an increasingly serious threat to global public health which includes the ever increasing infections caused by bacteria, parasites, viruses and fungi[4]. Polymeric nano-assemblies are emerging as important classes of biomaterials for antibacterial and antimicrobial applications[1]. This report is aimed to design and develop biodegradable homo and block cationic copolymers based on polycaprolactone[2-3] (PCL) and employ them for antibacterial activity. Multi-functional monomer was tailor-made with primary, tertiary and quaternary amine units and subjected to ring opening polymerization to yield well-defined cationic macromolecular architectures.[4] Monomer and polymers were characterized using ^{1}H NMR, ^{13}C NMR, and HRMS and the molecular weights of the polymers were determined by gel permeation chromatography (GPC). These cationic polymers exhibited very good solubility and self-assembled into 80-120 nm size nanoparticles. Water contact angle (WCA) of the cationic polymers were found to have WCA<50^o with respect to its hydrophilic nature. In vitro cytotoxicity studies showed that the polymeric nanoparticles were non-toxic in human cell lines. Antibacterial activity was investigated in *E. coli* (gram negative bacteria) and the polymer was found to show MIC values in the range of 5-10 μg/mL. The molecular weights of the cationic polymer were also varied by ROP route to study their role on the antibacterial activity. The cationic polymer acted through membrane-lytic mechanism in which bacterial killing is observed through electrostatic and hydrophobic interaction with the negatively charged bacterial membrane. Due to this non-specific mode of eradication, they show an edge over antibiotics in MDR bacteria. Confocal and Electron microscopy further reinstated the mechanism of action of these cationic polymeric scaffolds.



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PHCMD-50

pH Responsive Polysaccharide based Drug Delivery system

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Abstract

Polymer based drug delivery system (DDS), which comes with an added advantage of enhanced efficacy and reduced side effects are emerging as powerful therapeutics to combat cancer. Vesicles have an edge over a variety of self -assembled Nano scaffolds available because of their resemblance with the biological membranes which further enhances their cellular uptake due to like interactions. Polysaccharide based vesicles offer an exceptional ability of loading both hydrophobic and hydrophilic drugs owing to its bilayer structure that aids the delivery of more than one drug at specific cellular cites using both external and internal stimuli.[1,2] The pH of the endosomes and lysosomes typically varies in the range of 6.0–5.5 and a pH of 6.5 to 7.4 has been reported in breast tissue environment.[3] Delivery at tumour and cellular level can be orchestrated by tailoing the pH sensitive chemical linkage of the DDS. The present investigation reports dextran (polysaccharide) based pH responsive nano-vesicles which was contrutcuted using naturally occuring biodegradable resource called pentadecyl phenol (PDP) via imine linkage.[4] These structures self-assembled to form vesicles and are capable of loading a variety of cytotoxic drugs which can be released under acidic pH. The vesicular morphology was confirmed using AFM and DLS.

The fate of these nano-scaffolds can be futher monitored by tagging them with an aggregation induced emission (AIE) chromophore. For this purpose, Dextran vesicles were conjugated with carboxylix functionalized tetraphenylethene (TPE) derivatives and the resulting nano scaffold exhibited flourescence owning to the AIE properties of TPE molecule. Various dyes and cytotoxic drugs were then encapsulated and assessed for FRET, which in turn showed a clear dependance on pH. Curretly efforts have been put to exploit the tailr-made pH responsive fluorescent nano-vesicles for both thearpeauics and bio imaging purpose in cancer cells.

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PHCMD-51

Synthesis, characterization and drug delivery applications of copolymer blend membranes: Kinetics and mechanism of drug release profile

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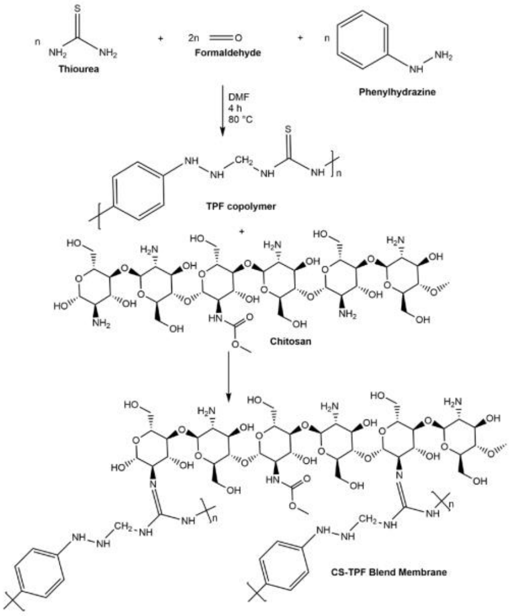
Abstract

A novel chitosan (CS) blended thiourea/phenylhydrazine/formaldehyde (CS-TPF) membranes of various compositions containing the metformin (MFN) drug were prepared. The membranes were subjected to elemental, SEM and FTIR analyses to investigate the empirical formula and weight and the presence of functional groups present in the matrix. The swelling behaviour, drug loading and release profile were extensively studied using UV-visible spectroscopy. The membranes exhibited a maximum swelling index 90.8% at 7h. The drug loading efficiency of the membrane was about 65.18%. The membranes showed a sustained drug release of around 75%. The higher percentage of chitosan content showed a remarkable improvement in swelling behaviour and leads to an effective drug delivery. Decrease in the polymer content and chitosan without the polymer does not enhance the drug loading and release profile. However, higher content of chitosan with lower concentration of polymer showed remarkable results of drug loading and release profile. The kinetics study shows that the drug release is in good agreement with the Ritger-Peppas and Higuchi model which follows swelling and non-Fickian diffusion controlled mechanism.

Keywords: Chitosan, copolymer, antidiabetic, drug delivery, kinetics



Scheme: 1 Reaction sequence of developed chitosan – copolymer membranes

PHCMD-52

Mechanistic and structural origins of the asymmetric barrier to prion-like cross-seeding between tau-3R and tau-4R

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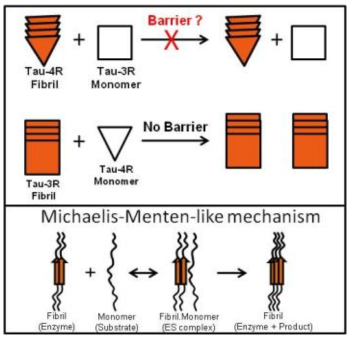
Abstract

Transmission of amyloid fibrils in the brain *via* a prion-like mechanism is a major feature of various neurodegenerative diseases. It is known that seeding barriers exist between different types (strains) of fibrils formed by any protein, but the mechanistic basis of the seeding barrier and propagation of fibrils is not well understood. Seeding is the only known way by which fibrils can spread within the brain from one cell to another: the seed induces the conformational transition of soluble monomer protein to fibril-like structure in every new cell reached. Structural compatibility between monomer and fibril regulates whether cross-seeding can occur, and also determines whether transmission of fibrils can occur across different species. A method to quantitatively analyze this compatibility is missing at present, and would provide detailed molecular level understanding of the cross-seeding mechanism. An understanding of the molecular mechanism of template-driven conversion of native soluble protein into structurally different type of fibrils will lead to a better understanding in general of the molecular basis of the seeding barrier in various neurodegenerative diseases, and will help in development of therapeutics for various protein aggregation diseases.

One example of a seeding barrier that exists between different types of fibrils, is the asymmetric seeding barrier between two isoforms of tau, tau-3R and 4R. Aggregates formed by tau-3R and tau-4R are associated with distinct tauopathies. In this study, the molecular mechanism of template-driven growth of the tau fibrils is shown to be describable by a simple Michaelis-Menten-like two-step model, in which monomers act like the substrate, and fibrils act like the enzyme. Modeling tau fibril growth to such a simple model provides a mechanistic rationale for the asymmetric seeding barrier which exists between two isoforms of the tau protein. Importantly, tau-4R (tau-K18) and 3R (tau-K19) are found to form structurally different fibrils: the structural core is more ordered in tau-K19 fibrils than in tau-K18 fibrils. These results provide a structural rationale for the asymmetric seeding barrier. Hence, the current study provides a detailed understanding of the molecular parameters which determine the pathological properties of amyloid fibrils.



PHCMD-53

Stimuli responsive polymer as an actuator for cellular signaling

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Abstract

Stimuli responsive polymers are of special interest for biological and biomedical applications such as biosensing, force clamps, cellular targeting and actuation and regenerative medicine [1-2]. Among different stimuli responsive polymers Poly (*N*-isopropylacrylamide) (PNIPAAm), a thermoresponsive polymer has been greatly explored for material science applications as well as in drug delivery systems [3]. PNIPAAm changes its physical properties according to surrounding temperature. Below or at the lower critical solution temperature (LCST) PNIPAAm is hydrophilic and hence soluble in aqueous environment, while above LCST it phase separates due to an entropically driven process, and falls out of solution [4]. We explored this thermoresponsive property of PNIPAAm to actuate cell signaling response mediated by a receptor tyrosine kinase- Epidermal growth factor receptor (EGFR) in cancer cells. When specifically targeted to EGFR, either with monoclonal antibodies or through binding to acceptor peptide expressed at amino terminal of the receptor, PNIPAAm could generate a rapid signaling response above LCST. Below LCST, though targeted to EGFR on cancer cells PNIPAAm did not induce any signalling response. Further analysis of PNIPAAm induced signaling actuation in cancer cells suggested the cellular response was comparable to canonical ligand-induced EGFR activation and signaling. PNIPAAm grafted proteins and specific targeting of PNIPAAm could be useful for non-invasive silencing or activation of cellular proteins. Similarly, it can find applications as a molecular remote control to actuate cell signaling.

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PHCMD-56

Fluonazole loaded polymeric nanoformulations for pH modulated effective antifungal activity

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Abstract

Human fungal pathogens such as *Candida*, *Aspergillus* and *Cryptococcus* cause high mortalities (> 40%) among patients having compromised immunity [1]. In India, *C. albicans*, *C. parapsilosis*, *C. glabrata*, *C. krusei*, and *C. tropicalis* are the dominant infective *Candida* species while *C. auris* is fast emerging as a drug resistant strain causing severe infection with high mortality [2]. The azole antifungal drugs, often used to treat fungal infections, are facing problems of resistance [1,2]. As the new drug antifungal pipeline lacks suitable candidates, the question arises that, can we can improve the antifungal efficacy of available drugs with newer approaches? Nanotechnology strategies for drug delivery improves the bioavailability, solubility, efficacy and reduces the toxicity [3]. In this study, natural and synthetic polymeric nanoparticles were synthesized for improved fluconazole delivery. Chitosan-PLGA nanoparticles (110nm) and chitosan-alginate nanoparticles (120nm) were prepared by solvent evaporation and ionotropic pre-gelation methods respectively. Drug loading on C-PLGA and C-ALG NPs was 80-84% (~ 8 weight %). The release kinetics displayed a burst release (50%) in 12 h for the nanoformulations at pH 4, associated with fungal cell wall milieu, whereas very poor release was observed at physiological pH 7. The nanoformulations showed a significant 6-fold reduction in the antifungal activity (MIC90 2.5 ug/ml) against *C. albicans* and *C. neoformans* as compared to the control. Post-antifungal effect showed no trailing growth as compared to the control. Thus, fluconazole polymer nanoformulations have great potential in increasing the efficacy of the drug and addressing the problem of resistance

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PHCMD-57

Selective Targeting of Breast Cancer Brain Metastases by Cisplatin Prodrug Nano-formulation

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Abstract

Breast cancer brain metastases (BCBMs) are common in patients with advanced breast cancer diseases. This is one of the breast cancer subtypes and its performance status are the major determinants of the course of the disease and survival time following a diagnosis of brain metastasis [1]. The unique challenges specific to the management of BCBMs includes, overcoming the blood-brain barrier (BBB) and resistance to conventional systemic therapies, as BCBMs typically occur in the pretreated patient population [2]. The development of new systemic and selective targeting nanoformulation based therapies for BCBMs has become increasingly important. In this work, we developed a cisplatin prodrug loaded brain accumulating nanoparticles to deliver the active drug cisplatin to the mitochondria of the cancer cells. Though the brain cell matrix is very complex and heterogeneous, we were able to show the selective targeting ability of these nanoparticles towards the BCBM cells over non-cancerous brain cells by crossing the BBB.

Acknowledgment: This work is supported by the Sylvester Comprehensive Cancer Center.

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PHCMD-58

Multifunctional Therapeutic Nanoparticles for Atherosclerosis

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Abstract

Macrophage derived foam cells contain high amount of choletserol which promote atheroma expansion and disruption of arterial plaques[1]. Human atherosclerotic plaques are predominantly M2 macrophages, enriched with macrophage mannose receptor (MMR) on their cell surface in addition to classically activated M1 macrophages[2]. High-density lipoprotein (HDL) exerts its protective property against atherosclerosis by removing cholesterol from lipid laden foam cells. Earlier, we have reported the development of synthetic polymeric hybrid nanoparticle (NP) using Food and Drug Administration approved poly(lactic-*co*-glycolic acid) (PLGA) having favorable organ distribution and anti-atherosclerotic property[3]. Herein, we describe the systematic design of a dual targeted synthetic therapeutic NP with both mitochondria and MMR-targeting surface functionalities loaded with a hydrophobic MRI contrast agent, Mito-magneto (MM), to achieve target-specific MRI contrast and therapeutic outcomes *in-vivo*. Macrophage targeting surface functionality on the HDL-NPs is expected to add another dimension to the construct by targeting and enabling better detection of plaques, and enhanced lipid reduction at the same time. In addition, the encapsulation of mitochondria acting coenzyme Q_{10} (CoQ_{10}) into the core of these NPs is extremely crucial to improve the cellular bioenergetics and reduction of oxidative stress in aortic smooth muscle cells for better prevention and treatment of heart related disease.

Acknowledgment: This work is supported by American Heart Association National Scientist Award and Sylvester Comprehensive Cancer Center.

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PHCMD-59

Synergistic Effect of Organocatalysts on the Ring-Opening Polymerization and its Application in Biocompatible Polyester Synthesis

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Abstract

The development of biocompatible materials for the medical applications from renewable resources have received significant attention.[1] Synthesis of polyesters generally employs transition metal catalysts, the residual metals are compromising the purity of the product. The polymer used for medical application should be free from metal contamination due to toxic effect of metal. Therefore, metal free approach of organocatalyst[2] provides the safe procedure for the synthesis of biocompatible polymer in medical applications. The aim of current study was to develop a general and simple procedure for synthesis of biocompatible Polylactic acid (PLA) using an organocatalysts, by controlled ring opening polymerization (ROP) of lactide monomer. In this study, the 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD) and 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) have been used. Present organocatalytic system contains electrophilic and nucleophilic centers that can activate the lactide monomer as well as the hydroxy end group simultaneously. The TBD catalyst activates lacide monomer whereas the DBU catalyst activates the nucleophilic centre of the hydroxy end group. The combination of two catalysts provide metal free biocompatible PLA throgh ROP of lactide in good yield.

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PHCMD-60

Surface Acetylated and Internally Quaternized Poly(propylene imine) Dendrimer as a Biocompatible Drug Carrier for Piroxicam

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Abstract

Surface acetylated and internally quaternized poly(propylene imine) (PPI) dendrimers with generation 2 and 3 viz., QPPI-NHAc (G2) and (G3) were synthesised and characterized. The drug carrying potential and biocompatible of the prepared drug carriers were evualuated using piroxicam (PXM, an anti-inflammatory drug) as a model drug with respect to aqueous solubility, *in vitro* release and cytotoxicity. Pharmacokinetic and biodistribution studies were also carried out in male albino wistar rats and the efficiency of modified dendrimer formulation was tested by carrageenan induced paw edema model. The observed results showed that the aqueous solubility of PXM significantly showed 50 fold increase in presence of QPPI-NHAc (G3) drug carrier as compared with its intrinsic solubility. The *in vitro* release of PXM was remarkably slow compared to parent dendrimers and thus proves their ability for sustained/delayed release of PXM. The cytotoxicity study in Vero cell line reveals that QPPI-NHAc (G2)/(G3) showed appreciable increase in cell viability and thus indicating the reduced cytotoxicity and improved biocompatibility. Biodistribution results reveal that in the case of QPPI-NHAc (G3)–PXM, 75% of inhibition was observed at the 4th h and this was maintained above 50% until the 8th h compared to plain PXM and proves that it was retained for longer time in the bio system. It is concluded that dendrimer–drug formulations not only enhanced the solubility but also controlled the delivery of bioactive material with localized action at the site of inflammation.

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PHCMD-61

Anion Selective Ion Channel Constructed from Self-Assembly of Bis(cholate)-Substituted Fumaramide

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Abstract

The self-assembled ion channel constructed from bis-cholate substituted fumaramide is reported. Such ion channel formation was favoured by intermolecular hydrogen bonding interactions among fumaramide molecules. The corresponding maleamide, which lacks sufficient intermolecular hydrogen bonding interactions, was less active. Fluorescence kinetics experiments and planar bilayer conductance measurements confirmed the selective chloride process through the fumaramide channel. Theoretical calculations were done to confirm the hydrogen bonding self-assembly of fumaramides and chloride recognition within the cavity.

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PHCMD-62

Interactions of Alpha Synuclein with Synthetic Single Stranded Oligonucleotides

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Abstract

The α-Synuclein protein aggregates were found to be the major components of Lewy bodies, the hallmarks of PD [1-3]. The structure of α-synuclein can be divided into three regions: the N-terminal region containing 1-60 aminoacids having four 11-amino acid imperfect repeats, the highly hydrophobic and amyloidogenic NAC region with 61-95 aminoacid residues and the highly acidic C-terminal region consisting of residues 96-140. The development of small molecules that specifically and efficiently inhibit the aggregation process is an effective therapeutic approach. In the present study, we have analysed the interactions of synthetic single stranded oligonucleotides with α-synuclein before and after fibril formation. The initial results suggest that the negatively charged oligonucleotide sequence could interact with the positively charged amino acids at the N-terminus of the α-synuclein, resulting in amyloid fibre disassembly. The fibrillation of α-synuclein under lab conditions is catalysed by the presence of preformed fibrils (seeds), which acts as nucleation sites for the formation of fibrils. This is known as nucleation dependent fibrillation. The uptake of the fibres into the human neuroblastoma cell line (SH-SY5Y) and the changes in the cell morphology are illustrated in figure 1. The cells in figure 1B show the uptake of aggregated protein Alpha synuclein (green) and the colocalisation (yellow) ofthe same with tyrosine hydroxylase (TH, red) present in the cytosol.

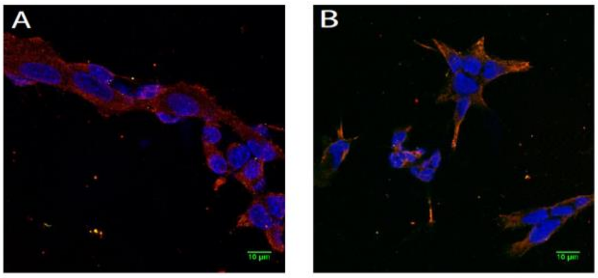

Figure 1: Uptake of Alphasynuclein protein fibrils by neuroblastoma cells. Antibody staining to detect pSER alphasynuclein (green), DAPI (nuclear stain, Blue) and TH (red), prove the uptake of α-synuclein in the cells.

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Theme –PREA

PREA-01

Assessing the Influence of Imidazolium Cations on Poly(arylene ether sulfone)s Block Copolymers for Anion Exchange Membranes

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Abstract

Polymer electrolyte membranes (PEM) for fuel cells are attractive choice to resolve the energy crisis and environmental problems because of their high energy density and efficiency. Nafion® (Dupont) is the most well-known and widely used as PEM material. The high cost of the membrane, use of precious metal catalyst and high degree of methanol crossover are the main drawbacks of the current PEM's. Nowadays, there has been a growing interest in alkaline fuel cells that utilize anion exchange membranes (AEM) as an electrolyte membrane because of higher fuel cell efficiency. The present AEM's suffer from poor chemical stability including cationic species and polymer backbone. The stability of various cationic head groups have been investigated such as quaternary ammonium, phosphonium, sulfonium, pyridinium, pyrolidiniium, piperazinium, guanidinium, morpholinium and imidazolium. Among the various cations examined, imidazolium has attracted extensive recognition due to its physiochemical properties, including electrochemical stability, non-flammability and high ionic conductivity. Due to its unique property, imidazolium is regarded as highly stable cation due to the presence π - conjugation over the heterocyclic ring. However, the positioning of imidazolium cations plays a significant role on the polymer backbone architecture. Herein, we prepared poly(arylene ether sulfone)s block copolymers containing imidazolium cations on main chain, side chain and comb-shaped structure. The synthetic routes, spectral analysis, thermomechanical, physical and electrochemical properties will be discussed.

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PREA-02

Synthesis and Properties of Novel Sulfonated Poly(oxyimide) (SPOI) - Membranes Bearing Quinoline Pendant Groups as Side Chains For PEM - Fuel Cell Applications

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Abstract

The most attractive and eco-friendly nature Proton exchange membrane fule cells (PEMFCs) are considered as powerful green energy sources for portable, stationary and tranport applications[1]. Till date, several Proton Exchange Membrane (PEMs) such as perfluoro sulfonic acid membranes (PFSAMs) namely, Nafion, Flemion, Aciplex, Dow membranes have been synthesized and extensivly used as PEMs[2]. However PFSAMs have two main limitations. The first one is their expensive cost. The second is that low proton conductivity at elevated temperature (> 100 ^{o} C) which emerged from evaporation of water[3]. Hence, in order to overcome these short comings associated with PFSA membranes considerable efforts have been explored to develop new cheaper alternative aromatic polyelectrolyte membranes including, sulfonated polyimides (SPIs), sulfonated poly (arylene ether) s (SPAEs) and sulfonated polybenzimidazoles (SPBIs) are the focus of current investigations on PEMs. Furthermore, several publications illustrated that the alternative polymer electrolytes with sulfonic acid groups on the pendants exhibited higher hydrolytic and oxidative stability than those with sulfonic acid groups attached directly to the polymer backbone. In the present work, we have design and successfully prepared novel aromatic diamine monomer with pendant sulfonic groups and synthesized a series of corresponding side chain type new sulfonated pol(oxyimides) (SPOIs) with different molar ratio. The structure of the resulted SPOI membranes have been characterized by ^{1}H-NMR, IR spectroscopic techniques. The membrane properties such as thermal, mechanical, crystallinity, morphology, solubility, oxidative, hydrolytic, IEC, water uptake, swelling ratio and proton conductivity were investigated in detailed. Finally, the resulted SPOI-xx membranes are expected to be promising PEM materials to be used for PEMFC application's.

Fig. 2. Photographs of SPOI -xx Membranes

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PREA-03

Electrical and Dielectric Studies on MnO_2 doped PVA/$NaClO_4$ Polymer Nanocomposite

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Abstract

In recent days, researchers are concentrated their attention towards polymeric materials, because of their wide applications mainly as optical, dielectric and insulating materials in solar cells, fuel cells, batteries, etc. The changes in polymer structure, composition and preparation conditions to be chosen to achieve the desired result of product as per the application requirement. In view of this, we have studied the effect of dopant Manganese Dioxide (MnO_2) on electrical, dielectric and structural properties of poly(vinylalcohol)(PVA)/sodium perchlorate ($NaClO_4$) nanocomposites. The pure and doped films of various concentrations of MnO_2 nanoparticle were prepared using solution casting method. The structural, thermal, electrical, dielectric and morphological properties of prepared polymer nanocomposite films were characterized using Fourier Transform Infra-Red (FTIR), X-ray Diffraction (XRD), UV-Visible, Fluorescence, DSC, TGA, Impedance Analyzer, AFM and SEM.

FTIR spectra were recorded in the wavenumber range of 400 to 4000 cm^{-1} and the results shows that the interactions are taken place between nanoparticle and polymer molecules. The UV-Visible spectra are recorded in the wavelength range 190 to 800 nm, which indicates the absorption bands around 270 nm assigned to $n \rightarrow \pi^*$ transition. The ionic conductivity increases as the concentration of dopant increases which is conformed from current-voltage (I-V) characteristic graph. The dielectric constant of the composites PVA/$NaClO_4$ decreases with increase in frequency with MnO_2 doping. The dielectric loss occurs due to inability of polarization process in electrolyte to follow the rate of change of oscillating applied electric field. The tensile strength, stiffness, Young's modulus reached maximum for 1wt% MnO_2 doped composites. This indicates that the film become more resistant to deformation. Morphological studies were carried out using the Atomic Force Microscope (AFM). Other characterizations such as XRD, SEM and TGA are in progress. In summary, the sodium perchlorate has modified the electrical and dielectric properties of the PVA/$NaClO_4$ polymer nanocomposite and with such modifications it may be used in electronic devices.

Acknowledgement: Authors are thankful to USIC, Karnatak University, Dharwad for providing experimental facilities and DST/SERB, Govt. of India for the research project (SB/EMEQ-089/2013). The authors are thankful to UGC, New Delhi for providing research grants under SAP-CAS Phase-II (F.530/9/CAS-II/2015 (SAP-I).

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PREA-04

2-Methyl-2-(N-(3-sulfopropyl)acrylamido)propane-1-sulfonic Acid Grafted Dehydrofluorinated Poly(vinylidene fluoride-co-hexafluoropropylene) based Cation Exchange Membrane for Electro-electrodialysis of HIx Mixture

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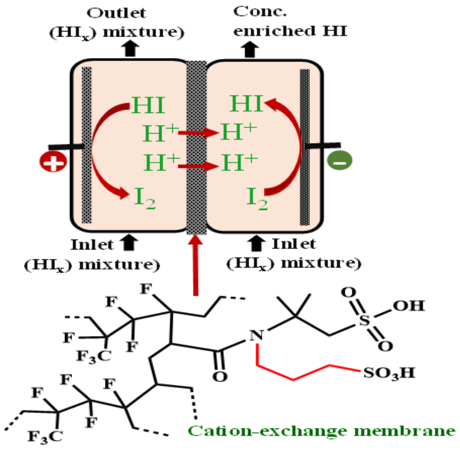
Abstract

To increase the HI (as H_2 source) concentration in the HI_x ($HI+I_2$) mixture produced by thermochemical water-splitting iodine-sulfur (Bunsen) process, electro-electrodialysis (EED) was performed using acid and oxidative resistant sulphonated copolymer cation exchange membrane (CEM). Reported CEM was prepared by chemical grafting of synthesized 2-methyl-2-(N-(3-sulfopropyl)acrylamido)propane-1-sulfonic acid (MSAPS) with dehydofluorinated poly(vinylidene fluoride-cohexafluoropropylene) (DPVDF) in presence of free radical initiator. Different PVSU membranes were characterized for their morphology, ion-exchange capacity (IEC), water uptake, conductivity, and stabilities (mechanical, chemical, and thermal) in compare with Nafion117 membrane. Most suitable PVSU-1.72 CEM membrane showed superior proton conductivity (5.15×10^{-2} S cm^{-1}) and IEC (1.72 m eq. g^{-1}) values in compare with different acid resistant CEMs reported in the literature. Further, PVSU-1.72 CEM consumed low electrical power (65.5 kJ/mol) in compare with Nafion 117 membrane (156.0 kJ/mol) during EED. EED process with PVSU-1.72 CEM showed close to 100% current efficiency (η^c and η^a), which demonstrates membrane suitability. The PVSU-1.72 consumes about 290 kJ mol^{-1}-H_2 energy to produce 1 mol H_2 by EED using energy, while Nafion117 membrane showed comparatively huge consumption (280.80 kJ mol^{-1}-H_2). These observations might be helpful for devising high performance EED process to increase the HI concentration as H_2 source.



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PREA-05

Development of Three Layer Geomembrane using Plasma Technology for Adverse Environment Applications.

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Abstract

The objective of this work was to determine surface properties of polymer surfaces after plasma treatment with the aim of further cytocompatibility tests. Geosynthetics are a family of plastic-based products that are helping us to protect the environment. These important products include geomembranes (liners). In most cases, geosynthetics are not only the most energy efficient and cost effective way of constructing infrastructure projects, but they simultaneously provide systems which helps to protect the environment. The plasma treated surface of HDPE material has provided the excellent adhesion strength with ply adhesion between HDPE layers and produced the same strength in 3 layers instead of currently used 5 layers. Therefore, this new approach is reducing the material quantity of geo-membrane with same or improved strength using environment friendly plasma treatment. Non-thermal plasma treatment leads to incorporation of polar groups into polymer surface and improves wettability which is advantageous in adhesion that inhibits delamitation of geomembrane. Moreover plasma treatment improves mechanical strength without changing the bulk properties. AFM analysis of the plasma-treated geomembrane shows that plasma treatment introduces greater roughness on the surface leading to the increased surface free energy.

Key Words: Geomembrane, Non-thermal Plasma, High Density Poly Ethylene.

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PREA-06

Flexible UV curable urethane films as polymer electrolyte in lithium-ion batteries

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Abstract

In this study, three kind of radiation curable polyurethane (PEG-UA) by isophorone diisocyanate and polyethylene glycol with different molecular weight (200, 400 and 1000 g/mol) was synthesized as a polymer electrolyte for lithium-ion batteries. PEG-UA structure was confirmed using FT-IR spectroscopy, thermal stability of the cured film was measured using thermal gravimetric analysis (TGA) and viscoelastic properties studied by dynamic mechanical *thermal* analysis (*DMTA*). Thermal stability of polymerized films provides acceptable safety for use at high temperatures (above 300 °C). According to the fact that proper temperature of battery life is 25-80 °C, it can be concluded that polymeric films produced can be used as polymer electrolyte in lithium-ion batteries. Also urethane acrylate film with polyethylene glycol with a molecular weight of 400 g/mol showed good mechanical strength and flexibility optimal that is a better option for use as a polymer electrolyte in lithium ion batteries. The results also showed that by increasing of molecular weight in the soft part of urethane acrylate, glass temperature transition reduces and freedom of chains increased. This increases the penetration and leads to further mobility of the lithium-ion polymer, and increases the ionic conductivity in the film. The results of the charge and discharge process are shown electrolyte polyurethane with PEG400 offers is very similar to a commercial separator film for lithium ion conduction.

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PREA-08

Alkali stable polymeric membrane with dual hydroxide ion conducting sites

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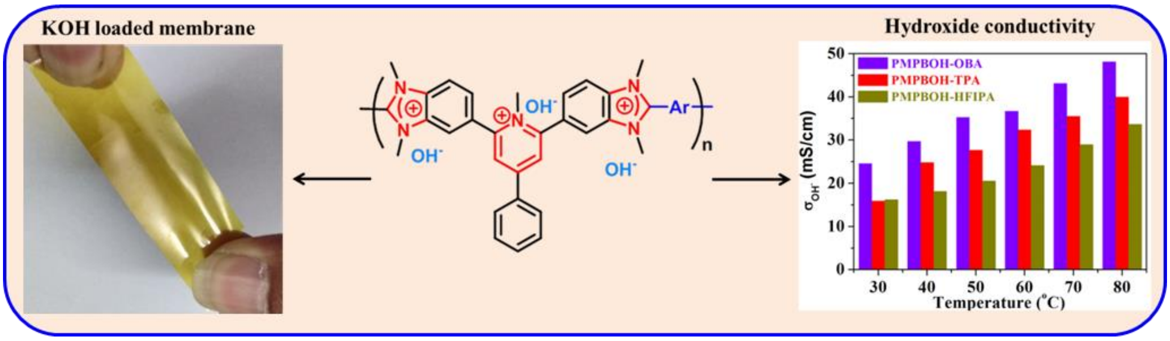
Two important concerns namely low hydroxide ion (OH^-) conductivity and weak alkaline stability of the polymeric membrane in regard to the development of alkaline anion exchange membranes (AAEMs) have been resolved in this work by synthesizing a series of pyridine bridged polybenzimidazole (Py-PBI) polymers consisting of dual OH^- conducting sites. Both the pyridine and imidazole functionalities of Py-PBI chains were quaternized by methylation to synthesize poly(methylated pyridinium benzimidazolium) iodide (PMPBI) which was readily converted to OH^- loaded AAEMs. The OH^- ion conductivities of KOH loaded PMPBI at 30 °C and 80 °C were found to be 24.6 and 48.1 mS/cm, respectively which are considerably higher than the most of the reported membranes. The simultaneous presence of dual OH^- ion conducting sites namely pyridinium and imidazolium in the polymer chain has been credited for very high ion conductivity of the AAEMs developed in this work. The current membranes showed excellent alkaline stability and mechanical robustness. The blocking of pyridinium α-positions in the PMPBI structure prevented irreversible oxidation of pyridinium into neutral pyridone which facilitated in improving alkaline stability.



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PREA-09

Conductive MoS_2 Quantum Dots/PANI Aerogel for High Energy Supercapaciator and Hydrogen Evolution Electrocatalyst

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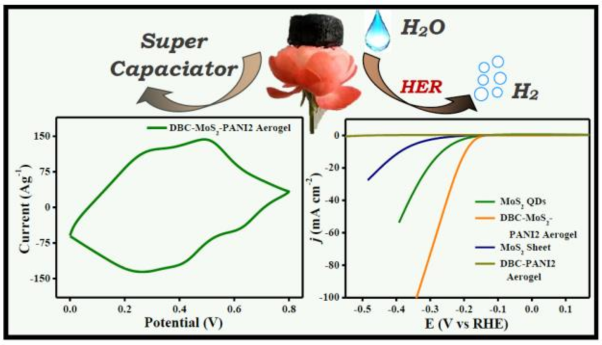
Abstract

The lower conductivity of MoS_2 sheet presents a huge barrier for the exploitation of its supercapacitor electrode application and electrocatalyst. To alleviate this difficulty, we have synthesized MoS_2 quantum dots (QDs) having greater quantity of catalytic edge sites by breaking up bulk MoS2 sheet using the solvent exfoliation technique. The synthesized MoS_2 QDs are embedded into polyaniline (PANI)-N,N-dibenzoyl-L-cystine (DBC) aerogel matrix for high energy supercapaciator and HER catalyst. Here, conductive PANI hydrogel are prepared by in situ polymerization of aniline where DBC acts as a gelator, dopant, and cross-linker. The DBC-PANI aerogel shows conductivity of 0.02 S/cm, specific capacitance of 278 F/g at a current density of 1A/g. The optimal MoS_2 QDs in DBC-PANI aeogel improves specific capacitance up to 796.2 F/g at 1A/g with superior rate capability (582 F/g at 20 A/g), and long cycling stability (86% after 5000 cycles). Also, the hybrid conductive DBC-MoS_2-PANI aerogels thus produced act as an efficient electrocatalyst showing lower HER overpotential in comparison to MoS_2 sheets and MoS_2 QDs. It exhibits an optimum overpotential value of 196 mV at 10 mA cm^{-2}, a favorable Tafel slope of 58 mV/dec, and an excellent electrocatalytic stability. Here, porous aerogel facilitate the fast diffusion of electrons/ions in the electrode, which can achieve high energy supercapaciator and the HER catalysis.



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PREA-10

Polyaniline Decorated MoO_2 Tube for Highly Efficient Flexible Solid State Symmetric Supercapacitor

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Abstract

For operation of different portable devices development of energy storage devices is a very imperative issue in our progressive society. Compare to other electrochemical energy storage devices supercapacitors have achieved a generous concern to the scientists as with its ultra-high power density and long cyclic stability it has prospect of reaching at battery like energy density. In that prospect herein we have grown polyaniline chain through MoO_2 hollow tube which exhibits excellent capacitive charge storage performance in both positive and negative potential region in H_2SO_4 electrolyte. The MoO_2/PANI nano composite possesses high areal capacity of 426.0 mC/cm^2 at 1 A g^{-1} current density with high retention of 61% at 20 A g^{-1}. Also it shows long cyclic stability of 91% after10000 cycles. Further the synthesized nano composite is utilised to fabricate all solid state flexible symmetric supercapacitor which holds very high energy density of 364 mW h/m^2 at 5100 mW/m^2 power density and delivers ultrahigh power density of 28140 mW/m^2 with energy density of 142 mW h/m^2 having energy efficiency of 89%.

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PREA-11

Improving Electrochemical Performance of Lithium-Sulfur Batteries using TiO_2 decorated Carbon Nanofibers

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Abstract

Lithium-Sulfur batteries (LSB) are regarded as the most promising candates for next generation electrical energy storage systems due to the low cost, nontoxic and naturally abundant sulfur based cathode, that endows the battery with a high theoretical specific capacity of 1675 mAh g^{-1} and energy density of 2600 Wh Kg^{-1}. However, the practical application of LSB's are hindered due to the electronically as well as ionically insulating nature of sulfur and it's final lithiation product, Li_2S, which results in low attainable capacity. Furthermore, the dissolution of lithium polysulfides in the liquid electrolyte causes loss of cathode material and lowers the cycle stability of LSB. To address these challenges, present study dealt the fabrication of TiO_2 decorated carbon nanofibers (TiO_2/CNF) with controlled properties of fiber diameter, surface area, interconnective porosity and conductivity. The TiO_2/CNFs are prepared by the carbonization of polyacrylonitrile(PAN)/Polystyrene (PS)/TiO_2 composite nanofibers fabricated by a facile electrospinning method. This unique fiber architecture further wrapped over the sulfur and used as the cathode active material for LSB. The fiber architecture is expected to provide rapid charge transfer pathway to improve the reaction kinetics and minimizes the diffusion of intermediate polysulfides via polar-polar interaction with TiO_2, which leads to the improvement in cycle stability of LSB. Moreover, the simple processing route used in the present study for the fabrication of cathode material is expected to open new avenues for practicle application of LSB.

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PREA-12

Polyelectrolyte as a Multifunctional Conductive Binder for High-Performance Lithium-Sulfur Batteries

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Abstract

Lithium-Sulfur batteries (LSBs) with high specific capacity are considered as one of the most promising next-generation energy storage devices. However, the shuttle effect of lithium polysulfide makes it difficult to commercialize stable LSB. Exploiting advanced binder systems is an effectual and simple strategy to improve the electrochemical performance and this method has the inherent advantage of not introducing additional weight and volume to the cell. Traditional PVDF binder fails to withstand mechanical instability of high S-loaded electrode. Moreover, the binder possesses poor affinity towards polysulfides, making it unsuitable for LSB. Hence, employing advanced binder systems is urgently required to fabricate high S-loaded electrodes.

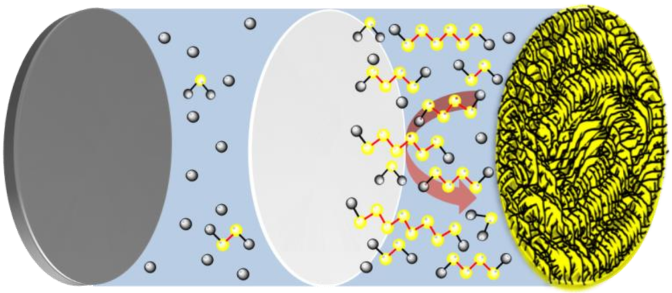

Figure 1. Schematic illustration of polysulfide trapping by PAMPS binder

In this work, we have explored the potential of a polyelectroyte, poly(2-acrylamido-2-methyl-1-propanesulfonic acid) (PAMPS) as multi-functional binder. Compared to the conventional PVDF binder, this PAMPS binder has uniform dispersion, higher adhesion strength and and stronger chemical interaction with polysulfides, which helps to keep the polysulfides within the cathode region, thereby improving the the capacity and cycle performance of the battery. As a result, sulfur electrode with PAMPS binder delivered a high initial discharge capacity of 1293.3 mAh g^{-1} and capacity retention up to 83% after 100 cycles at 0.1C with sulfur content of 70 wt% in the cathode, which are significant improvements compared with the corresponding LSBs with a conventional PVDF binder. Additionally, preparation of the cathode material with this new binder uses water as the solvent, avoiding the use of toxic organic solvents such as N-Methyl-2-pyrrolidone (NMP).

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PREA-13

Integrating Polymer Electrolytes with $Li_4Ti_5O_{12}$: A Safer All-Solid Li-Ion Battery

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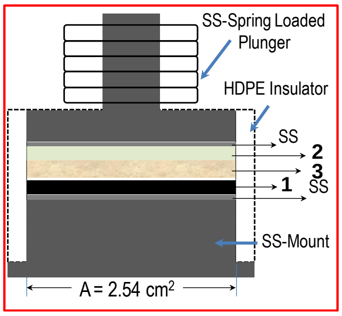
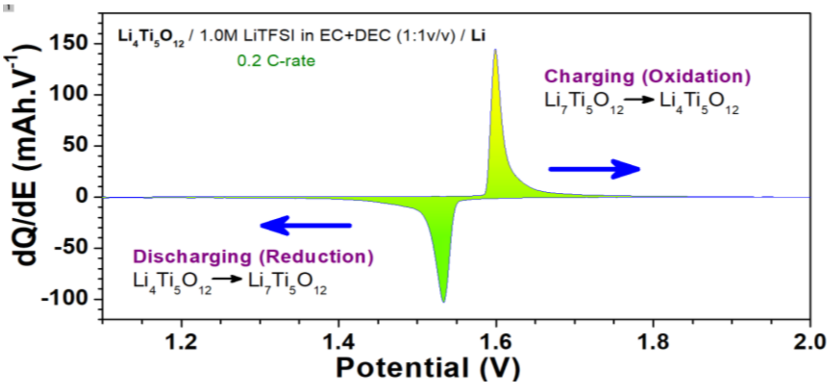
Abstract

Rechargeable Li-ion batteries although efficiently power small portable devices, implementation in electric vehicle mobility to assuage environmental concerns demands batteries possessing higher power densities and capacities while being compact and safer. Recent research is hence focused towards developing battery components that can sustain high charge-discharge rates while addressing the safety issues.

It is now apparent that *nanostructured materials* with their envisaged applications would soon mature to become the major driver in Li-ion battery research. In our recent research efforts, we have focused on nanostructured lithium titanate ($Li_4Ti_5O_{12}$) as an alternate anode material. Effect of synthesis parameters on phase, size, and morphology is expected to have a huge impact on the capacity, power density, performance and lifetime of the devices. Concurrently, the prospect of integrating polymers as electrolyte matrices to achieve safe, *all-solid state devices* are projected to address multiple issues related to device performance, however, factors such as relatively low ionic conductivity, sluggish kinetics and the high interfacial electrode-electrolyte impedances are still major roadblocks. In recent years, our group has reported some key breakthroughs achieved in the area of polymer electrolytes.





Integrating the two strategies, we have made an endeavour to pair the nanostructured $Li_4Ti_5O_{12}$ as active electrodes with a polymer electrolyte system, evaluate the redox performance and demonstrate device feasibility. Certain bottlenecks still exists; nevertheless, we were successful in overcoming some of the major challenges relating to interfacial resistances and achieve a battery operating at ambient temperatures. This report will provide a brief overview and summarize our recent findings.

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PREA-14

Synthesis and Characterization of Fused 5,11-dihydrothieno- [3',2':5,6]indolo[3,2-b]thieno[3,2-f]indole Containing Polymers

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Abstract

In this work, a series of new 5,11-dihydrothieno[3',2':5,6]indolo[3,2-b]thieno[3,2-f]indole based polymers were synthesis with the insertion of various alkyl and donor groups for used as an active p-channel semiconductor in organic field-effect transistors (OFETs).[1] The obtaining polymers showed small optical band gaps pooled with low-lying HOMO energy levels and established semiconducting activities in OFETs. OFETs were exhibited (Figure 1)high hole mobility up to 1.4 x 10^{-2} – 2.5 x 10^{-2} $cm^2V^{-1}s^{-1}$ and high on/off ratio up to 10^4 for series.[2] These materials were functioning as hole-transporting materials (HTMs) in fabricating mesoporous $TiO_2/CH_3NH_3PbI_3$/HTMs/Ag solar cells device with power conversion efficiency up to 12.6% with an active area of 1.74 cm^2.

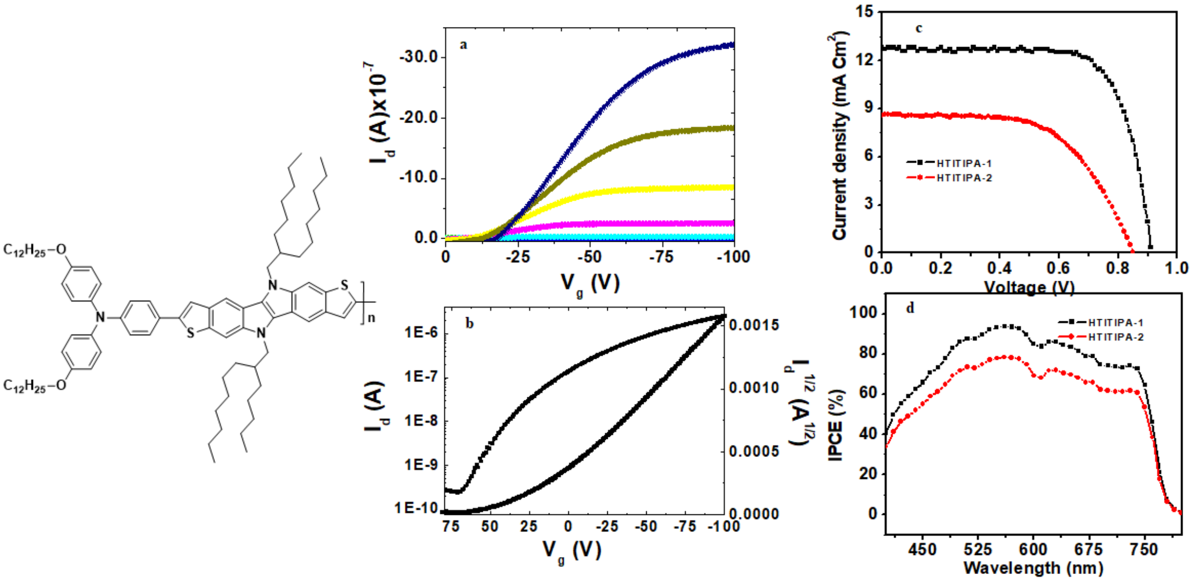

Figure 1 Output (top) and transfer (bottom) features for HTITIPA-1 in bottom gate and bottom contact (a, b) and power conversion efficiency and IPCE curves (c, d) device structure

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PREA-15

Generating PPy Nanotubes in Microwave for Energy Storage

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Abstract

We report a direct solution combustion microwave-assisted route for generating PPy nanotubes as an electrode material for supercapacitor cells. PPy well-known as an intrinsic conducting polymer finds use in electrochemical sensors, energy storage devices, microwave shielding, organic solar cells, electroactuators, electronic devices etc. due to its high conductivity, good thermal & environmental stability, redox properties and low toxicity [1]. In particular, synthesis of one-dimensional (1D) PPy nanostructures like nanowires, nanofibers, nanotubes etc., is of great significance for charge storage applications and has widely been explored using different protocols [2]. Microwave irradiation methods are not only simple and encompass the advantage of reduced reaction durations, but also suppress side reactions which improves the reproducibility [3,4]. Nanotubular conformation for PPy is verified by SEM & TEM, besides the structural integrity is supported by XRD & IR characterizations. The PPy nanotubes exhibit high specific capacitance (315 F g^{-1} at scan rate 5 mV s^{-1}) within a potential window -0.3 to 0.6 V as determined using three electrode assembly in 1 M KCl electrolyte. The research work bestows promising pseudocapacitive material for energy storage devices and opens up new frontiers in the field of 'polymer chemistry' that deals with the development of methods for synthesizing nanostructures of polymers.

Keywords: polypyrrole; nanotubes; solution combustion microwave synthesis; pseudocapacitance

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PREA-16

Semiconducting Properties of Modified Styrene- Maleic Anhydride Nanocomposites

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Abstract

Designing new semiconductor materials includes efficient tuning of electronic and optical band gaps and the charge-carrier transport properties of the material involved. Organic Polymers with extended pi-electron system serves as good candidates for building up a semiconducting material. Addition of heteroatoms to the matrix further provides the advantage of extra electronic mobility in the form of lone pair of electrons. The semiconducting properties experience a perceptible increase on the inclusion of nanoparticles. The semiconductor-electrolyte interface, the type of semiconductor and its charge-carrier densities can be studied in detail using the Mott-Schottky analysis. In the present work, a thiadiazole moiety is hooked on to Styrene-Maleic Anhydride copolymer. The incorporation of ZnO nanoparticles were effectively carried out on the polymer matrix. Spectral and thermal analysis was carried out on the samples. Electrochemical impedance data and the subsequent linear fit were performed. The impedance analysis was useful in obtaining the Mott-Schottky plot and it helped in confirming the semiconducting nature of the nanocomposites and the type of semiconductor formulated.

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PREA-17

Polymer-ZnO Nanocomposites as Electrodes for Supercapacitor Applications

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Abstract

Polyimides are thermally stable polymers with good chemical resistance that are often based on solid aromatic backbones. Polyimides are used as cathode materials for rechargeable lithium batteries. A polyimide is synthesized using 4, 4' diphenyl diamine methane (DDM) and poly(styrene-*co*-maleic anhydrides) (SMA). The modified styrene-*co*-maleic anhydride is taken as the matrix into which ZnO nanoparticles are incorporated. This polyimide nanocomposite was characterized by spectral and thermal analysis. The surface morphology was studied using Scanning Electron Microscopy (SEM). Supercapacitor electrodes have been fabricated using different composition of the Polymer Nanocomposite-Activated Carbon (AC)-Binder. Electrochemical properties of the fabricated composites has been studied using Electrochemical Impedance Spectroscopy, Cyclic Voltammetry (CV) and *Chronopotentiometry* (CP) techniques using 1 M KOH as the electrolyte. The cycling stability and the charge-discharge time were noted to establish its applicability as an efficient supercapacitor.

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PREA-18

Synthesis & Characterization of Polymer Microencapsulated Fatty Acid as Phase Change Materials (PCMs) for Thermal Energy Storage (TES) Applications: A Renewable Approach

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Abstract

Currently, efforts in search of renewable and sustainable energy sources are hiked over the past few decades. For regulating energy consumption, storage of energy is a present day challenge to the technologists. Phase Change Materials (PCMs) are well known for Thermal Energy Storage (TES) applications not only bridges the gap between supply and demand but also improves the performance and efficiency of energy systems and plays a vital role in conserving the energy. PCMs are promising for use in energy storage and delivery since they can store or release thermal energy at nearly constant temperature and provide a large thermal storage capacity during phase transformation. Microencapsulated Phase Change Materials (MEPCMs) are little containers/capsules made of polymers as shell containing PCMs inside as core to avoid PCMs from leakage during the phase change and reducing the reactivity of the PCMs with external environment in their applications. The present study focuses on preparation and thermal characterization of Polymethyl Methacrylate (PMMA) microcapsules enclosing fatty acid (Lauric Acid) as Phase Change Material (PCM) for Thermal Energy Storage formed by Suspension Polymerization Method. Fourier Transformed Infrared spectroscopy (FT-IR) was used to perform the chemical characterization of the shell microcapsules. Thermal properties and thermal stability of prepared MEPCMs were determined using Differential Scanning Calorimetry (DSC) and Thermal Gravimetric Analysis (TGA). Micro PCMs can be used for thermal energy storage and thermal regulatory applications like solar energy utilization, thermal insulation, energy conservation in buildings, thermal regulating textile materials etc.

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PREA-19

Efficient Nanogenerator for Energy Harvesting Using Processed Poly(vinylidene fluoride)

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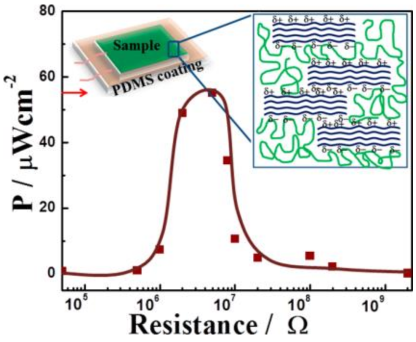
Abstract

Poly(vinylidene fluoride) (PVDF) is processed at high temperature to generate energy from waste mechanical energy. The piezoelectric β-phase has been induced through uniaxial elongation of polymer films at high temperature. The extent of β-phase has been confirmed from a deconvoluted XRD pattern, found to be ~75% of the electroactive phase, and able to demonstrate high piezoelectric effect as evident from the measured piezoelectric coefficient of −30 pC/N after a suitably processed and poled specimen. Bulk morphology and spectroscopic studies support the structural alteration. Following the direct piezoelectric effect, energy harvesting devices have been fabricated which show very high power output of 55.2 μW/cm^2 using the processed and poled specimen. The use of nanogenerator in practical applications also been shown by measuring output power by various human motions. The nanogenerator is also able to light up the LEDs. Thus, robust and easily processable polymeric material having very high energy conversion efficiency is demonstrated which is sufficient to power miniaturized devices.



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PREA-20

Enhanced piezoelectric response in nanoclay induced electrospun PVDF nanofibers for energy harvesting applications

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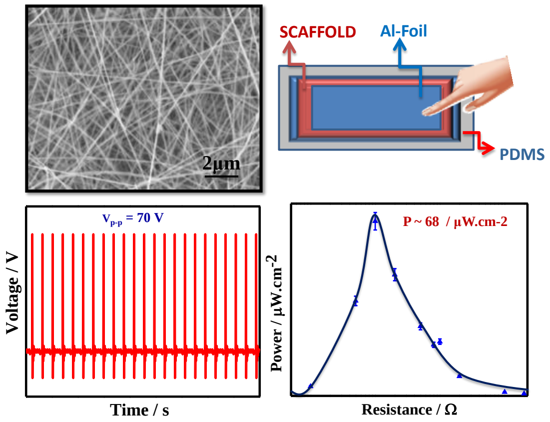
Abstract

Electrospun nanofibers of poly (vinylidene fluoride) have been designed in the template form on top of two dimensional modified nanoclay for energy harvesting applications. Nanoclay has been used at different concentration with the polymer matrix to examine the alteration in structure and morphology. Nearly 90% of electroactive piezo-phase has been stabilized in presence of nanoclay through optimized electrospinning. Nanohybrid is found to be stiffer and tougher than pure polymer which favoured the flexibility of the nanogenerator. Power generation up to 100ms has been able to conceive through the unimorph of the nanohybrid which was higher as compared to the pristine polymer. The electrospun nanohybrids were fabricated into a device to observe the electromechanical response produced via different human movement. Considerable voltage and power output has been obtained from the different mode of human movement e.g. finger tapping, bending, twisting, walking and foot tapping. The maximum voltage and power of 70 V and 68.1 μWcm^{-2} has been recorded through finger tapping. The processed nanohybrid is capable to transform the waste mechanical energy to useful energy which can be understood through the charge separation mechanism in template system.



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PREA-21

Cardo Fluorene based Semifluorinated Polyamides : Gas Transport Properties and Molecular Dynamics Simulations

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Abstract

Researches on polymer membranes are of great technological interest for a range of molecular separations due to its technical advantages. The advancement of the membrane based separation technology depends on the availability of the superior membrane materials with high gas permeability and gas selectivity.[1,2] Here, a series of new processable polyamide (PA) membranes were prepared by long-branched chain containing cardo fluorene diamine monomer with four commercially available diacids via conventional polycondensation method.[3] The synthesized PAs showed high thermal stability (up to 365 °C in air, for 10% weight loss) and tensile strength up to 85 MPa. The permeability of four different gases CH_4, N_2, O_2 and CO_2 through these PA membranes was investigated at 35 °C under a defined applied upstream pressure. PAs showed high gas permeability (P_{CO2} up to 142 and P_{O2} up to 18 barrer) and high permselectivity (P_{CO2}/P_{CH4} up to 60 and P_{O2}/P_{N2} up to 7.6). The gas transport properties have been correlated with the polymer structures with respect to their experimental and simulated molecular modelling, fractional free volume (FFV), size-distribution function of free-volume and intersegmental distance (d_{sp}).[4] Gas diffusivity is supported by extensive studies of individual penetrant molecule trajectories (fig. 1) and mean-square displacements in a polymer matrix.

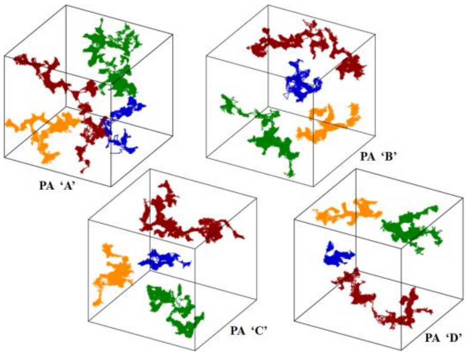

Fig. 1. Trajectories of gas molecules in a PAs matrix
(O_2 = red, CO_2 = green, N_2 = orange, CH_4 = blue)

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PREA-24

Continuous Flow Synthesis of High Performance n-type Polymers based on Naphthalene and Perylene diimide

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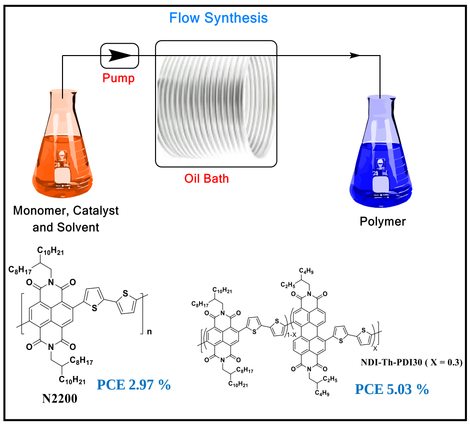
Abstract

Polyera Activink or N2200 or P(NDI-2OD-T2) is an n-type polymer that has found wide application in the field of all-polymer solar cells (PSCs) and OFET because of its desirable semiconducting and photo-physical properties.[1] This polymer exhibits good solution processability, high crystalline nature and broad absorption in IR and near visible region. The properties of P(NDI-2OD-T2) polymer were tuned by random incorporation of PDI as a co-acceptor. [2] Generally these polymers were synthesized via Stille polycondensation reaction in batch reactors. The batch-to-batch variability in molecular weight characteristics developed by batch process is a hindrance to reproducible device performance in photovoltaic applications. The continuous flow method of developing conjugated polymers affords a reproducible and scalable method to develop high performance materials that can exhibit enhanced efficiencies in photovoltaic device applications. [3] P(NDI-2OD-T2) was synthesized in the lab by batch process and varying amounts of the higher analogue perylene diimide was introduced into the polymer, which resulted in enhanced all-polymer solar cell device performance due to better blend morphology. Here we report the synthesis of these polymers (P(NDI-2OD-T2) and NDI-Th-PDI-30) by stille polymerization by continuous flow process. P(NDI-2OD-T2) showed very high molecular weight Mn=64900, Mw=585000, PDI=9.01 compared to batch synthesize one of Mn=26400, PDI=5.7. Further optimization is ongoing.



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PREA-26

Fabrication of low cost Functionalized PVDF membrane for fuel cell applications

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Abstract

The nanochannels are created in polymer and its nanohybrid by bombarding particle radiation of high energy (swift heavy ions) (SHI). The pore dimensions of the nanochannels are varied from 80 to 100 nm. The wall of nanochannels is grafted with the conducting monomer using the free radicals caused by SHI followed by their functionalization. Organically modified nanoclay enhances the piezoelectric β-phase in polymer and their extent gets enhanced after irradiation, grafting and functionalization leading to a better material for different electrical applications. Functionalization of membrane and its relevant properties has been measured by different spectroscopic techniques such as NMR, IR, UV-visible, and water uptake. The structural variation after the grafting and functionalization measured by the XRD pattern. The Current-voltage (I-V) characteristic of functionalized nanochannels is studied through the parameter analyzer of the bulk film in the semiconducting range against the insulating nature of the neat polymer. IV characteristic of the membrane exhibits superior conduction in functionalized nanohybrid. Proton conductivity of the functionalized nanohybrid is 4.22×10^{-2} S cm^{-1} and neat polymer is 4.0×10^{-2} S cm^{-1} at 25^0C, while methanol permeability drastically reduces indicating higher values of the selective parameter (SP) of the developed membrane as compared to Nafion117. Membrane electrode assembly (MEA) studies of functionalized nanohybrid show superior efficiency as compared to standard nafion117 membrane. Above functionalized membrane also sutiable for radioactive waste sepration in nuclear power plants.

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PREA-27

Cross-Linked Polybenzimidazole as Proton Exchange Membrane

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Abstract

Water-free, proton-conducting polymer electrolytes have been attracting attention because of their possible application as fuel cell membranes at intermediate temperature (100 to 200 °C). Covalently cross-linked polymer membranes have been developed from pyridine bridged oxy-polybenzimidazole (Py-OPBI) and brominated polyphenylene oxide (BrPPO). The crosslinked Py-OPBI-BrPPO membranes exhibited better solubility, stability up to 85% in phosphoric acid, improved conductivity ,high resistance to swelling in concentrated phosphoric acid solutions and excellent stability towards the radical oxidation. The acid-doped membranes displaced improved mechanical strength compared to pristine Py-OPBI. The superior characteristics of the cross-linked PyOPBI membranes absorbed higher acid and hence showed higher proton conductivity (0.12 S/cm^{-1}) as compared to pristine Py-OPBI (0.001 S/cm)

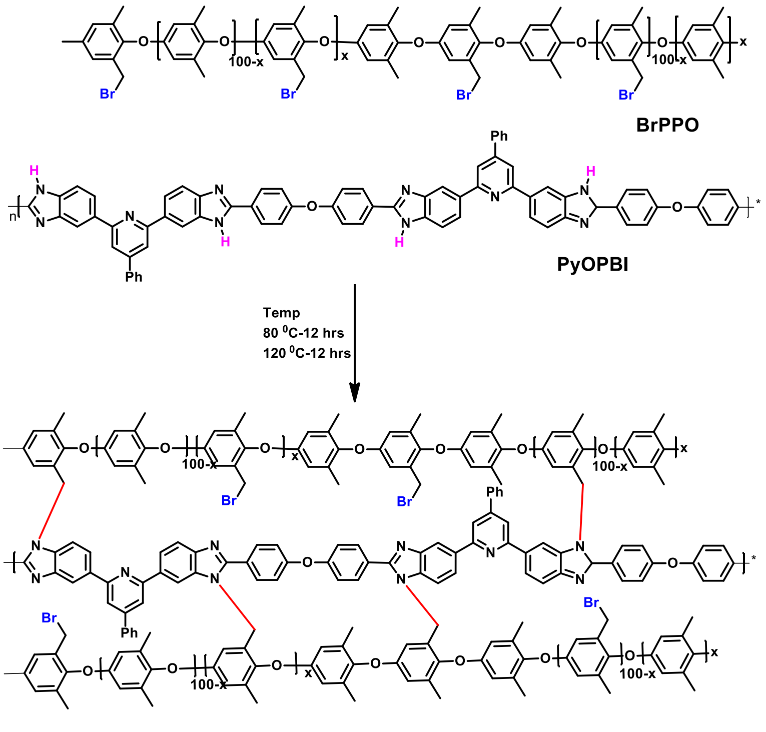

Fig: Development of cross-linked PEM from PBI and PPO

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PREA-28

Sulfonated polybenzimidazole homopolymer as proton exchange membrane.

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Abstract

Polybenzimidazoles are promising materials for the use as proton exchange membranes (PEM) in fuel cell. Here we have synthesised sulfonated polybenzimidazole homopolymer by monomer modification. The main motto for introducing sulfonic group in to the polymeric backbone is that, it can be used both for low temperature fuel cell, where water acts as conducting media and also for high temperature fuel performance, where phosphoric acid act as electrolytic media. The polymer structure was confirmed by NMR and FTIR analysis. The thermal stability and mechanical stability was analysed by TGA, DMA and UTM, respectively. Microbial fuel cell (MFC) study was performed where water doped membrane was used as PEM and the result showed comparatively higher power density than the Nafion. For high temperature PEM application, the membrane was doped in phosphoric acid (PA). It was observed that SO3Na form of membrane display higher PA doping and conductivity as compared to SO3H form of membrane. The sulfonic group which is attached to the polymer in the SO3H form of membrane is not helping in proton conductivity at the same time it is deactivating the imidazole group for up taking more acid. This is because SO3H group is acidic and imidazole group is basic in nature. Both are deactivating each others contributions for helping in proton conductivity. But in SO3Na form there is no interaction between imidazole group and sulfonic group. Hence the basicity of the imidazole group is unaltered. So it is absorbing more phosphoric acid as compared to SO3H form and simultaneously showing more conductivity.

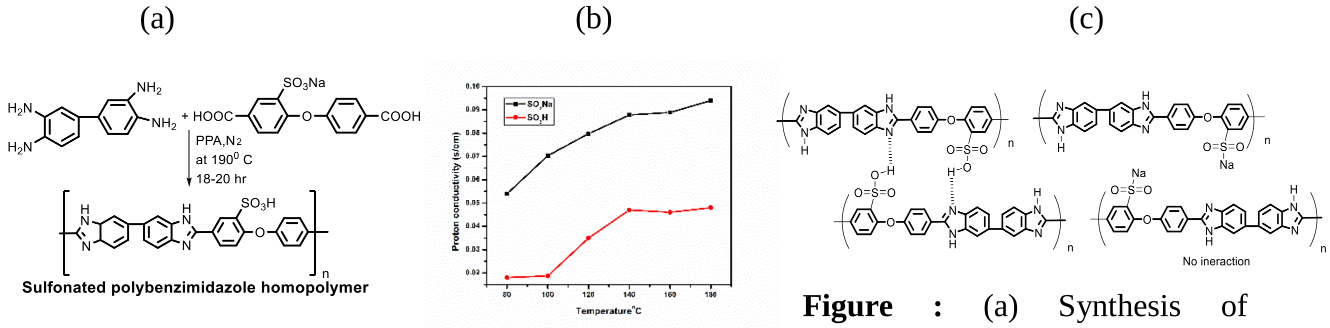

Figure : (a) Synthesis of sulfonated polybenzimidazole, (b) conductivity of SO3Na and SO3H form of membrane, (c) possible interaction between sulfonic group and benzimidazole group

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PREA-30

Multi-Chromophoric Truxene Derivatives to Realize Solution Processable Blue Emitting Materials: A Combined Experimental and Computational Study

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Abstract

One-pot modified Debus-Radziszewski reaction was used to design and synthesize truxene derived novel blue-emitting materials bearing phenanthroimidazole substituents. The materials were prepared non-catalytically, under ambient conditions using a triamino based derivative of truxene as a key precursor in good yields. The positions 5,5',10,10',15,15'- of the truxene were alkylated to render solubility to the molecules, making the materials solution processable. The substituted phenanthroimidazole moieties were introduced at the 2,7,12-positions of truxene to synthesize the target molecules. The materials were prepared by varying the phenyl group attached at the C2 position of phenanthroimidazole moiety, designated as T_1 for phenyl, T_2 for 4-methoxyphenyl and T_3 for 4-cyanophenyl substituent. From the photophysical studies, T_3 was found to have charge transfer character dominant in its excited state. Also, the materials exhibited photoluminescence quantum yield as high as 0.83. The optimized geometries obtained from the computational studies revealed that the molecules are highly twisted, with dihedral angles of ~75°. The HOMO-LUMO distributions were found to be well separated showing the bipolar character of the compounds. The emission spectra in the solid state gave maxima at 402 nm for T_1, 412 nm for T_2 and 450 nm for T_3. The materials were thus found to be emitting in the blue region of the visible spectrum. The TCSPC and TRPL studies were done to explore further the excited states of the molecules, wherein radiative pathways were found to be dominant. The TDDFT computations were done to obtain the vertical transitions energies of the possible excitations, their respective contributions and the oscillator strength.

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PREA-31

Intrinsically Stretchable and Self-Healable Semiconducting Polymer Based on Urethane Side Chain Engineering

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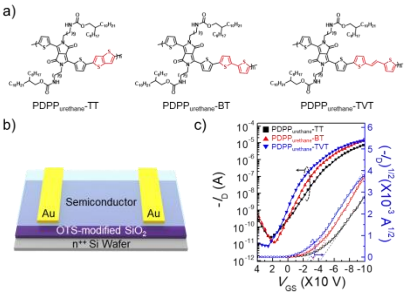
Abstract

Stretchable electronics with high electronic performance and mechanical stability has highly been desired for the application area of the next-generation electronics.[1-4] Mostly, the fabrication of stretchable semiconducting devices have been carried out based on the materials which could endure the mechanical deformation[14] or introduction of the blended composite system of intrinsically not stretchable semiconductors and elastomeric polymers. However, these approaches typically have unavoidable limits such as low electrical performance and structural complexity impeding the fabrication of integrated circuitry. Herein, we present the intrinsically stretchable and self-healable DPP-based semiconducting polymers with urethane-containing side chains. The urethane-containing side chains provide dynamic bonding moieties, facilitating the stress dissipation of the polymer thin films during the mechanical deformations. The mechanical and electrical characteristics of the DPP-based polymers with urethane side chains have investigated by varying the spacers in the backbone of the DPP-based polymers; namely, $\text{PDPP}_{\text{urethane}}$ derivatives. The thin films of $\text{PDPP}_{\text{urethane}}$ derivatives showed excellent stretchability up to 100% of external strain without degradation of electrical performance confirmed by utilizing an organic field-effect transistor (OFET) platform. Furthermore, the self-healing properties of $\text{PDPP}_{\text{urethane}}$derivatives have also been investigated to confirm the effects of the dynamic H-bonding from urethane side chains, showing both the phase reconnection of polymer thin films and the recovered electrical properties after post-treatment. Our works reported herein provide a viable approachfor the realization of stretchable and self-healable electronics based on intrinsically stretchable semiconducting polymers based on a novel side chain engineering.



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PREA-33

Synthesis of Graphene from Biowaste and Graphene-Polymeric hybrid materials for CO_2 Capture

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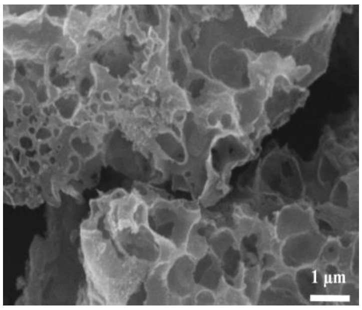
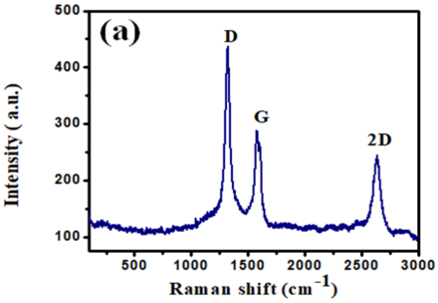
Abstract

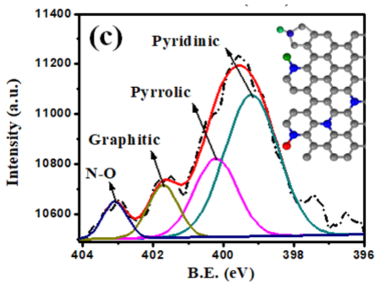
Anthropogenic emissions of CO_2 concentrations are increasing rapidly in the atmosphere, hence, it is very essential for the efficient and selective capture of CO_2 from fossil-fuelled power plants. Flue gas also contains moisture which affects the adsorption process in the recently developed materials. Therefore, there is a quest worldwide to develop new polymeric material having hydrophobic nature, highly thermally stable during the CO_2 capture and bead-like structure for packing. Nowadays, graphene is receiving tremendous attention in the CO_2 capture due to its unique molecular structure and exceptional properties. However, the major disadvantages are cost and use of toxic solvents during preparation. Therefore, the scientific challenge is to adopt the eco-friendly method in order to overcome these problems. Here, we highlight the preparation of graphene from biowaste (waste leaves) and its incorporation during *in situ* polymerizations of Styrene-Divinyl Benzene (SDBC) to obtain Graphene-SDBC hybrid material for CO_2 capture. Chemical activation and carbonization of biowaste were carried out at different temperatures i.e. 500, 600, 700 and 800˚C respectively. *In situ* suspension polymerization of styrene-divinyl benzene was carried out in presence of prepared graphene to obtain Graphene-SDBC hybrid material. These materials were characterized using DSC, DLS, WAX-XRD, FESEM, BET, RAMAN and XPS. The results showed different crystallinities as well as morphologies at various heat treatments (temperature ranging from 500 to 800˚ C). The results showed that the naturally doped nitrogen in graphene in hydrophobic polymeric spherical hybrid beads. These hybrid materials also showed a high surface area, optimum pore volume for CO_2 capture.



SEM image of graphene (700 ˚C)



Raman Shift of graphene (700 ˚C)



XPS results of graphene(700 ˚C)

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PREA-34

Organic Acid Doped Polyaniline Nanotubes as Electrode Materials

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Abstract

Among the conducting polymer family, polyaniline (PANI) is the popular conducting polymer due to its easy of synthesis, environmental stability, its profound reversible electronic structure conversion ability (due to charge transfer doping/ dedoping) and associated optical and electrical properties that make PANI attractive as an electronic material for potential use in a variety of applications. Making of PANI nanotube is much more attracting over the bulk PANI as it generates much controlled architectures as the available surface area required for enhanced performances. Herein, template-free method have been developed to make easy preparation process that is capable of producing more amount of pure and uniform PANI nanotubes with various organic acids (like benzene tetracarboxylic acid (BTCA), benzene tri-carboxylic acid (BTA) and terephthalic acid (TA)) upon the polymerization of aniline in presence of APS (ammonium persulphate). Subsequently, these composites have been utilized as electrode materials for capacitive measurement. Morphological investigations reveal the formation of nanotubular shape of PANI as observed under FESEM study (Figure 1a). Spectral characterizations would be done by UV-Vis and XRD studies. Capacitive behaviour would be explored by cyclic voltammetry and galvanic charge discharge (GCD, Figure 1b) techniques to judge the suitability of these composites as energy storage materials.

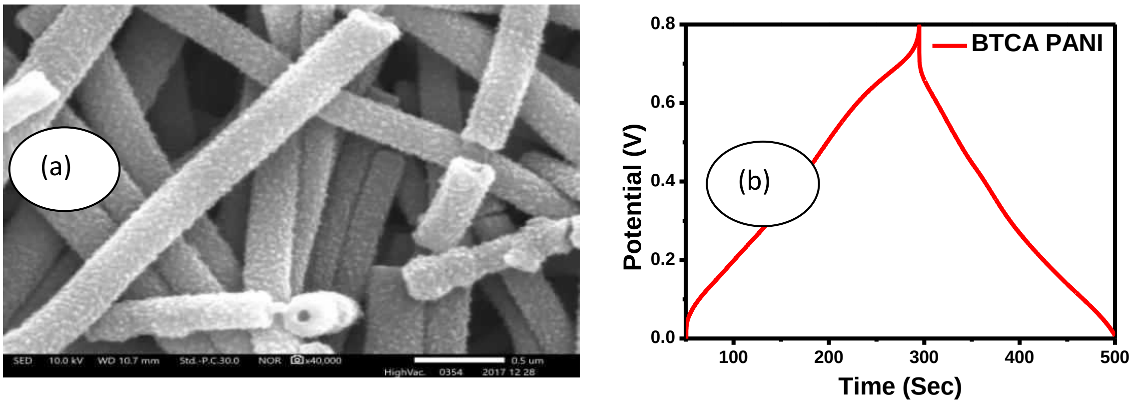

Figure 1: Representative (a) FESEM images and (b) GCD data of BTCA-PANI composites

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PREA-35

Non-Fullerene small molecule Naphthalene diimide acceptor based for organic solar cells

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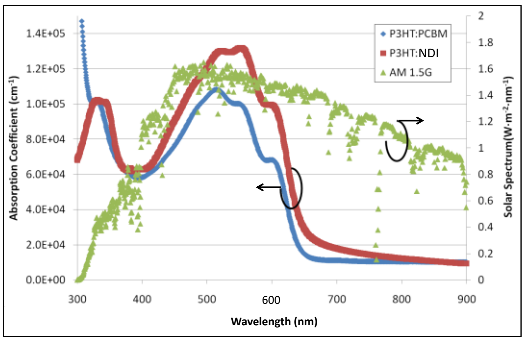
Abstract

Organic solar cells (OSC) has traditionally been dominated by bulk-hetrojunction(BHJ) solar cells using blends of a donor polymerblendedwith a fullerene acceptor (FA).FAs have weak absorption in the visible region and have limited energy level variability, thermal stability and solubility[1]. To overcome thesedrawbacksinFA molecules, research efforts on non-fullerene electron acceptorsare being actively pursued with impressive OSC performance results [2].In line with looking for non-fullerene acceptor molecules for OSC, we have synthesized naphthalene diimide (NDI) based small moleculesas an electron acceptor.NDIare easy to synthesis, exhibit a stronger absorption in the visible region, have excellent solubility in common organic solvents and allow good electron mobility[3].The superior poly 3-hexyl thiophene (P3HT):NDI based blend absorption is compared with traditional FA BHJ blend in the figure below (left). Using NDI acceptors synthesized by us, we are fabricating BHJ OSCwith P3HT:NDI blends (figure below right). The device characteristics and their comparison with traditional FA BHJ solar cells will be shared at the conference.



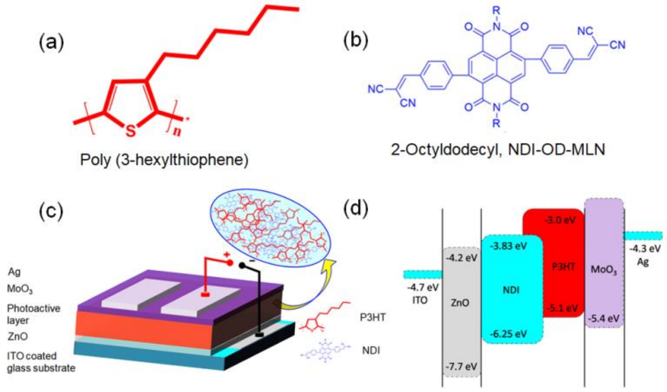


Figure (left):NDI:P3HT blend absorption in solar spectrum is better than traditional P3HT:PCBM blend. **(right)**(a) Molecular structure of donor poly(3-hexyl thiophen donor; acceptor (b) 2-Octyldodecyl,NDI-OD-MLN materials; (c) schematic of device structure; and (d) energy level diagram for device stack.

Acknowledgement: Device fabrication supported byNational Centre for Flexible Electronics, IIT Kanpurthat is funded by MeitY, Govt. of India.

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PREA-39

A polymer and graphene layer to increase dye regeneration and suppress back electron transfer in dye sensitized solar cells

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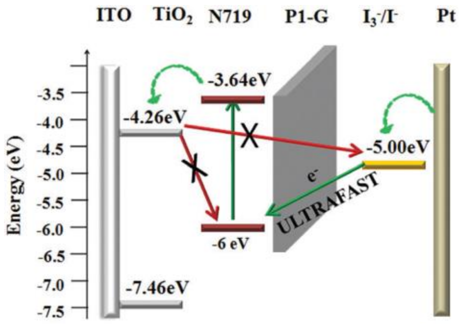
Abstract

Dye regeneration and back electron recombination (BET) are the key events to determine the performance of the DSSCs. BET process occurs between electrons in conduction (CB) of TiO_2 and holes in either electrolytes or dyes [1]. P1 (P2) polymer slows the dye regeneration [2] process (electrolyte to dye). Contrary, CB of the TiO_2 to FTO conducting glass occurs at a 10^{-3}s [3] and this high residence time of electrons in the CB of the TiO_2increase the chance of BET. We have envisioned that the fast dye regeneration is an alternate method for increase power conversion efficiency (PCE) and stability. Hence, in order to make faster electron transfer to TiO_2 CB, we have come up with the idea of using highly conducting material to make a composite with P1. We realized the P1 polymer composites with graphene (P1-G) have found to increase the ultrafast dye regeneration. These composite materials in the photoactive layer can result in a greater dye regeneration process and decrease the BET (synergetic effect). The PCE was increased drastically by 7.51% to 10.41% (with P1-G) with excellent stability.



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PREA-40

Perylene Based Small Organic Molecule as Cathode Material for Lithium Ion Battery

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Abstract

The Lithium ion batteries based on Organic molecules are attractive due to the possibility of fabricating light weight batteries with high energy and power density, long life and environmental friendliness for mobile applications and flexible devices. However, the organic lithium batteries have high capacity and large serial parallel numbers which coupled with such problems as safety, durability and cost. Often, the experimental specific capacity is very low during charging and discharging process as compared to theoretical capacity while discharging the battery at moderate and high C rates. To prevent these problems, we designed as many as maximum active sites with Perylene based small conjugated organic molecule. The fabricated Li-ion battery using lithium salt of Perylene hexa carboxylic exhibits 100% coulombic efficiency and specific capacity while discharging at 5 C. The control experiments confirm our hypothesis of using the maximum number of active sites in smaller organic molecule improve the performance of organic lithium battery.

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PREA-42

Effect of heteroatom(S/Se/N) juggling in anthraquinone and benzochalcogenadiazole/benzotriazole based (D-A-D-A′) copolymers: Synthesis, photophysical and electrochemical properties.

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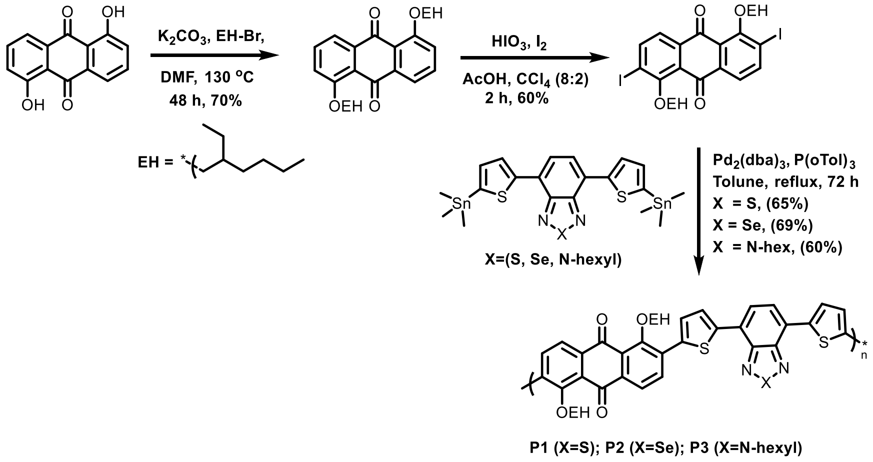
Abstract

Three donor-acceptor(1)-donor-acceptor(2) (D-A-D-A′) copolymers **1-3** have been synthesized, where thiophene was used as donor and alkyl substituted anthrarufin and benzochalcogenadiazole/benzotriazole were used as acceptor(1) and acceptor(2), respectively. Their photophysical and electrochemical properties were studied. The polymers **1-3** showed large Stoke's shift. The polymers **1-3** possess significant crystallinity in the solid state and showed sharp diffraction peaks in powder XRD data. Hence, they are expected to be a promising candidate for the organic field effect transistors (OFET).



Scheme 1

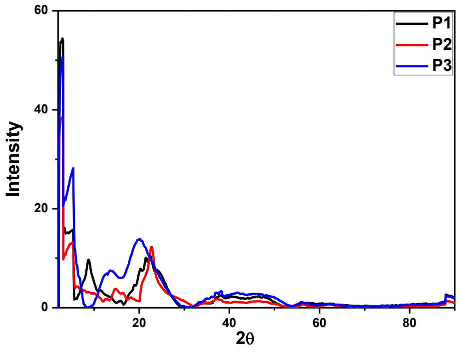


Figure 1: Powder XRD data of the three copolymer (P1, P2, P3) respectively.

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PREA-43

BODIPY-Isoindigo Based Polymer For Organic Field Effect Transistors

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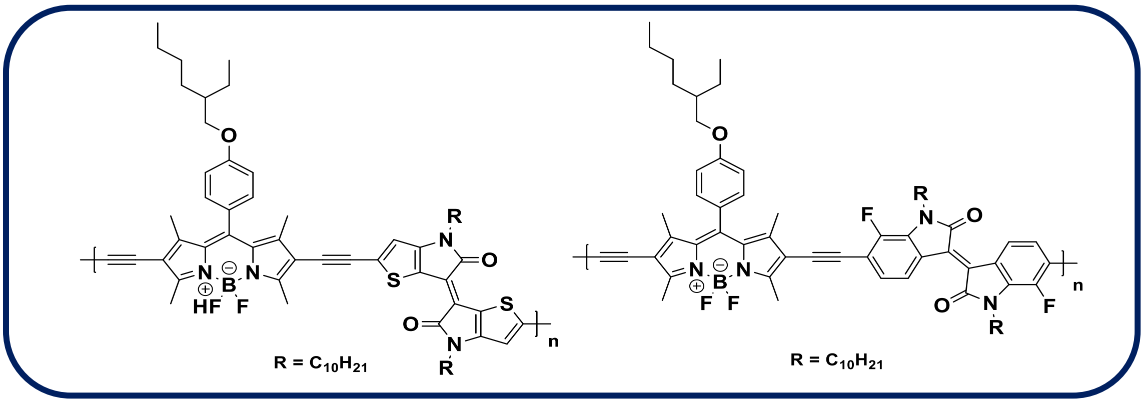
Abstract

BODIPY (4, 4-diflouro-4-bora-3a, 4a-diaza-s-indacene) fluorophores have been used in variety of applications such as sensors, biological labelling, photodynamic therapy, etc. because of its excellent thermal/photochemical stability, sharp fluorescence peak, tuneable emission and high quantum yields.[1] Despite, these BODIPY semiconductors are rare. There are few reports of BODIPY based systems for OFETs, but charge carrier mobility values have been moderate so far. In this work, we have attempted to design two novel π-conjugated D-A copolymer.[2] It is proposed that BODIPY unit with ethylene linkage will act as a donor[3] and as acceptor thino- fused isoindigo, 7, 7´ difluoro substituted isoindigo will be used. Isoindigo having π-core and lactum group behaves as a acceptor and this property can be alter by attaching thiophene or more electron withdrawing element like fluorine. These polymers will be synthesized by palladium catalysed sonogashira coupling and expected molecular orientation and film formation will improve charge carrier property.



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PREA-45

Electrochemical and Electronic Properties of Transparent Coating from Highly Solution Processable Graphene Using Block Copolymer Supramolecular Assembly: Application toward Metal Ion Sensing and Resistive Switching Memory

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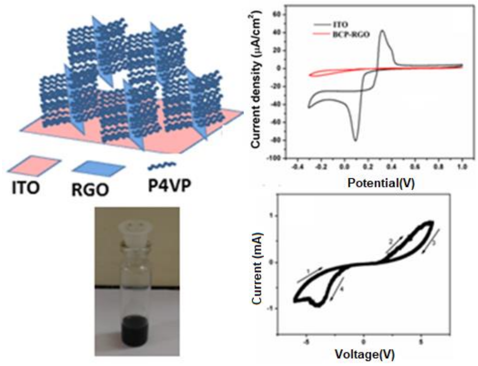
Abstract

Here, we have discussed the fabrication of a highly solution processable graphene from a novel supramolecular assembly consisting of block copolymer polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) and pyrenebutyric acid (PBA)-modified reduced graphene oxide (RGO). The H-bonding between the carboxylic acid group of 1-pyrenebutyric acid (PBA) and the pyridine ring of P4VP forms the supramolecular structures. Highly transparent and mechanically stable thin films can be deposited from these supramolecular assemblies on a relatively smooth surface of different substrates such as silicon wafer, glass, indium tin oxide, and flexible polymer substrates like poly(ethylene terephthalate). The graphene surface modifier (PBA) can be selectively removed from the thin film of the hybrid material by simple dissolution, resulting in a porous structure. Hybrid thin films of around 50 nm thickness exhibit interesting electrochemical properties with and a real capacitance value of 17.73 μF/cm^2 at a current density of 2.66 μA/cm^2 and good electrochemical stability. The pendent P4VP chains present in the composite thin film were further exploited for electrochemical detection of metal ions. The electrical measurement of the thin film sandwich structure of the composite shows a bipolar resistive switching memory with hysteresis-like current−voltage characteristics and electrical bistability. The OFF state shows ohmic conduction at a lower voltage and trap-free space-charge-limited current (SCLC) conduction at high voltage, whereas the ON state conduction is controlled by ohmic at low bias voltage, trap-free SCLC at moderate voltage, and tarpassisted SCLC at high voltage.



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PREA-47

Amphiphilic polymer rich amphiphilic-acid blend membranes and their properties

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Abstract

The main objective of this study is to obtain dimensionally stable amphiphilic polymer rich amphiphilic-acid ionically crosslinked blend membranes. The commercially available high ion exchange capacity value based sulfonated poly(arylene ether sulfone) (IEC: 2.08 meq. g^{-1}; SES0005) is used as an acid polymer. Amphiphilic homopolymer i.e., sulfonated *para*-polybenzimidazole (s-*p*-PBI) have been synthesized by solution polycondensation, of 3,3'-diaminobenzidine and 2-sulfoterephthalic acid monosodium salt in an inert atmosphere with polyphosphoric acid medium successfully. The formation of resultant brown color polymer fiber structure indicates that the high molecular weight based s-*p*-PBI has been attained under specific synthetic conditions. The synthesized s-*p*-PBI is soluble in polar aprotic solvents. It indicates that amphiphilic polymer has been suitable to prepare miscible blend membrane with acid polymer. The FT-IR characterization result of s-*p*-PBI proves expected polymer structure and presence of functional group, respectively. Different compositions of amphiphilic polymer containing amphiphilic polymer rich amphiphilic-acid blend membranes are prepared by using DMAc solvent. Membrane properties such as thermal stability, mechanical strength, ion exchange capacity, solvent uptake are in progress. The characterization studies such as ^{1}H-NMR, Dimensional stability (Fig.2) and ATR-IR are studied.

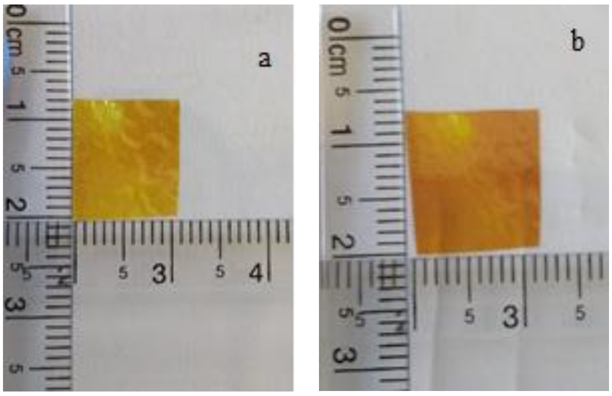

Fig 1: ATR-IR graph of Blend membranes; Fig 2: Dimensional stability of the amphiphilic polymer rich amphiphilic-acid blend membrane (BM-P) in deionized water at 70 ºC for 2 hours (a) Before the stability test, and (b) After the stability test.

Acknowledgement: The authors would like to thank DST-SERB (ECR/2015/000014) for granting financial support.

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PREA-48

Conducting polymer-rGO composite based high performance asymmetric supercapacitor

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Abstract

Supercapacitors are those charge storing devices which have high power density but low energy density. In this respect, asymmetric supercapacitors are highly recognized in recent years due to the smart alteration in voltage window thus exhibiting a high energy density along with high power density. Here we have made an asymmetric supercapacitor employing two dissimilar material, polyaniline and reduced graphene oxide in an aqueous gel electrolyte. The capacitance, energy and power densities, cycling stability of our asymmetric supercapacitor was found to be remarkable.

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PREA-49

CONDUCTING POLYMER FOR THE ELECTRODE MODIFICATION TO ENHANCE THE BIO-ELECTROCHEMICAL REDUCTION OF CARBON DIOXIDE

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Over the most recent many-year, there has been developing awareness among the scientists over the globe to explore alternative source for the generation of fuel and power. Various advancements are at the phase of research and improvements for example chemical, electrochemical, photochemical, biological, inorganic changes and transforming which utilize carbon dioxide (CO_2) for the generation of purported Carbon-neutral fuels. Of these techniques, electrochemical reduction of CO_2 appears to be most encouraging because it expends less energy than traditional chemical reduction processes and can proceed at a moderate temperature and atmospheric pressure. Researchers are investigating ecologically well-disposed strategies to accomplish the fixation of CO_2.

MICROBIAL ELECTROLYSIS CELL (MEC) can be improved when accelerating the cathode substrate reduction, electron transfer, and mass transfer. To promote the cathode substrate reduction and electron transfer, exploring effective cathode material is of great importance since the cathode is not only the carrier of the electrogenic bacteria but also the conductor of the electron. A high-performance cathode material should have the following characteristics, excellent conductivity, good chemical stability, strong bio-compatibility, large surface area, and low cost. The most versatile cathode material for MECs is carbon (felt, cloth, paper, and fibers). Carbon materials have little electrocatalytic activity and thus modification of carbon material is the main approach to improve their performance. Recent studies demonstrated that carbon cathode modified by the used of Polyaniline (PANI) and Polypyrrole (Ppy) to modify cathode which delivered more current density and accelerated the extracellular electron transfer from electrogenic microbes to the cathode, thus promoting the CO_2 reduction for biofuel production. The cathode surface was characterized by employing various surface characterization techniques such as scanning electron microscopy (SEM), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

Keyword: Bioelectrochemical cell , Carbon Dioxide, Electrolysis, Reactor, PANI & Ppy ,.

PREA-50

Highly efficient color amalgamation system for fine tuning of white light-PLEDs using blue and red chromophores

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Abstract

White light emission and tuning of colors were directly obtained by mixing of blue and red polymeric chromophores. The present work focuses on fine tuning of colors to achieve the white light emission from primary blends of blue and red emitting conjugated polymers. The binary luminescent polymers (blue & red) were synthesized and characterized by different standard techniques. The polymers were confirmed by FT-IR and NMR techniques, while the GPC result illustrates the polymeric properties of the materials. The absorption peak of ppy 1 and ppy 2 is 375, 426 nm. The emission peak of the materials at 473 (ppy) and 603 (ppy2) nm demonstrates that the materials belongs to red and blue emissive category. The highlight of this work is that the color tuning and achieved white color emission by mixing the different ratio of the compound.

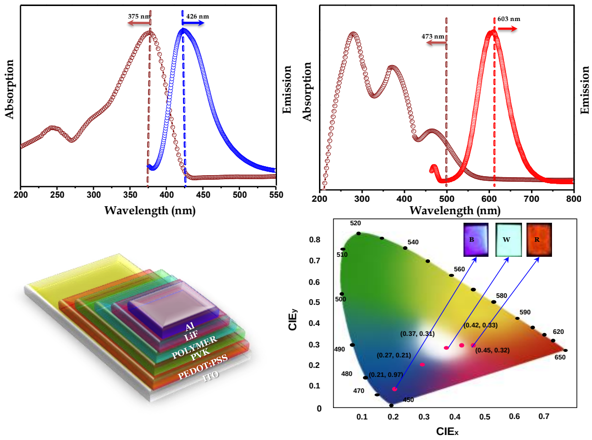

Fig. 1. Optical Properties and white light CIE coordinates of polymers

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PREA-51

Organic Solar Cells based on P3HT: Stability and Efficiency Improvements

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Abstract

Finding an inexpensive, clean and completely renewable energy source is the most pressing challenge of current times. Solar energy has long term potential because the earth receives enough energy from the sun in just one hour to meet all human energy requirements for an entire year. Current silicon-based solar technologies lead the market in terms of device efficiency and lifetime but they are expensive to implement on a global scale.[1] This is the major motivation for the development of organic solar cells (OSCs), which recently attracted much attention due to their low-cost, flexibility, lightweight and their use in large-area devices.[2] OSCs are not without their problems, most notably lifetimes, which can be as low as 5 years. The individual layers play a vital role contributing towards the performance and lifetime of the final solar-powered device.

Block copolymers (BCPs) have long-term structural stability and also their solid-state morphology being of the appropriate dimensions to efficiently perform charge separation and transfer to electrodes.[3] Our aim is to improve further the efficiency and lifetime of OSCs by creating highly original and industrially viable novel block copolymers. Hence, we focused on the synthesis and photovoltaic application of BCPs based on poly(3-hexylthiophene) (P3HT) due to its high hole mobility, good processibility and ease of synthesis.[4] Herein, the novel synthesis of the latest BCPs based on P3HT will be presented and explored their detailed study of self-assembly and device performances.[5]

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Theme : SMR

SMR-01

Biopolymer Assisted Drug Carrier and Release Hydrogel Systems

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Abstract

Hydrogels consists of three dimensional net-work structures with highly hydrophilic character and can be obtained in different macromolecular structures that include the following cross-linked or entangled networks of linear homopolymers/copolymers (block or graft), complexes of polyions with multivalent ions, other polyions and also H–bonded complexes. Because they are available in different physical forms, their utility in diverse fields especially in biomedical application is well known. We will present our results on the weak physical gels formed by the biopolymer aqueous solutions, viscoelastic gels of drug anion containing amphiphilic ionic liquid and also their solution blends as drug carriers and release systems. The agar gels in aqueous media are prepared in dexamethasone, a hydrophobic drug solubilized in micellar solutions and drug release is monitored from gel media and also dry cast films of the gels. In the second approach acetyl salicylate is incorporated into an amphiphilic ionic liquid which forms large entangled viscoelastic micellar gels in aqueous sodium salicylate solutions. The solution blends of such gels with the agar or chitosan are also prepared. The rheological features in terms of storage modulus, loss modulus and complex viscosities as a function of temperature, frequency and biopolymer nature are measured and the results are interpreted in terms of morphological features of the gels. The sustained release profiles of the drug species were modelled to understand the release mechanism. It is concluded that gels of varying nature can be designed and the drug release can be promoted from the films.

SMR-02

Development of a novel chitosan based biocompatible and self-healing hydrogel for controlled release of hydrophilic drug

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ABSTRACT

Smart polymeric hydrogels of chitosan and acryloyl-phenylalanine having potential of fast intrinsic shape memory properties (self-healing), non-toxic, biocompatible with moderate mechanical strength have been developed. The hydrogel has been formed by linking its network with flexible pendant side chains of chitosan and acryloyl-phenylalanine (exhibiting optimal balance of hydrophilic and hydrophobic moieties). The non-toxic and biocompatible behavior of the synthesized chitosan based hydrogel reveals its potential use towards the biomedical field. The side chain of hydrogel consists of amine and carboxylic acid groups and these moieties allow non-covalent interactions (H-bonding) across its interface. Thus, synthesized hydrogel shows very good self-healing property. Further, it has shown remarkable swelling (at different pH *viz.- 2*, 7, 9), cell viability (HEK-293 cells up to 200 µg/mL), cell proliferation, and controlled drug release and thus found multi-responsive.

SMR-03

Stimuli-Responsive Coordination Polymer Based Metallogels: Synthesis of Ag Nanoparticles and Sensing Hazardous Gases

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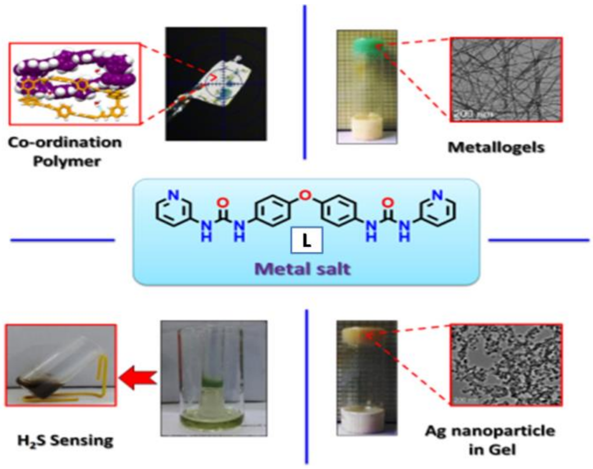
Abstract

Metallogels[1] are special types of supramolecular gel[2] where metal ion is a part of gel network thereby playing a crucial role in gelation. Research on developing metallogelators is important as such metal containing soft materials offer various potential applications that include catalysis, nanoparticle synthesis, sensing etc. However, designing metallogelators is difficult because of the lacking molecular level understand of gelation. The design principle exploited in the present work[3]is based on a structural rationale that suggests that lattice occluded crystalline solids (LOCS) do have potential to produce gels under suitable condition as akin to LOCS, gels do have large amount of solvents immobilized within the gel network. An oxo-bridged bis-pyridyl-bis-urea ligand (**L**) was thus designed and synthesized. Reaction of **L** with various metal salts produced single crystal X-ray quality crystals that turned out to coordination polymers when subjected to single crystal X-ray diffraction (SXRD). Gelation studies revealed that many such coordination polymers produced metallogels. One of the Ag coordination polymer based metallogels in the series produced Ag nanoparticle without the assistance of external reducing agent. One of the Cu coordination polymers metallogels showed interesting hazardous gas sensing ability.



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SMR-04

Exploring Orthogonal Hydrogen Bonding in Designing Supramolecular Gelators for Biomedical Applications

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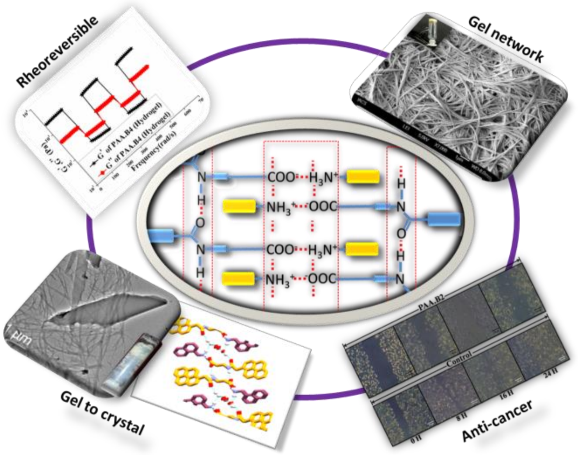
Abstract

Gels are visco-elastic soft materials that are commonplace in everyday life. Supramolecular gels are formed through the formation of self-assembled fibrillar networks (SAFiNs)[1] that hold the flow of solvent via capillary force action. Designing supramolecular gelators is important as this class of soft materials offer various potential applications including therapeutics. Importance of 1D supramolecular synthon involving hydrogen bonding in gelation is well established.[2] In this work,[3] orthogonal hydrogen bonding involving amide…amide and primary ammonium monocarboxylate (PAM) synthons has been exploited to get an easy access to a series of supramolecular gelators. For this purpose, a series of PAM salts derived from β-alanine derivatives of pyrene and naphthalene acetic acid were synthesized. Gelation studies revealed that ~50% of the salts were gelators. Single crystal X-ray diffraction (SXRD) studies on some of the salts and the parent acids revealed that orthogonal hydrogen bonding indeed played a crucial role in gelation. A pyrene based PAM salt in the series selected based on MTT assay was studied for anti-cancer activity on a highly aggressive human breast cancer cell line MDA-MB-231 by cell migration assay. Internalization of the anti-cancer salt was probed by cell imaging studies.



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SMR-06

One-dimensional luminescent electrospun polymer nanocomposite materials; Rheological and Optical studies

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Abstract

Photoactive rare earth oxide electrospun polymer nanofibers are promising candidate for their potential utilization in photonic applications. Electrospinning is a simplistic and novel route for the formation of one dimensional luminescent material, with their large surface to volume ratio, uniform diameter and tunable porosity. Cerium oxide nanoparticles have number of fascinating properties, such as narrow emission band, high quantum yields, long life time, chemical stability which have been considered as good additives for making luminescent electrospun nylon 6,6 nanofibers. Herein, Cerium oxide nanoparticles (Ce Nps) have been synthesised using hydroxide mediated method, characterized and introduced into electrospun Nylon 6,6 (Ny) nanofibers. These were studied by X-Ray diffraction (XRD), Fourier transform infrared (FT-IR), scanning electron microscope (SEM), Optical microscope, Thermal gravimetry (TGA) techniques and investigated their luminescence property by using photoluminescent Spectroscopy (PLS) and also investigated its rheological property. The prepared Ce NPs/Ny nanofibers showed good optical and mechanical properties which are useful for optical and sensor devices.

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SMR-07

Decontamination of wastewater containing cationic dyes by thiol-norbornene photo cross-linked polymer network

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Abstract

The present work focuses on the UV curable synthesis of an organogel based on thiol-norbornene click chemistry. Characterisations of the material are accomplished by standard spectroscopic and analytical techniques. Viscoelastic property of the as synthesised material is investigated systematically. Rheological measurements reveal higher values of storage modulus (G') than loss modulus (G") within the linearity limits of deformation, indicating the predominance of elastic property in the network. Swelling behaviour of the gel is thoroughly analysed in various solvents with dielectric constants (ε) ranging from 1.88 to 80.1. Additionally, this material exhibits significant mechanical and thermal stability. Especially,the gel possesses excellent proficiency towards the removal of cationic dyes as well as heavy metals (e.g. mercury) from wastewater. DFT calculations suggest the favourable interaction energy between the dyes and the gel is crucial for the selective uptake of cationic dyes by the gel. To the best of our knowledge, the efficiency of norbornene based photo cross-linked network towards removal of toxic dyes has not been investigated so far. Further, minimum water uptake during dye removal process keeps maximum amount of water available for future usage thereby making it an inexpensive material that has potential applications in toxic organic dye containing wastewater treatment.

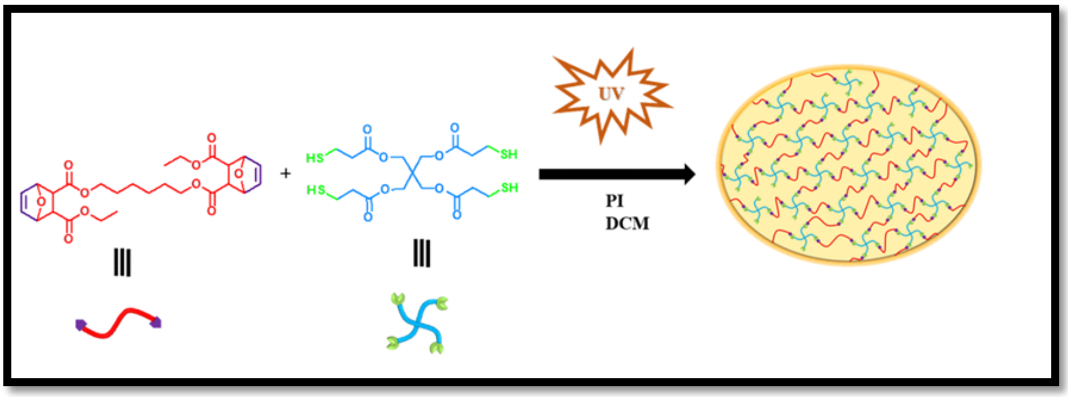

Figure 1. Synthesis scheme of the gel.

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SMR-08

Injectable Hydrogel of Vitamin B9 for Controlled Release of Both Hydrophilic and Hydrophobic Anticancer Drugs

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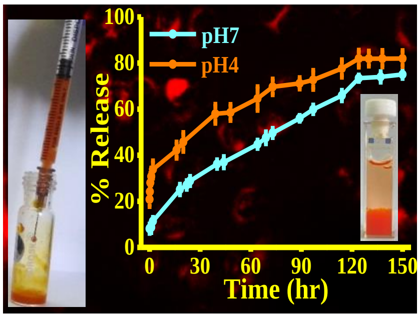
Abstract

Folic acid (FA), vitamin-B9, is a good receptor of drugs triggering cellular uptake via endocytosis. FA is sparingly soluble and here a new approach for formation of FA hydrogel at physiological condition is reported using hydrolysis of glucono-δ-lactone in PBS buffer. The gel has fibrillar network morphology arising from intermolecular H-bonding and π-stacking interaction. Thixotropic property of gel is utilized for encapsulation of both hydrophilic (doxorubicin, DOX) and hydrophobic (camptothecin, CPT) drugs. The loading of DOX and CPT in the gel is attributed to H-bonding interaction between FA and drugs. The release of DOX, is sustainable at both pHs and Peppas model indicate that at pH7 diffusion of drug is Fickian but, non Fickian at pH4. The release of CPT is documented from fluorescence study which also corroborates combined release of both the drugs. MTT assay of hydrogel shows nontoxic behaviour and cytotoxicity of DOX loaded FA hydrogel is lower than pure DOX.



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SMR-10

SYNTHESIS AND CHARACTERIZATION OF COLLOIDAL LATEXES OF BUTYL ACRYLATE AND ITS COPOLYMERS

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Abstract

This investigation reports the synthesis and characterization of colloidal latexes of butyl acrylate (BA) and its copolymers with vinyl acetate (VAc), styrene (Sty) and acrylonitrile (ACN). All the copolymers of BA with VAc (BA-*co*-VAc), Sty (BA-*co*-Sty) and ACN (BA-*co*-ACN) were prepared via emulsion polymerisation using two different thermal initiators, ammonium persulfate (APS) and potassium persulfate (KPS). Sodium dodecyl sulfate (SDS) was used as surfactant in all cases. The polymerisations were carried out at 70°C. Attempts had also been made to prepare copolymers of various compositions by varying the monomers concentration in the feed. The progress of the polymerizations was monitored by measuring the conversion of monomers time to time. The conversion of monomers was measured gravimetrically. The prepared latexes were characterized by GPC, UV-Visible, FT-IR and ^{1}H NMR analyses. All the prepared latexes were found to be nearly transparent as evident by the UV-Visible analysis. The FT-IR analysis of the purified copolymers confirms the successful preparation of the copolymers. ^{1}H NMR analysis also confirms the successful incorporation of the co-monomer in the copolymer. The molar composition of the co-monomers in the prepared copolymer was calculated by comparing the areas under the characteristics ^{1}H NMR peaks of the repeating units of the two co-monomers.

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SMR-13

Enhancing the properties of shear thickening fluids by addition of nanoclay and modification of the suspension medium

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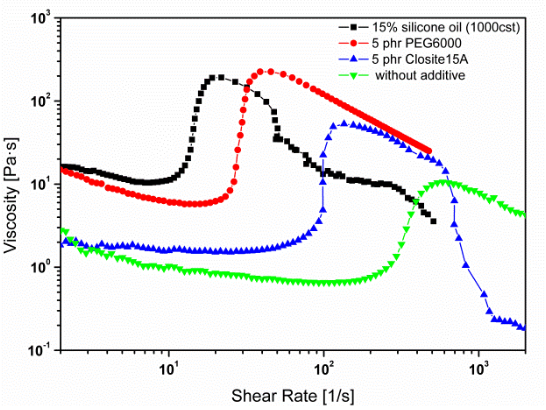
Abstract

Shear-thickening fluids (STF) are concentrated colloidal suspensions of hard nano-particles in a carrier fluid that show a non-Newtonian behavior i.e. a steep and reversible rise in viscosity when subjected to shear. Mechanical properties such as energy absorption, flexibility, impact resistance and reduced weight etc. make them suitable in engineering application in state of art technologies such as soft body armor systems, damping devices and smart structures. A typical example of an STF would be a suspension of nano-fumed silica (11 nm) particles in a carrier fluid like polyethylene glycol (PEG 200). Modifications of conventional STF with improved elasticity and stability can be used to develop STF which can be used for improved or new applications. The first approach involved modifying the hydrodynamic forces by adding high aspect ratio particles: four types of nanoclays to a suspension of 20 wt% fumed silica in PEG200. Among them,Closite® 15A demonstrated significant enhancement in shear thickening properties in dynamic state and stability at low and high temperatures. The second approach involved modifying the particle-fluid interaction and depletion forces by blending fluid with other fluids with a specific chemical functionality such as addition of viscoelastic fluids: high molecular weight PEGs and high viscosity silicone oil where, PEG with molecular weight of 6000and silicone oil of 1000cst showed promising properties.Such STF combines the material properties of the additives.Thus, current trends towards using nanoparticles and viscoelastic polymers is leading to enhanced performance of STF.



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SMR-17

The effect of segmental compatibility imposed over metal based polybutadiene polyurethane

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Abstract

A series of metal based polyurethanes (PUs) have been synthesized from hydroxyl terminated polybutadiene (HTPB) with combination of a potential energetic material, 1-chloro-2,4-dinitrobenzene (DNB) and burn rate enhancer vinylferrocene (VF) with an objective to exert more flexibility into the hard, rigid PU membrane. Butadiene polymer has been functionalized first with DNB at the terminal carbon through terminal functionalization technique and then VF has been grafted radically as polyvinylferrocne (PVF) chain onto the pendant vinyl double bond of the backbone. The polymer was characterized by NMR, IR, UV, GPC. The variation indegree of VF grafting has a large influence on the viscosity. The mechanical stability of cured polyurethanes have been tested by universal testing machine (UTM), thermal properties have been studied by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). From FTIR spectroscopy, the physical interactions between DNB and PVF chain have been interpreted. To understand the existence or lack of phase separation, dynamic mechanical analysis (DMA) has been performed. Morphology of the domain formation observed from FESEM, have been further investigated by small angle X-ray scattering (SAXS), wide-angle X-ray diffraction (WAXD). The presence of DNB at the chain end of soft segment (SS) causes strong segmental mixing between SS and hard segment (HS) domain. This helps to increase the elasticity of SS chain by increasing the inter polymer chain distance; have been found to be responsible for being more elastomeric.

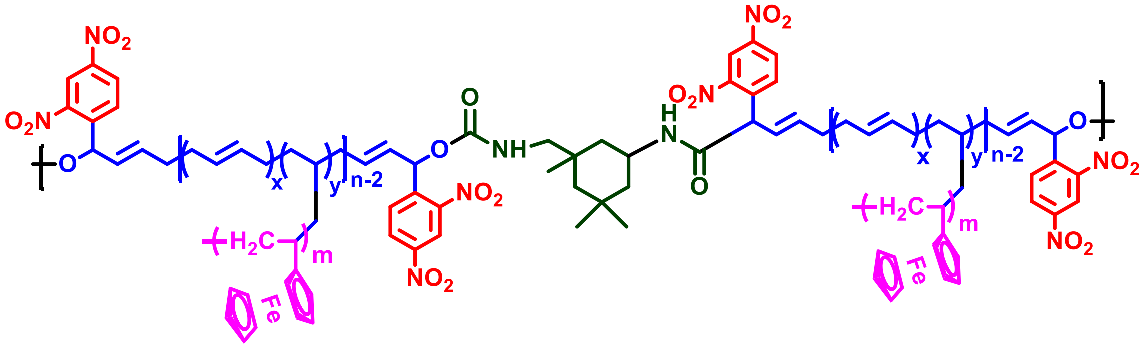

Figure: Ferrocene grafted nitrobenzene containing polybutadiene polyurethane

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SMR-18

Architectural Influences on the Properties of Amphiphilic Double-Brush Polymers

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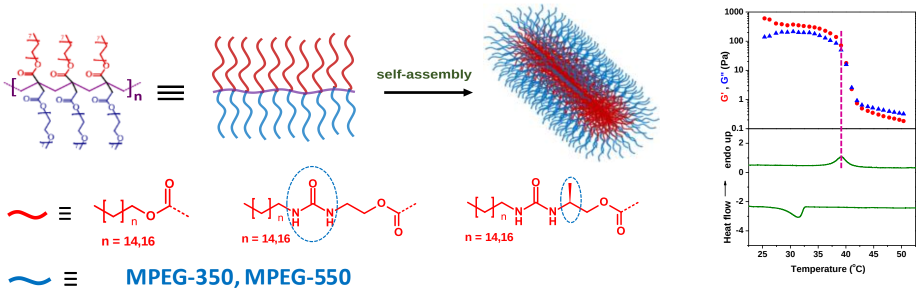
Brush polymersare a special case of graft copolymers where the polymeric side chains are closely spaced along the polymer backbone. Double-brush polymers are a subclass of brush polymers where two different polymeric side chains emanate from a single junction on each repeat unit of polymer backbone. In case of double brush polymers, the immiscibility between the two side chains on each repeat unit could lead to the formation of *Janus*-type structures, as depicted in the scheme below.



Polymerizable amphiphiles, where a polymerizable group is located at the junction of the hydrophobic and hydrophilic segment is one of the simplest approaches to prepare amphiphilic double-brush polymers. Itaconic acid is an interesting bio-sourced molecule that can be readily *hetero*-functionalized to generate amphiphilic itaconate diesters; polymerization of these have led to polymers with interesting properties.[1,2] Recently, Chakrabortyet al.examined the behavior of a series of amphiphilic double-brush polymers based on itaconate diesters;[3]the system carrying acetyl chain as hydrophobic unit and heptaethylene glycol, monomethylether(HEG) as hydrophilic unit generated shear-and thermo-responsive hydrogels, above a critical concentration; this presumably is because of the formation of worm-like micellar structures, wherein the crystallization of the cetyl chains was shown to be responsible for the physical crosslinking, as supported by DSC and temperature-dependent rheological studies (see above).

The objectives of the present study is to probe the influence of different structural features on the physical properties of the hydrogels; specifically - i) variation of the segment lengths of the alkyl and PEG segments; ii) influence of H-bonding units installed within either the hydrophobic or hydrophilic segments, and the effect of their location; and iii) the effect of a chiral center present on either of the side chains. Based on our preliminary studies it is evident that a fine balance between the alkyl and PEG segment lengths is critical to stabilize the hydrogel; furthermore, rheological studies of some of the hydrogels appear to indicate that the LCST behavior of the PEG segment introduces a rather interesting temperature-dependent variation wherein viscosity appears to go through a maximum at a specific temperature. The poster will examine this and several other interesting properties of these rather unique class of itaconate-based amphiphilic polymers.

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SMR-19

Stimuli Responsive and Stretchable Self-Healing Hydrogels of Chitosan-Formaldehyde in Presence of CTAB Surfactant

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Abstract

We report the synthesis of a hydrogel system by employing Chitosan (CS) and Formaldehyde (FD) as cross-linker. The modification of viscoelastic properties of the prepared hydrogel system was carried out by utilizing CTAB surfactant. These properties were studied under changing concentrations of CTAB and it was revealed that only at a particular CTAB concentration viscoelastic behavior of Chitosan-formaldehyde (CS-FD) hydrogels could be optimised.The hydrogels were characterized by Fourier Transform Spectroscopy (FTIR), Thermogravimetric (TGA), Scanning electron Microscopy (SEM). The structural properties were investigated by considering Rheometric observations like viscosity measurements, oscillatory frequency sweep, oscillatory temperature sweep, and dynamic strain sweep , revealing that G' and G" values were found to be different than normal Chitosan-formaldehyde hydrogels dependent on the CTAB concentrations taken. The temperature sweep data revealed the modulation of gelation temperature at different CTAB concentrations. The CS-FD+CTAB hydrogel were found to retain their elastic behavior at high frequency. The Hydrogels after exposing to some experimental concentrations of CTAB showed an abrupt change in the stretching behavior and the stretching properties could be seen 10-20 times than that of normal CS+FD hydrogel system and as such we have successfully achieved a hydrogel system with tremendous stretching properties. Hence it can be shown that the rheological properties of the CS-FD hydrogels system can be controlled by polymer concentration, surfactant concentration and cross linker concentration.

Keywords: Chitosan (CS),Formaldehyde (FD),Hydrogels,Rheology,Stretching Behavior,CTAB.

SMR-20

Magneto-rheological fluids of spherical and flake shaped iron particles

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Abstract

Magneto-rheological (MR) fluids are the suspension of magnetizable micron sized particles in base fluid. The base fluid is selected from liquid such a silicone oil,mineral oil, synthetic oil, water or ethylene glycol. The magnetizable particle include carbonyl iron, electrolytic iron and their alloys. Additives are used to keep the particle suspended in base fluid.The rheological beheviour of these fluids can be varied within milliseconds on application of magnetic field. Under influence of magnetic field the suspended magnetic particles gets aligned in the direction of the applied magnetic field and interacts to form a structure that can resists shear deformation or flow. This change in the material results into a semisolid state that restricts the flow of the fluid with improved shock absorbing properties. On the removal of the magnetic field from the system the suspended particles gets free for the movement which results in the reduction in the viscosity.

These MR fluid may find applications as shock absorbing fluid in automobile, active vibration control in heavy duty vehicle, breaks and bridges etc.

MR fluids developed using spherical carbonyl iron and flake electrolytic iron as magnetizable particles and silicon oil as base fluid. Lithium grease is used as an additive for keeping the particle suspended in base fluid. The samples were characterized for off state viscosity, shear stress, relaxation time under magnetic field to understand the effect of particle shape.

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SMR-21

Topological Influence of the Cubic Lyotropic Liquid Crystalline Phases on the Dynamics of Confined Water Molecules

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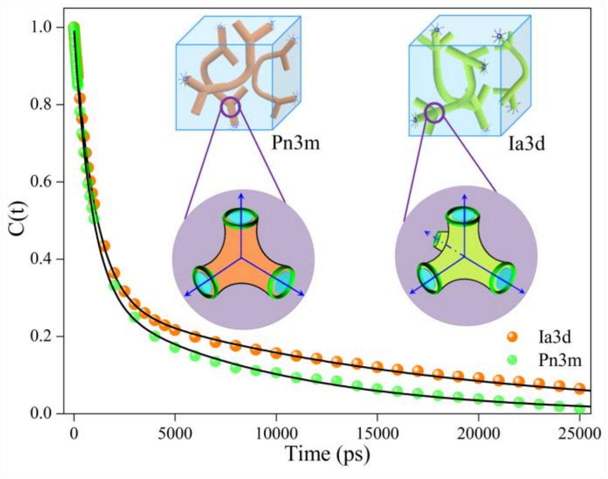
Abstract

Lyotropic liquid crystals are a class of organized nanostructured materials, based on the self-assembly of short surfactants and polymers, which have garnered popularity in the last decade because of their wide scope of applications in multiple fields.[1] The structural features of LLC cubic phases for instance, allow transport of both hydrophilic and lipophilic targets and have been utilised extensively for *in vitro* and *in vivo* delivery of drugs and oligopeptides.[2] The cubic phases have also been used to facilitate the crystallization of large proteins inside its nanochannels which do not crystallize in the bulk.[2] Different applications of these cubic phases are majorly dependent on the nature of nanochannels, dynamics of water molecules and interfacial hydration,[3] thus exploring the behaviour of water molecules at different regions of the nanochannels is important to improve their applications for future use. In our work, we have utilized two coumarin probes of varying hydrophobicities to map the micropolarity, microviscosity and solvation dynamics of the confined water molecules by the time-dependent Stokes shift method at different water layers inside the nanochannels of two cubic phases, Ia3d and Pn3m. It is important to understand the effect of the structural disparities between the two cubic phases on the behaviour of water molecules. We have observed hydration dynamics corresponding to three discrete water networks with the hydration considerably slower in Ia3d phase than the Pn3m phase. This has been attributed to differences in topology, curvature, elastic and hydrophobic stress and the radius of the nanochannels between the two phases.



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SMR-22

Evolution of conformations and consequent rheological changes in casein solution during drying

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Abstract

Caseins arephosphoproteinsextracted from milk. The rheological and structural aspects of these proteins are mainly studied for their application in food, pharmaceuticals and adhesives. Drying is an integral step of processing these products, which can affect the protein conformations. The functionality of proteins is determined by their structural composition which makes it important to identify such effects. In this study, we show that the conformational changes in casein during drying of the solution affect their rheological behaviour. Rheologicalcharacterization as well as the conformational changes in proteins are well studied. However, the present work is first attempt to correlate the conformational changes and rheology of casein solution during drying. It is observed that casein solutions with high initial fraction of random coil structures evolve to α-helical structures as the drying proceeds. Steady state and oscillatory shear experiments carried out on drying solutions show the corresponding changes in the rheological behaviour. Carreau-Yasuda model is used to capture the rheological behaviour of the drying solutions. A significant increase in the zero-shear viscosity, elastic modulus and shear thinning was observed with structural changes as the drying proceeds. Proteins are known to be highly sensitive to the changes in pH and temperature. The effect of each of these factors during drying was studied in detail and found that pH is a crucial factor determining the conformational evolution.

SMR-23

SYNTHESIS, STRUCTURE, SPECTRAL CHARACTERIZATION AND BIOLOGICAL STUDIES OF (E)-N'-(2HYDROXYBENZYLIDENE) HYDRAZINE CARBOTHIOHYDRAZIDE

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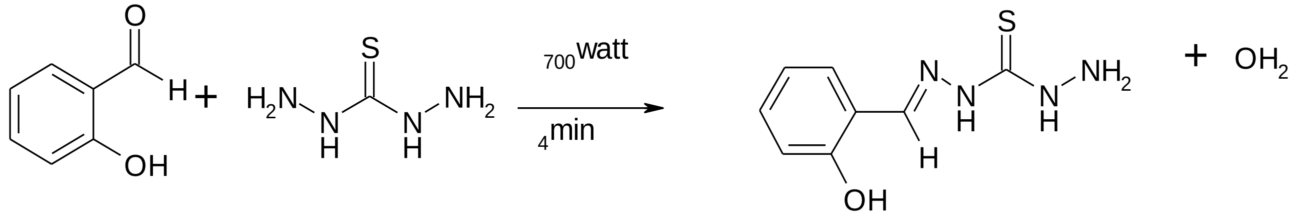
Abstract

A (E)-N'-(2-hydroxybenzylidene)hydrazinecarbothiohydrazide viz. (2-hydroxy B) HCT has been synthesized by reacting 2-hydroxy benzaldehyde and thiocarbohydrazide under microwave irradiation without use of catalyst and solvent , as a green chemistry approach. The reaction occures within a few minutes giving high percentage of the product. The compound was characterized by elemental, IR, NMR and mass spectra. Evaluation of antibacterial activity against Staphylococcus aureus and Escherichia coli and antifungal activity against Aspergillus niger and Rhizopus sps was studied for compound. The compound is biologically active in very low concentration.



4-methyl Benzaldehyde

thiocarbohydrazide

(E)-N'-(2-ydroxybenzylidene) hydrazinecarbothiohydrazide

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SMR-24

Synthesis of Triarylamine-Cored Dendritic Organogel: Efficient Colorometric, Fluorometric, and Impedometeric Detection of Picric Acid

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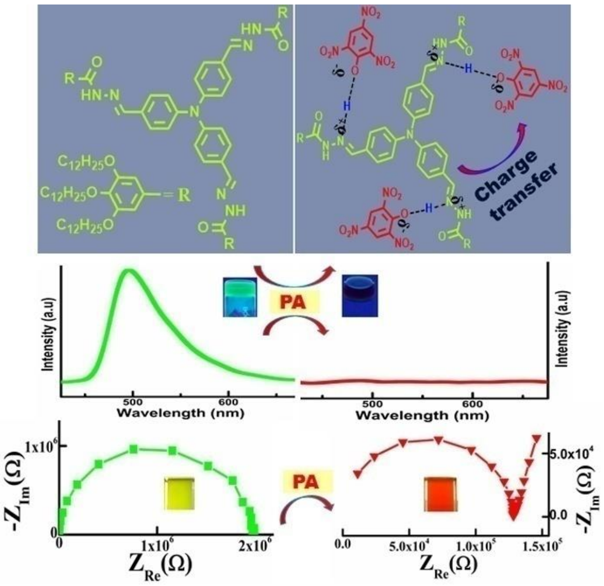
Abstract

Detection of nitroaromatics at ultralow concentration is a major security concern in defense, forensics, and environmental science. To this end, a new triarylamine-cored dendritic gelator (OGR) was synthesized, which produced thermoreversible, thixotropic, and fluorescent gels in n-octanol. On gelation, both π–π* transitions and the emission peak of the gelator show redshifts with a 4.5-fold increase of fluorescence intensity in the gel state indicating J aggregation. The nitrogen lone-pair electrons of OGR make it a donor, and electron transfer occurs to acceptor nitroaromaticscausing fluorescence quenching, which is further promoteddue to its acidity. The Stern–Volmer rate constants measured for different nitroaromaticsshowed that it senses picric acid (PA) best. The contact-mode technique with OGRtreatedpaper strips can allow naked-eye detection of PA under UV light down to 10^{-11}M concentration within 30 s. Reusability of the gel is achieved by treating OGR@PA_x with NaOH solution. Impedance spectroscopic results indicates a decrease of both charge-transport resistance and Warburg impedance on successive addition of PA. The limits of detection of PA determined from fluorescence and impedance measurements match well. Thus, the OGR gel is a reusable, low-cost, specific sensor for PA by naked-eye colorimetric, fluorescence, and impedance techniques.



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[5]

SMR-25

Adsorption of Malachite green with regenerative cellulose nanocrystal (CNC) synthesized from lignocellulose

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ABSTRACT:

Advancement in technology has given human ease in life but has developed huge concerns. Recently, the improvement of nanomaterials has attracted researchers in the preparation of CNC (cellulose nanocrystal) nanoparticles from lignocelluloses and their application in waste water treatment. Here cellulose nanocrystals obtained by acid hydrolysis of Crotalaria juncea has been characterized by Fourier transformed infrared (FTIR) spectra, thermo gravimetric analysis (TGA), X-ray diffraction (XRD), dynamic light scattering (DLS), field -emission scanning electron microscope (FESEM).Nanocrystalline cellulose aerogels were produced using different binders such as PEG and Glutaraldehyde. These aerogels were used as adsorbent for the removal of malachite green and the adsorption characteristic was compared with that of pristine CNC. Adsorption studies were designed using central composite design to fully reflect the effect of parameters on the process. The extents of removal achieved were determined via UV-Vis Spectroscopy. The stability of nanocellulose as adsorbent also shows good prospects in upgrading scale as regenerative aspects indicates good performance after several adsorption-desorption cycle. This study provides a comprehensive analysis on the use of nanocellulose and its modified forms for the wastewater treatment.

SMR-26

Research on fabricated bio-filler for Light weight natural fiber flame retardant polymer nano composite

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ABSTRACT:

Nano-structured platforms have been explored in the context of enhanced absorption in photovoltaic systems [1, 2]. However facile fabrication of nanostructures remains a challenge. Also identification of important device length-scales over which nano-scale effects result in enhanced and combined opto-electronic performance is a problem seldom addressed. We present our work on identification of enhancement mechanisms in both the optical and electrical domains, in a proof of concept polymer photovoltaic system shown schematically in Figure 1(a). The experiments are carried out a nano-structured platforms fabricated by facile methods involving template-based moulding. The nanostructured device are seen to result in a significantly improved photocurrent, as seen from the external quantum efficiency curves in Figure 1(b) and the enhanced absorptance of the structured architecture in Figure 1(c). We see that the enhancement in due to simultaneous improvements in optical absorptance and charge transport. Further we also present our findings on the effects of the length scales of the various layers in the device architecture and the consequent trade-offs between nano-structured enhancement and increased parasitic losses with nanostructures. This leads to design rules for geometry and material selection in the general context of thin film photovoltaic devices. Further, our novel fabrication method opens up a simplified experimental method to make device quality nano-patterned substrates at an applied level, and studying nano-scale phenomena at the fundamental level.

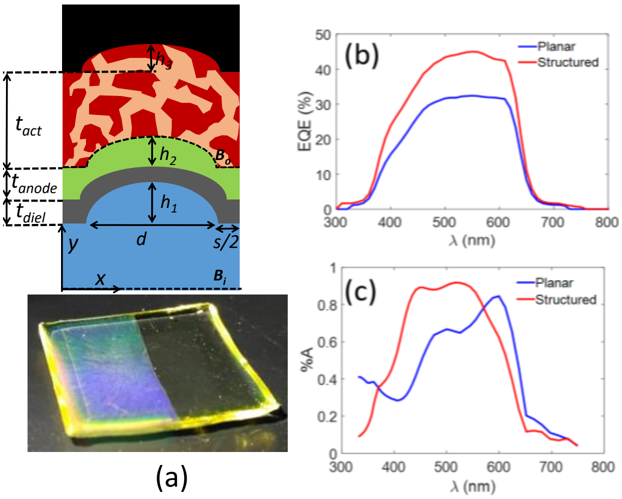

Fig. 1 (a) Schematic device architecture employed (above) and structured substrate (below), (b) External quantum efficiency of planar and structured devices, (c) Computed absorptances of planar and structured devices.

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SMR-27

Structure and Properties of Star Telechelic Poly(lactide) Ionomer

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ABSTRACT

Poly(lactide) (PLA) has reached commercial success in view of its biodegradable and biorenewable "green" nature. Making ionomers by introducing few ionic groups (upto 15 mol %) on polymer chains is an interesting and potential approach to improve several properties of the base polymer including melt rheology. Ionomers of star poly(L-lactide) (PLLA) melt exhibited qualitatively and quantitatively different rheological behavior than that of star PLLA. The star PLLA ionomer showed dominantly elastic response, and both elastic and viscous moduli were at least three orders of magnitude higher than the moduli of the star PLLA melt. In this work we report for the first time an anomalous inverse temperature dependence of shear viscosity and linear viscoelasticity of a melt of star telechelic ionomer of poly (D, L lactide). We also report unusual transients in isothermal oscillatory shear tests. We propose that these interesting rheological properties result from rearrangement of dipolar clusters with temperature. Equilibrium and non-equilibrium atomistic molecular dynamic simulations of star telechelic PDLLA ionomers supported this hypothesis. SAXS experiments supported this hypothesis. Further, equilibrium and non-equilibrium atomistic molecular dynamic simulations of star telechelic PDLLA ionomers also supported this hypothesis. These results could have important implications on improving melt processibility of polylactide.

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Theme- TSMP

TSMP-01

Structure and dynamics of aqueous solutions containing poly-(acrylic acid) and non-ionic surfactant octaethylene glycol n-decyl ether ($C_{10}E_8$)

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Abstract

We present the first computational (molecular level) study of Polyelectrolyte-Non-ionicsurfactant-water solution system to the best of our knowledge. The self-assembly of non-ionic surfactant octaethylene glycol n-decyl ether ($C_{10}E_8$) in aqueous solution containing anionic poly electrolyte poly (acrylic acid) PAA was investigated via atomistic molecular dynamics (MD) simulations. The concentration of surfactant (C_s) was varied in the range0.01–0.3 M (dilute to concentrated) while polymer concentration (C_p) was in dilute condition (i.e. C_p= 0.01 M). The binary and ternary system show a*micelle* like aggregates at low C_s and*lamellar* aggregates at high C_s. Strong intermolecular interaction is observed between PAA and $C_{10}E_8$ at low C_s in agreement with experimental data [1]. PAA chain wraps around the surfactant micellar aggregates. Compared between the binary system of the two surfactants $C_{10}E_8$ and C_8E_5, micelles were formed at a lower C_s in $C_{10}E_8$ system than in C_8E_5 system, this infers that on increasing the tail length of the surfactant CMC value decreases, this kind of behavior is in agreement with experimental data [2].In the case of the lamellar phase the PAA chain shows slight polar interaction with the hydrophilic moieties of the surfactant molecules. This interaction was originating from the (COOH) groups of the PAA with the (CO) groups of the $C_{10}E_8$ molecules. This result was supported by computational analysis such as RDF's, solvent accessible surface area, atom density profiles.

Keywords: Surfactant, Poly (acrylic-acid), micelles, lamellar aggregates.

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TSMP-02

Structure and dynamics of hydrophobic graft-co-polymers ofpoly (vinyl amine) in dilute solution using molecular dynamic simulations

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Abstract

Structural changes and dynamics of graft-co-polymers of PVAm in dilute solution were investigated as a function of degree-of-ionization (*f*) and degree-of-substitution (DS) of grafts. The graft-co-polymers studied were hydrophobic derivatives of PVAm constituted by hydrophobic moieties, viz. dodecyl (C12-PVAm), octyl (C8-PVAm) and n-benzyl (Mebz-PVAm), were grafted on PVAm amine group. The DS for C12-PVAm was 9.5 % and 20 %, C8-PVAm was 17 % and 34 % and for Mebz-PVAm was 28 %, 52 %, 100 % and 150 %. Atomistic molecular simulations were carried out with a modification of GROMOS53a6 forcefield for primary amines and tertiary amines.

These polymers show chain expansion with increase in *f*. The expansion occurs in the range of $f = 0.3 – 0.5$ beyond which no significant expansion takes place. The range of *f* at which the maximum expansion occurs depends on DS and chemical nature and size of the grafted moieties. The chain expansion was correlated to the available DLS-data for a validation of the simulations. Significance of these factors on polymer-solvation behavior is inspected using radial distribution functions, hydrogen bond dynamics and backbone dihedral dynamics. For radial distribution functions, water-chain, residue-water and atomistic radial distribution between amine-nitrogen and water-oxygen were used. The findings showed charge-charge repulsion and couterion-chain interaction plays crucial role in chain-hydration. The presence of stiff, bulky and short graft, made the solvation of Mebz-PVAm challenging. Implications of these structural feature also has found to have effect on the solvation dynamics and were analyzed by hydrogen-bond-relaxation-time (τ_{HB}) and backbone-dihedral-relaxation-time (τ_{RB}).

TSMP-03

Effect of Polymer Charge and Interface Concentration on Structure of Poly(acrylic acid) at Oil-Water interface

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Abstract

Understanding the factors that govern adsorption of polyelectrolytes and the structure of adsorbed polyelectrolyte layers is important to control the stability of emulsions and to regulate the properties of macromolecular monolayers. Adsorption behavior of *isotactic*Poly(acrylic acid) (*i*-PAA) at CCL_4-H_2O interface was studied by performing atomistic molecular dynamics simulations. The effect of polymer charge and interface monomer concentration on the conformation, orientation and hydration properties of *i*-PAA was determined by calculating various structural and solvation properties. *i*-PAA at the interface shows a planar extended conformation which is different from its random coiled conformation in bulk water. The ordered orientation of adsorbed *i*-PAA was analyzedin terms of orientation distribution of carbonyl and hydroxyl groups which shows characteristic orientation of each of these groups. The simulations showed that adsorption occurs only for low values of degree of ionization (f<0.2), which is in reasonable agreement with experimental observations [1].The effect of interface concentration was studied for uncharged *i*-PAA at the interface.*i*-PAA chain undergo structural change from extended planar conformation to random coiled conformation upon increasing the interface concentration. This conformational change is reflected in torsion angle distribution of backbone dihedrals and orientation distribution side groups. The preferential orientation of backbone and side groups disappear with increase in interface concentration. The morphological properties of adsorbed film such as film thickness and interface coverage were calculated. Along with the detailed structural analysis, the solvation behavior of COOH groups [2] of *i*-PAA in water through hydrogen bonding interactions will be presented.

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Complexation between Poly(methacrylic acid) (PMA) and Poly(allylamine hydrochloride) (PAH) in aqueous solution: A Molecular Dynamics Simulation Study

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Abstract

Polyelectrolytes are polymers consisting of positive or negative charge groups in its backbone or side-group respectively. These groups dissociates into the aqueous medium leaving charges in the polymer and counter-ion to the solution. Behaviour of these charged polyelectrolytes are different than neutral polyelectrolytes in aqueous solution. The electrostatic interaction between oppositely charged polyelectrolytes leads to interpolymer ion condensation and formation of polyelectrolytes complex (PEC) or aggregated system. In addition, inter-macromolecular interactions are involved in the formation of PEC structures such as hydrogen bonding, van der Waals forces, hydrophobic and dipole interactions. The nature of PEC is different than individual polycation or polyanion polymer in solvent. Because of their difference in nature PEC are used in biological and chemical system, gene therapy, drug delivery, membrane manufacturing and solid-liquid separation. To study the atomistic nature and behaviour we have carried out explicit-solvent molecular dynamic (MD) simulations between oppositely charged polyelectrolyte in aqueous solution at different degree-of-ionization (*f*). Poly(methacrylic acid) (PMA) is used as polyanion while poly(allylamine hydrochloride) (PAH) as polycation. Both polyelectrolytes having same number of monomers and are present in stoichiometry proportion and water is used as solvent. The following analysis of the PEC will be presented: equilibration of PEC ($<R_g>$), intermolecular structure (RDF) between PMA & PAH, hydrogen bond (H-bond) dynamics and H-bond relaxation time, the atomistic RDF between pair of atoms, and their contribution in the solvent.

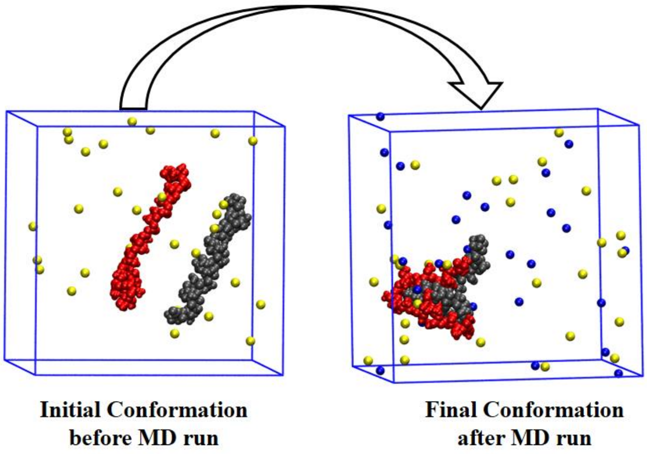

Fig. Snapshot of initial and final conformation of PMA (grey) and PAH (red) complex system at $f = 1$. (water molecules are not shown here for better clarity). (Cl^-: yellow, Na^+: blue).

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TSMP-05

Chain Conformational and Hydration Structure of Poly(itaconic acid) in aqueous Solution: A Molecular Dynamics Simulation Study

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Abstract

The polycarboxylic acid poly(itaconic acid) (PIA) is used in ophthalmic drug delivery to controlled release of the opthalmological drug through the human cornea.Atomistic molecular dynamics simulations of homopolymer of poly(itaconic acid) (PIA) in dilute aqueous solution were performed for study of chain conformation, hydration behaviour and thermodynamic properties of PIA. Several properties of PIA such as Radius of gyration (R_g), dihedral angle distribution, radial distribution function, hydrogen bond dynamics with water and hydration enthalpy were simulated and analyzed. The influence of tacticity on chain dimensions, backbone and side-group dihedral distribution and intermolecular hydrogen bonding was also studied for 30-mer stereoregular (*isotactic* and *atactic*) polymer chain as a function of degree-of-ionization (f) in explicit solvent medium and counterions. The chain expansion of PIA is found to be different than other known polyelectrolytes. The radius of gyration $<R_g>$ of PIA increases for $0<f< 0.5$ beyond which it decreases. The hydration behavior of the PIA chain was investigated using the radial distribution function with respect to different atom types for PIA-water and PIA-Na^+. The non-bonded interaction energy such as electrostatic and dispersive contributions of hydration enthalpy are calculated for both types of stereoregular chains as a function of f. Detailed results will be presented.

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Molecular Simulation Studies of Glassy and Melt Phases of Polybutylene Terephthalate (PBT)

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Abstract

Atomistic simulations are carried out for glassy and the melt phases of PBT using high molecular weight and simulation trajectory. Analysis of the melt are carried out specifically to investigate short time dynamics, conformational dynamics and effect of different preparational methods on the equilibration time. Glassy phase analysis is done primarily to gain an in-depth understanding of the different structural aspect of the polymer. For the preparation of the glassy samples, chains are packed in a large box initially and then the system is compressed to achieve the required experimental density, while for the melt phase the initially prepared low density samples are brought down to the melt temperature either by quenching or the stepwise heating method. In order to have an extensive covering of the phase space and to have appropriate statistical sampling five samples are prepared for the glassy phase and five samples for the melt phase. The equilibrated samples areanalysed for the molecular physical structure and thermodynamic properties. Structural analysis included dihedral angle distribution, intrachain and interchain radial distribution functions, radius of gyration of polymer and torsion angle distribution for conformations, free volume, and orientation distributions of interchain phenylene rings of the polymer. Solubility parameter estimation gave excellent match with experimental data for both the glassy and the melt phase (quenching method). Free volume analysis of these polymers show correct behaviour as a function of probe radius. The calculated average fractional free volume is in the range seen previously for chemically similar polymers.

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Molecular dynamics simulations of structure and thermodynamic properties of symmetric poly (styrene-*block*-methacrylic acid) (PS-*b*-PMAA) micelle in salt-free aqueous solution

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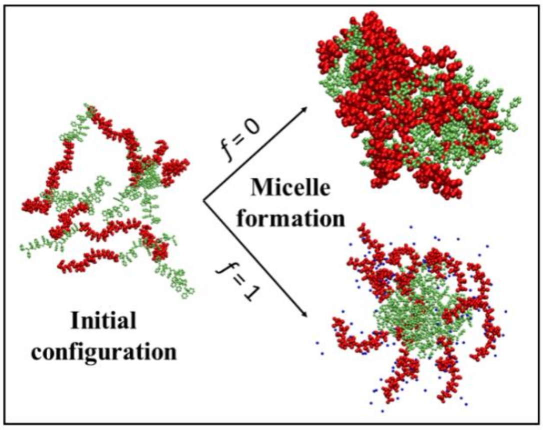
Abstract

The formation of micelle with amphiphilic molecules in aqueous solution is important for many applications in biological and industrial applications. The growth of micelle is a multistage pH dependent process. Atomistic molecular dynamic simulation study has been carried out for structural and thermodynamic properties of self-assembly of pH sensitive symmetric di-block copolymer of styrene and methacrylic acid in salt free solution at different degree-of-ionization (*f*). The molecular dynamic (MD) simulation of 30-mer chains having equal block length have been performed for *atactic*employing bernoullian statistics and straight configuration with variation of *f*.These micelle were characterized based on structural properties such as radius of gyration (R_g) for homopolymer (PS,PMAA), shape of micelle, radius of core and micelle and surface area of micelle and thermodynamic property like hydration enthalpy. The R_g of PS atoms remains constant as function of *f* however R_g of PMAA atoms increases with increase in *f* due to chain gets coiled to extended conformation. The radius of core and micelle were increases with increase in *f*, showed good agreement with experimental data. The shape of micelle is transformed from ellipsoidal to spherical as increase in *f* and the surface area of micelle decreases due to spherical shape. The number of hydrogen bond for PMAA-water group increases for unionized to fully ionized PMAA block. The distribution of sodium ions were observed near corona layer with radial density profile and pair correlation function. Solvation enthalpy contribution of PMAA-$Na^+$and the nature of the interaction between Na^+ ions and PMAA confirms the micelle being in "Osmotic" regime in agreement with experiments.



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Molecular Simulation Studies of Glassy and Melt Phases of Polybutylene Terephthalate (PBT)

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Abstract

Atomistic simulations are carried out for glassy and the melt phases of PBT using high molecular weight and simulation trajectory. Analysis of the melt are carried out specifically to investigate short time dynamics, conformational dynamics and effect of different preparational methods on the equilibration time. Glassy phase analysis is done primarily to gain an in-depth understanding of the different structural aspect of the polymer. For the preparation of the glassy samples, chains are packed in a large box initially and then the system is compressed to achieve the required experimental density, while for the melt phase the initially prepared low density samples are brought down to the melt temperature either by quenching or the stepwise heating method. In order to have an extensive covering of the phase space and to have appropriate statistical sampling five samples are prepared for the glassy phase and five samples for the melt phase. The equilibrated samples areanalysed for the molecular physical structure and thermodynamic properties. Structural analysis included dihedral angle distribution, intrachain and interchain radial distribution functions, radius of gyration of polymer and torsion angle distribution for conformations, free volume, and orientation distributions of interchainphenylene rings of the polymer. Solubility parameter estimation gave excellent match with experimental data for both the glassy and the melt phase (quenching method). Free volume analysis of these polymers show correct behaviour as a function of probe radius. The calculated average fractional free volume is in the range seen previously for chemically similar polymers.

References

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The Study of Swelling Kinetics of Polyelectrolyte (PE) Gels

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Abstract

Analytical and numerical solutions to the equations of motion of swelling kinetics of polyelectrolyte (PE) gels with fixed and variable charges in a salt-free solvent in both the linear and spherical geometries are being studied in this work. Two methods for the swelling kinetics - the Bulk Modulus Method (BMM), which uses a linear stress-strain relationship, and the Stress Relaxation Method (SRM)[1], which uses a phenomenological expression of osmotic stress, are explored to provide the spatial profiles for polymer density, osmotic stress, and degree of ionization, along with the time evolution of the gel size. Further, we obtain an analytical expression[2] for the elastic modulus for linearized stress in the limit of small deformations. We match the BMM – SRM profiles to estimate the effective diffusion coefficient (D) of swelling and also capture its variation with the effective charge of the PE gel. In addition to that, we obtain the effects of hydrophobicity, gel cross-link density on D as well as the total swelling time of spherical PE gels. Our numerical results are in line with the experimental trends available in the literature.

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Development of Frequency Dependent Hyper Elastic Material Model for Nitrile Butadiene RubberTargeting Aerospace Applications

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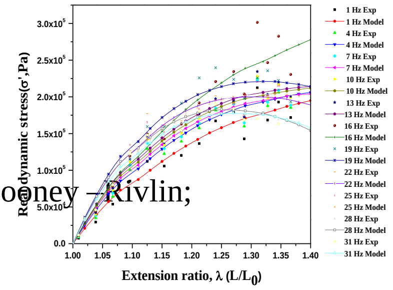
Abstract

Majority of the aerospace structures used in satellite launch vehicles and aircrafts are embedded with hyper elastic materials mainly consisting of specialized elastomeric compositions to ensure attenuation of the undesirable structural vibrations induced during its regime of operations. Finite Element Analysis (FEA) based structural dynamic assessment of structural subcomponents like O rings, seals; bellows need a dedicated frequency dependent hyper elastic modelfor assessing safety margins for safe operations of aerospace structures.
In the recent past, very little work has been carried out on the prediction of frequency dependence of hyperplastic material constants at high deformation. Trisha Sain,*et al.*,have developed a finite deformation viscoplastic rate dependent model for polyurethane nano composites under finite strain regime of 10% and frequency of 100 Hz[1]. Kamal Jahani *et al.*,reported that Mooney-Rivlin constants for incompressible materials are stronglydependent on frequency and dynamic strain [2].
This paper details the work carried out for the development of a frequency dependent hyper elastic model based on the two parameter Mooney-Rivlin strain energy density function. The development of the model is based on the analogy of strong frequency dependence of Mooney-Rivlin constants C_1 and C_2. The vital steps in the development of this frequency dependent hyper elastic model is the segregation of frequency dependence of real (C_1´and C_2´) and complex(C_1´´and C_2´´)counter parts of Mooney-Rivlin constants in the strain energy density function (W). The frequency and stretch ratio dependence of real and complex counter parts of the dynamic stress was simulated by conducting the dynamic mechanical response experiments of nitrile rubber at varying frequencies in the range of 1 Hz to 100 Hz, dynamic strain (0.05 to 0.36) and static strain (0.01-1.5).The frequency dependence of real and complex Mooney Rivlin coefficients, bulk modulus and Poisson's ratiowerealso estimated from the experimental dynamic stress-strain response.The prediction based on the developed model shows excellent agreement with the experimental data up to 40% dynamic strain and 100 Hz frequency.Complex Mooney-Rivlin model formulation

$$W = \{\mathbf{C_1}'(\boldsymbol{\omega}) + \mathbf{jC_1}''(\boldsymbol{\omega})\}\{\mathbf{I_1} - \mathbf{3}\} + \{\mathbf{C_2}'(\boldsymbol{\omega}) + \mathbf{jC_2}''(\boldsymbol{\omega})\}\{\mathbf{I_2} - \mathbf{3}\}$$

W: $Strain\ energy\ density$;
$I_1 \& I_2$: $Principal\ strain\ invariants$
, C_1'', C_2', C_2'': Mooney – Rivlin constants



Keywords:
Hyperelastic, dynamic, frequency, Strainenergy, Mooney –Rivlin;

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TSMP-14

Dynamics of end-pulled polymer translocation through a nanopore

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Abstract

Polymer translocation through a narrow pore has been an active field of research because of its importance in many biological and technological processes such as transport through membrane channels, virus injection, gene therapy, DNA sequencing etc.[1,2] Many advances are made to understand the translocation process from experimental, theoretical and computational perspectives.

In the present study[3], we look into the translocation of a polymer pulled through a narrow pore with high driving force, applied at the one end of the polymer by Langevin dynamics computer simulation method. These kinds of studies on end pulled translocation are equivalent to experimental studies where a polymer is pulled through a pore at one end by optical/magnetic tweezers or atomic force microscope (AFM). We look into the role of applied force on the translocation dynamics from the translocation time distributions, waiting time distributions and velocity propagation calculations along the backbone of the chain. The results were qualitatively explained with the iso-flux tension propagation (IFTP) theory on a coarse grained level. Our studies revealed a complicated dependence of chain configurations on the translocation dynamics. Further extension of end pulled translocations has been done to study the translocation of folded polymers.

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TSMP-18

Life Span Prediction for Lap Shear Jointsof Aerospace Grade Aluminium Substrates Bonded Using Epoxy Adhesive Based on Maximum Strain Principle

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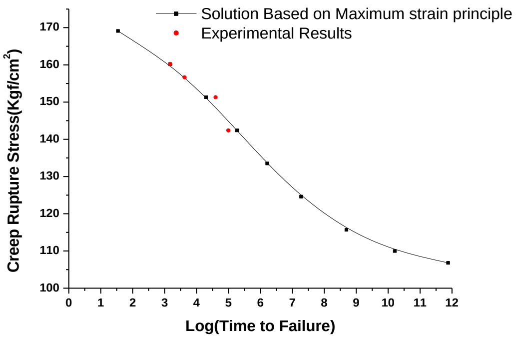
Abstract

In the recent past years epoxy based adhesive joints have attracted attentions of several industries viz. aerospace, automobile, electronics for its high dampening capability, durability, high specific strength and excellent resistance towards fatigue. However, epoxy adhesive joints are extremely sensitive towards the continuously growing monotonic creep loading due to its time dependentvisco-elasto-plastic behavior.Several researchers have performed studies in order to assess the failure behavior of adhesively bonded joints. S Kumar, *et al.*, have performed nonlinear computational analysis of single lap shear joint of aluminum- FM73 adhesive system under the failure stress ratio of 0.5 based on fatigue crack propagation and initiation method [1]. They found close agreement of predicted life time with experimental values. The cohesive failure of the adhesive layer is solely dependent on the energy stored and dissipated during the creep loading under continuous monotonous loading. M Guedes has proposed a free energy based cohesive zone failure criteria of polymeric material [2].

Present work details the failure life prediction methodology of epoxy adhesive bonded single lap shear joint under creep loading based on maximum strain principle in conjunction with time temperature superposition principle.Creep experiments of epoxy adhesive coupons were performed in the temperature range of 30°C to 100°C and time duration of ~ 2500 sec using dynamic mechanical analyzer in order to develop master creep compliance curve based on Arrhenius rate theory. The master creep compliance curve was extended up to 2.42x 10^8 sec based on power law method in order to represent the long term behavior. A theoretical model for the prediction of time for failing epoxy adhesive lap joints under creep load was developed based on the obtained long term creep compliance behavior and maximum failure strain theory. Further experiments were also performed under different creep load to validate the proposed model. The proposed model exhibited fair agreement with the experimental results.



$$\left\{\frac{1}{t_{Rupture}}\right\} = \left[\left\{\frac{\left(\frac{J_{\infty}}{J_0} - 1\right)}{{\tau_0}^n}\right\}\left\{\frac{\sigma_0}{\sigma_{Rupture} - \sigma_0}\right\} - \left\{\frac{1}{{\tau_0}^n}\right\}\right]^{\frac{1}{n}}$$

$t_{Rupture}: Time\ to\ rupture$

$J_{\infty}: Equilibrium\ creep\ compliance$

$J_0: Initial\ creep\ compliance$

$\tau_0: Retardation\ time; n: Power\ law\ index$

$\sigma_0\ : Applied\ stress;$

$\sigma_{Rupture}\ : Ultimate\ tensile\ stress$

Keywords: Epoxy, Arrhenius, TTS, Power law, Strain;

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TSMP-20

Mathematical Modeling in Polymeric Liquid Membranes

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Abstract

Liquid membranes have been attractive to separation scientists due to several advantages over conventional techniques[1]. The advantages include: ease of operation, simultaneous extraction and stripping, easy scale-up, etc. A liquid membrane is prepared by soaking the extracting ligand (solvent) in the pores of the polymeric membrane sheet. The membrane is sandwiched between feed and strip solution as shown in the Figure-1.Feed and strip solutions are continuously stirred at optimum speed to minimize the thickness of resistive boundary layer at both feed and strip side. The extraction of metal ion takes place at feed-membrane interface, followed by the diffusion of metal-ligand complex through the membrane. The metal-ligand complex is then stripped at membrane-strip interface. The transport behavior of metal ion can be mathematically simulated by taking following assumptions: (i) stripping is instantaneous i.e. no mass accumulation in membrane phase, (ii) the process is diffusion controlled, (iii) the concentration gradients are linear[2-4]. The equations are formulated by considering Fick's law of diffusion and assuming the pseudo-equilibrium. In this work, extraction of metal ion by ligand will be discussed. The basic experimental parameters will be evaluated and diffusion coefficient of the metal-ligand complex through the membrane phase will be calculated by the time-lag experiments carried out. The model also considers the extraction of acid (H^+ ion) by the ligand. The transport of metal ion will be simulated by solving the governing differential equation using MATLAB or suitable mathematical software. The simulated data results will be compared with the available experimental data.

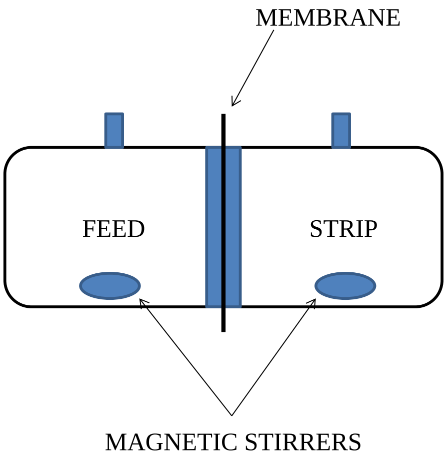

Figure-1: Schematic diagram of Flat Sheet Supported Liquid Membrane (FSSLM)

Acknowledgement: The authors acknowledge NIT Uttarakhand for supporting this work.

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TSMP-21

Demonstration of a Preliminary Simulation Framework for Foam Blow-Molding for Novel Polymeric Applications

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Abstract

The use of foaming overlaid with blow-molding and thermoforming processes for production of net-shaped complex polymeric parts is gaining widespread attention -- motivated by novel sophisticated needs from various commercial applications, and also enabled by the availability of better process-control and instrumentation technologies for foaming and forming. For these state-of-the-art processing technologies, the development of fundamental body of research providing insights and understanding on processing –structure – property relationships lags the actual empirical and commercial development of applications and instrumentation.

This studyattempts to bridge these gaps in understanding, through demonstration of a modeling and simulation framework for foam-blow-molding. The framework accountsfor the morphology-rheology interrelationships within the foam at high temperatures and high strains, and correlates the strains developed during blow-molding to the morphological aspects in the blow-molded part.

These aspects are addressed using simulations of uniaxial tensile deformation of a virtual representative volume element (RVE) of a foam microstructure to derive the nonlinear-tensileresponse of the foam at high temperatures. The simulated stress-strain curve is employed to parameterize a nonlinear rheological constitutive equation. These parameters are then employed for homogenized representation of the foam in the blow-molding simulation. The simulated uniaxial strains in the deformed parisonare then mapped back to the expected local foam morphology using the transfer functions derived from the RVE simulations.

This simple frameworkcan be detailed further with experimental rheological information on actual foamed parisons and more detailed post-processing algorithms to correlate multiaxial elongations with microstructure.

TSMP-22

Study of structure and hydration of cyclodextrin through molecular dynamics.

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Abstract

Cyclodextrins(CDs) are a class of cyclic oligosaccharide formed by the degradation of the amylose fraction of starch [1].These oligosaccharides are composed of monomers of α D-glucose units joined together by 1-4 glycosidic linkage. The cyclodextrins mainly available in nature can be classified into α, β and γ forms comprising 6, 7, and 8 monomer units, respectively. CD has a truncated cone structure with inner hydrophobic cavity and outer hydrophilic rims. Thus, CDs can form inclusion complex with various molecules in its cavity through non-covalent interactions. Due to the presence of large number of hydroxyl groups, CDs are soluble in water [1], [3]-[5].

When a CD molecule is solvated in water, there are certain changes which occurs in its structure. The change in the structural and hydration properties in the CD molecule in water as compared to that in the vacuum is quite evident through molecular dynamics study. The interaction of a CD molecule in water leads to the change in its adjacent rim-oxygen distances and dihedral angles. It also affects the circularity of the molecule. This change is a result of the ring puckering occurring in one or two of the individual glucose units. The naturally abundant 4C1 configuration in α D-glucose is changed to a boat or skewed form or inverted to 1C4 configuration [2]. It has been observed that the hydrogen bonding pattern is also dependent on the flipped glucose units. The β CD has lesser number of flipped units as compared to α and γ forms. Thus it has a more stable intramolecular hydrogen bonding leading to its lesser solubility in water.

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TSMP-23

Kinetics of conformational changes in polyelectrolyte systems

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Abstract

Equilibrium phase behaviour of charged-polymer (polyelectrolyte) systems has been well-studied over past several decades. Interest in the kinetics of conformational changes in such systems, however, has been sporadic, but has received recent attention given their relevance to biological problems like protein-folding or biomedical processes like drug-delivery. Our group has been working on studying the time-dependent, inhomogeneous profiles of physical variables, such as mass and charge densities and osmotic stress, related to such kinetic processes. We will present our understanding that we have developed on this topic over the past two years, especially for two systems - polyelectrolyte gels, and single, isolated, polyelectrolyte chains. Our study considers important issues like charge-regularization and role of elasticity and electrostatics to modulate the spatially varying osmotic forces, which drive these diffusive conformational changes. The major results we have obtained include estimation of effective modulus of charged gels, time-dependency of the size of a gel or a single chain as a function of its charge content, temperature, density of cross-links, and chemical affinity of the polymer and the solvent, relaxation time of swelling as function of the above parameters. The non-linear theory we propose addresses arbitrary deformation, which is in accessible to prevalent linear theories.

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TSMP-25

Design and Development of Theoretical Model to enhance the hole mobilityin Polymer based LED devices

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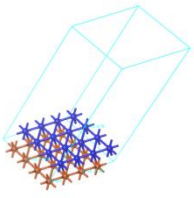
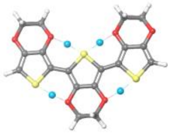
Abstract

Poly-3,4-ethylenedioxythiophene:polystyrenesulfonate (PEDOT:PSS) is a conducting polymer used as hole transport material in light emitting devices(LED) but its conductivity (< 10 S cm $^{-1}$) and hole mobility ($< 10^{-3}$ cm ^{2} V $^{-1}$ s $^{-1}$) is not satisfactory. Its due to the formation of insulating PSS outer layers and inhibit the formation of well-aligned PEDOT conducting chain networks. To resolve the issue we developed a theoretical model. In our work, we mainly focused on the quantum mechanical analysis of PEDOT PSS with different synthetically feasible transitional metal nano wires. In this work neutral (PSSH,PEDOT) and charged (PEDOT^{+},PSS^{-}) trimers were considered for theoratical studies. Solid state Transition metal nanowire properties were analysed by DFT using GGA,PBE functional. A 70 ns MD simulation using NVT ensemble done for analysing mobility in amorphous state.





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TSMP-26

Molecular View of CO_2 Capture by Polyethylenimine: Role of Structural and Dynamical Heterogeneity

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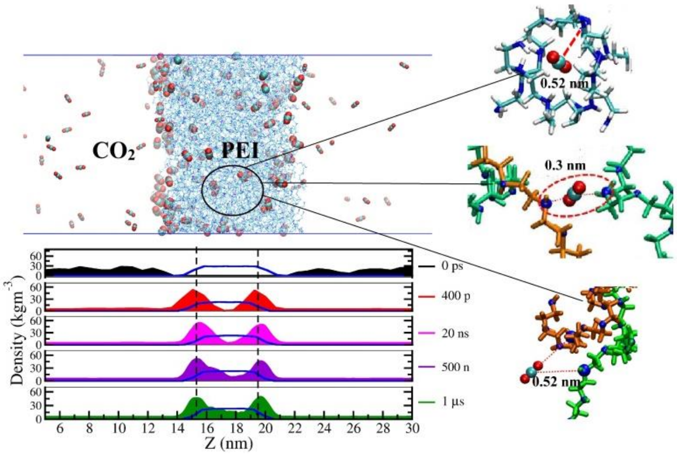
Abstract

Solid-supported polyamines have emerged as promising substitutes to aqueous amine solutions. Tunable porosities and thermal stability with added chemical selectivity due to polyamines make these solid adsorbents efficient candidates for CO_2 capture. Among polyamines, polyethylenemine (PEI), having low volatility and high amine density in the backbone, has been extensively used for CO_2 capture. The molecular thermodynamics and kinetics of CO_2 sorption in Polyethylenimine (PEI) melt have been investigated systematically using GCMC and MD simulations. We elucidate presence of significant structural and dynamic heterogeneity associated with the overall absorption process. CO_2 adsorption in a PEI membrane shows a distinct two-stage process of a rapid CO_2 adsorption at the interfaces (hundreds of picoseconds) followed by a significantly slower diffusion limited release toward the interior bulk regions of PEI melt (hundreds of nanoseconds to microseconds). The spatial heterogeneity of local structural features of the PEI chains lead to significantly heterogeneous absorption characterized by clustering and trapping of CO_2 molecules that then lead to sub-diffusive motion of CO_2. In the complex interplay of interaction and entropy, the latter emerges out to be the major determining factor with significantly higher solubility of CO_2 near the interfaces despite having lower density of binding amine groups. Regions having higher free-volume (entropically favorable) viz. interfaces, pores and loops demonstrate higher CO_2 capture ability. Various local structural features of PEI conformations, for example, inter- and intrachain loops, pores of different radii, and di- or tricoordinated pores are explored for their effects on the varying CO_2 adsorption abilities[1].



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Theme FPC

FPC-01

Superior thermomechanical and electrical properties of reduced graphene oxide reinforced PANI-DBSA/DVB nanocomposites

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Abstract

Various efforts are going on to improve electrical properties of epoxy-based carbon fiber reinforced polymer (CFRP) composites. In presentstudy, 1st time in addition to conducting polymer polyaniline (PANI), another conducting phase reduced graphene oxide (RGO) was incorporated in PANI based system. The RGO was synthesized and incorporated in different weight (0 to 0.5 wt%) fraction in dodecylbenzenesulfonic acid (DBSA) doped PANI-divinylbenzene (DVB) polymer system to get PANI-DBSA/DVB nanocomposite. RGO was characterized by various technique, which confirmed the availability of oxygen-based functional groups on surface and edge. It is observed that PANI-DSBA/RGO-DVB composite with 0.3 wt% RGO content shows significant improvement in flexural strength and modulus i.e. 153% and 32% respectively that of neat PANI-DBSA/DVB nanocomposite. Theelectrical conductivity ofPANI-DSBA/DVB system is 0.075 S/cm and reached is maximum 0.301 S/cm at 0.3 wt % of RGO. The storage modulus, glass transition temperature (T_g) and thermal stability are maximum in case of 0.3 wt% RGO incorporated PANI-DBSA/DVB nanocomposite. The FTIR, Raman spectroscopy and HR-TEM confirmed improved interfacial bonding by H-bonding and π-π interaction. Thus, RGO is constructive for improving the thermo-mechanical and electrical properties of PANI based system which can be used for development of conducting CFRP for structural applications.

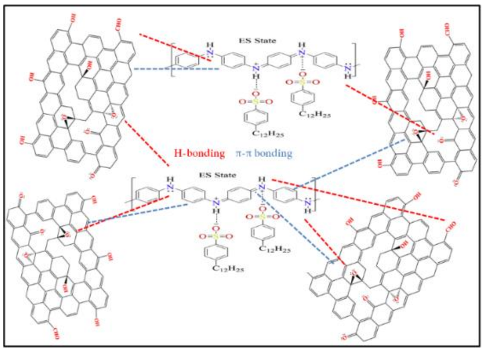

Figure 14: Proposed schematic of interaction between RGO and PANI-DBSA polymer system.

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FPC-02

Synthesis of surface molecularly imprinted polymer for determination of bisphenol (A) from aqueous solution

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Abstract

Bisphenol-A (BPA), identified as one of the endocrine disrupting compounds, may be present in the contaminated surface and ground water and therefore, poses a threat to the environment [1]. It is therefore essential to quantitatively and selectively detect and remove BPA from aqueous solution by imprinted crosslinked polymeric matrix. Compared to traditional imprinting polymerization technique, surface imprinted polymerization is fast emerging as an effective technique due to its improved binding kinetics and recognition ability [2]. In this study, a surface molecularly imprinted crosslinked polymer (SMIP) matrix was prepared for determination and removal of BPA from aqueous solution. Surface imprinting polymerization technique was applied on amino functionalized silica microsphere with optimized concentrations of methacrylic acid and 4-vinyl pyridine as dual functional monomers in presence of ethylene glycol dimethacrylate as crosslinker and 2-2'-Azoisobutyronitrile as initiator. FTIR spectra and SEM images confirmed the formation of dual-polymer crosslinked imprinted coating on the surface of silica microsphere. Compared with the adsorption capacities of non-imprinted polymer, SMIP showed higher selective adsorption of BPA from aqueous solution.

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FPC-03

Polymer Metal/semiconductor Nanocomposite Thin Films: Catalysis, Electrocatalysis and Fluorescence

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Abstract

Polymer nanocomposites are extremely interesting and useful because of the synergistic effects that modify the attributes of the nanoparticles and the polymer matrix in constructive ways.In our study, metal/metal oxide nanoparticles and nanoclusters embedded in polymer thin films are synthesized *in situ* by spin coating a mixture of metal precursor and polymer solution on suitable substrate followed by thermal annealing at an optimal temperature.

Platinum nanoparticles embedded poly(vinyl alcohol) (PVA) thin films were fabricated and application of these films in catalytic reduction of methylene blue (MB), 4-nitrophenol reduction and 4-nitrophenyl piperazine was explored. The films are reusable at least for 10 cycles in the catalysis of reduction of MB with higher TON, TOF than earlier reports (Fig. 1a).The utility of the polymer nanocomposite thin films is now extended to electrocatalysis. Nickel-iron oxide nanoplate - embedded chitosan thin films coated on conducting substrates are shown to give 10 mA/cm^2 current density at an overpotential of260 mV (Fig. 1b) with very low Tafel slope, high Faradaic efficiency and extended stability for OER.

Fluorescent gold nanoclusters (GNCs) with tunable emission characteristics (Fig. 1c) were generated in poly(methyl methacrylate) (PMMA) films using its weak reducing capability by mild and short thermal annealing.[3] The mechanism involved, possible ways of enhancing emission and stability by the addition of polystyrene (PS) and incorporation of thiourea (TU) respectively are explored. Potential application of GNC-PMMA/PS films as detector for $POCl_3$, an important precursor for nerve agents is investigated.

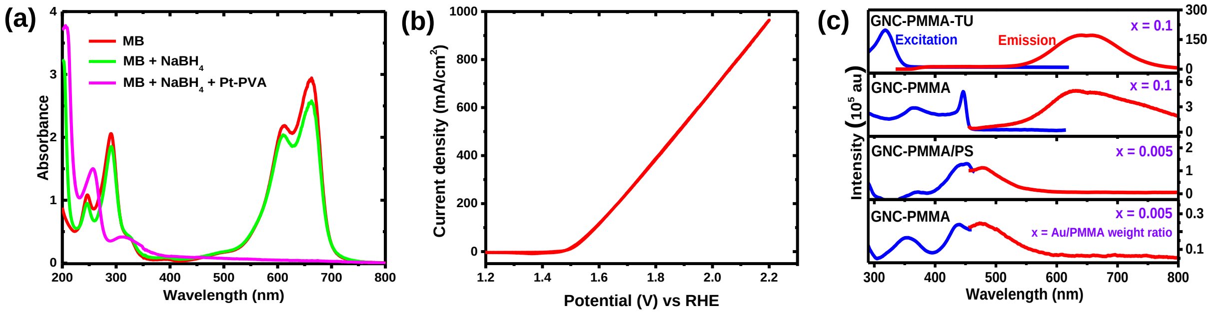

Figure 1. (a) Absorption spectra showing the reduction of MB,**(b)**cyclic voltammogram using [Ni,Fe]O-CS film on Ni foam substrates, in 1 M aq. KOH and**(c)**excitation and emission spectra of GNC-PMMA films of different metal/polymer weight ratio (x) and GNC-PMMA/ PS and GNC-PMMA-TU films.

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FPC-05

Thermal and TribologicalProperties of Graphite Nanoplatelet (GNP) filled High Performance Poly(aryletherketone)Nanocomposites

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Abstract

Poly(aryletherketone) (PEK) reinforced with graphene or graphite nano platelet (GNP) polymer matrix nanocomposites were fabricated using planetary ball milling followed by hot compaction.It was found that the experimental density of the nanocomposites is very close to that of theoretical density. Scanning electron microscope shows uniform distribution of the GNP in the PEK matrix. Thermal stability of the PEK/GNP nanocomposites was increased by 11ºC compared to pure PEK. The percentage crystallinity and glass transition temperatures of the nanocomposites were not affected by the addition of GNP content in the matrix. Microhardness of the nanocomposites was increased from 29.4 (for pure PEK) to 32.7 kg/mm^2 for the 2 wt %nanocomposite. The specific wear rate was found to reduce with increasing GNP content up to 2 wt.% (or 1.21 vol.%), i.e. the specific wear rate for the pure PEK and 2 wt %nanocomposites was found 160×10^{-6} mm^3/N.m and 13×10^{-6} mm^3/N.m, respectively which indicates a significant improvement in wear resistance of the nanocomposites. Coefficient of friction of the nanocomposites first increased and then decreased with increasing GNP content in the matrix.

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FPC-06

Recycling of plastics: Waste rubber, plastics and silica derived bricks

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Abstract

Rubber based tyres are used in automobile, trucks, buses and aeroplanes due to its properties and advantages. Rubber industry is key industry sector in Indian economy. India is third largest producer and fourth largest consumer of rubber. Used tyres are generated one million tonne every year in India. Waste rubber is used for land filling, erosion control, playground equipment etc. Plastics exhibit wide variety of property from flexible soft to rugged hard. 47% of plastics is used for packing applications. After use flexible plastics is discarded which creating pollution. In India 25,000 tonnes plastics is produced per day. Recycling of plastics is one of viable option to tackle the problem. Producing suitable value added product from waste rubber and waste plastics will be one of the option. The end product will have flexibility, plasticity and water repellence.

In the present study we have prepared bricks from waste tyre rubber, waste plastics and sand/bricks/saw dust. Various composition of waste rubber, plastics, fillers (sand/bricks/saw dust) have been blended and final products properties were examined. The best suitable composition for bricks applications as waste tyre rubber (30%), waste plastic bag (30%) sand/bricks (30%) and other fillers/processing aids. Brick can be prepared in any size, shape, colour and density. Physical, chemical, thermal, mechanical, biological properties and weather ability of bricks were tested (**Table 1**). Plastics bricks were used preparing wall around tree pit to check the suitable application (**Fig 1**). It is a effort to recycle the waste rubber/plastic to value added product. Developed bricks are suitable for application in defence, road construction, compound wall, sea shore, railway track, light weight bricks suitable for earth quake affected area, bullet proof walls.

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Sample	density	tensile strength	IPDT value
	(g/ml)	(kg)	(oC)
Prb[a]	0.89	9.5	455
Prb-S[b]	1.21	12.5	889
Prb-B[c]	1.28	1.5	1197
Prb-W[d]	1.03	1.5	486

a-no filler; b-sand filler; c-brick filler; d-wood floor

Fig. 1: Photo of brick sample

Table 1; Various properties of bricks

Keywords: Waste tyre, waste plastic ,sand ,wood floor, brick filler,bricks.

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It is part of M Sc students dissertation work in collaboration with Supreme Gold Irrigations Limited Nanded and Pawan Tyres Nanded.

FPC-08

Synthesis, Characterization and Photophysical properties of AIE active Conjugated Polymer: Facile Encapsulation of AIE polymer into Meso porous Silica Nanospheres for Bioimaging application

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Abstract

Polymeric luminogens are the promising materials for applications in various areas, such as PLED, plastic lasers, fluorescent chemosensors and bio-probes.[1-3] In this journey a large number of conventional luminescent polymers usually undergo aggregation caused quenching, which limits the bright emission imaging application. In contrast, conjugated polymers with aggregation induced emission (AIE) characteristics are strong emission in their aggregate states and have been an ultimate field for developing highly emissive nanomaterials fluorescent meso porous silica nanoparticles for cell imaging application. In this work, tetraphenylethene (TPE) units, one of the typical aggregation induced emission (AIE) moieties, are utilized to construct a new functional AIE conjugated polymer, which exhibits the exciting property of AIE with hole transporting triphenylamine. An AIE active conjugated polymer was synthesized with good yield using conventional Wittig polymerization reaction. The structure of the monomers and polymer was confirmed by FT-IR and NMR spectroscopic techniques. Synthesized AIE polymer is weakly emissive in solutions. They however, in aggregate states emit intensively with absolute quantum yield up to 37%. For efficient cancer cell targeting, synthesized Green emissive AIE conjugated polymer was encapsulated into meso porous silica nanoparticles (P-AIE-MSNPs) via simple non covalent approach, which afforded better emission. In addition, anti-EpCAM aptamer specific to cancer cell was functionalized on the surface of P-AIE-MSNPs for targeted cancer cell imaging.

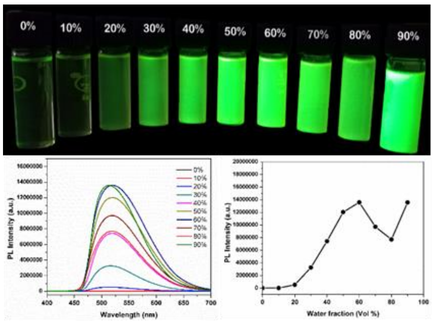

Figure 1. Photographs of Polymer in THF/water mixtures with different fractions of water taken under UV illumination

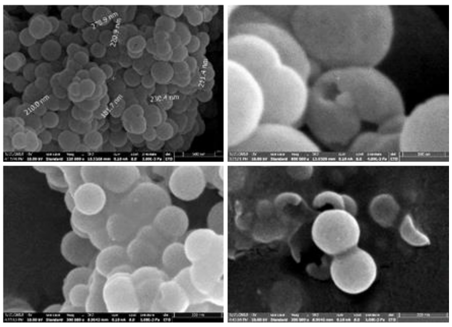

Figure 2. FESEM images of polymer encapsulated mesoporous silica nanospheres

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FPC-09

Surface modification of electrospunsilk/PEO nanofibresby dielectric barrier discharge plasma: Enhanced surface and mechanical properties and *in vitro*biocompatibility

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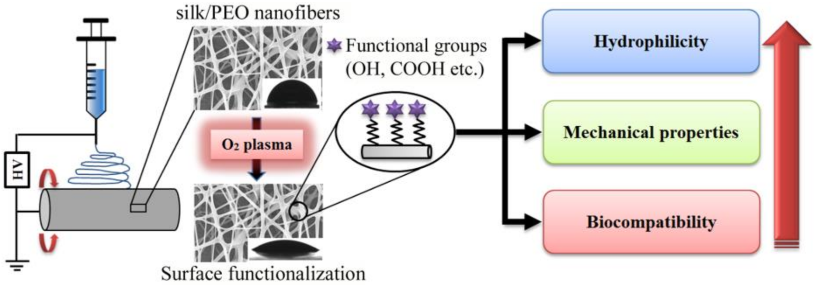
Abstract

With significant development of biomaterials for clinical and healthcare applications, there is a growing interest to develop electrospun polymeric nanofibers with multi-functionality and superior properties by modifying the surface chemistry [1, 2]. In this work silk protein produced by *Bombyxmori* silkworm is blended with polyethylene oxide (PEO) to fabricate nanofibersby electrospinningfollowed by surface treatment using dielectric barrier discharge (DBD) plasma. Plasma treatment of electrospun silk/PEO nanofibers is carried out with oxygen (O_2) gas at atmospheric pressure.Thesurface properties of silk/PEO nanofibers before and after O_2 plasma (silk/PEO/O_2) treatment are characterized by water contact angle measurement, field emission scanning electron microscope (FESEM),atomic force microscope(AFM) and attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy. It is found that the hydrophilicityof silk/PEO nanofibers is improved due to incorporation of polar functional groups and there is an increase in nanostructured roughness induced by O_2 plasma etching effect [3]. The changes in surface chemistry and properties of silk/PEO/O_2nanofibers lead to a remarkable improvement in mechanical properties of the nanofibers without affecting their blood compatibility. Cell viability and cell proliferation assessment results further reveals improvement in biocompatibility of silk/PEOnanofibers after O_2 plasma treatment. The experimental findings show that plasmatreatment is an efficient surface modification technique to improve mechanical properties and biocompatibility silk/PEOnanofibersand can be used to develop electrospun silk-based nanofibersfor wound dressing, drug delivery and tissue engineering applications.



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FPC-10

Development of High Strength PEK/MWCNT Composites for Wide Range EMI/RFI Shielding Applications using Multifunctional MWCNTs.

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Abstract

Multiwalled –walled carbon nanotube (MWCNT)- polymer composite have beeen fabricated to evaluate the electromagnetic inerferance (EMI) shielding efectiveness (SE) of Multifunctional MWCNTs .The small diameter, high aspect ratio, high conductivity, and mechanical strength of carbon nanotubes (CNTs), including SWNTs, MWNTs and functionalized MWCNTs make them an excellent option for creating conductive composites for high- performance EMI shielding materials at low loading . In this work MWCNTs functionalized with Silicon Carbide (SiC) and Polyphospazene respectively . With the aim to study the effect of fuctionalization of MWCNTs in PEK (Poly ether ketone) based nano composite, PEK/funtionalized MWCNTs nano composite were prepared by melt blending using twin screw extruder.Transmition electron microscopy (TEM) and Scanning electron microscopy (SEM) images showed uniform disperson of multifunctional MWCNTs in PEK/functionalized MWCNTs nano composite even at loading 5%.The mechanicalproperties of the PEK/functionalized MWCNTs nano composites were enhanced as the loading of MWCNT increased. EMI SE was tested in the frequency range of 26.5GHz to 40 GHz(Ka band) and the highest EMI sheilding efficiency (SE) was obtained for 5% functionalized MWCNTs and reached to the total Sheilding effectivness (SE_T) 40 dB with very high Sheilding effectiveness due to absorption.The resulting the conductive polymer composite materials will be used in applications for semiconductive,static-dissipative,anti-corrosive, electromagnetic interference (EMI) shielding and stealth composite coatings.

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FPC-11

Fabrication of Anti-bacterial Electrospun Acrylonitrile Butadiene Styrene/ZnO Composite Membranes for Oil/Water Separation

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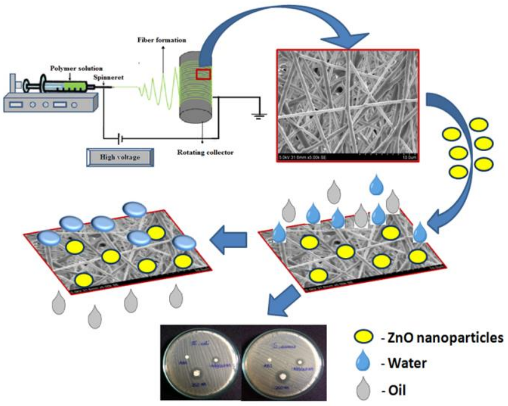
Abstract

The present work reports the fabrication of electrospun acrylonitrile butadiene styrene (ABS) polymeric membrane. The effect of spinning parameters, such as nature of solvent, solvent ratio, distance between syringe and mandril, and applied voltage on the fabrication of samples was discussed. The optimized membrane was further used for the preparation of potential ABS/ZnO electrospun composite membrane by post surface modification. The composite membrane showed excellent anti-bacterial and oleophilic properties. It could effectively separate both natural oils (coconut oil, sun flower oil and gingelly oil) and mineral oils (kerosene, diesel and petrol) from water without any external energy. The prepared membrane containing 5% ZnO nanoparticles possesses substantial anti-bacterial activity against *E. coli* and *S. aureus* bacteria. Both the pristine ABS and ABS/ZnO composite membranes showed water contact angle of 135˚ and 130˚ respectively and the oil drops were found to absorb in the surface of the composite membrane. The composite showed better mechanical and thermal properties than pure ABS membrane. This work introduces a novel and sustainable technique for the separation of oil and water, which have potential application in industries for waste water management.



A schematic representation of ABS/ZnO electrospun membrane fabrication and its applications

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Enhanced Ionic Conductivity in Catechol Based Phosphorus Containing Polymer Electrolytes for Lithium Battery Applications

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Abstract

Rechargeable Li-ion batteries are major components of a vast variety of electronic devices. Flame-retardancy is a major challenge in battery synthesis as the temperature increase during a thermal runaway may result in fire or explosion. A completely solid state battery concept is of utmost interest due to assured energy density and safety parameters[1]. Four different phosphorus containing polyethers (P1-P4) for solid polymer electrolyte applications in Li-ion batteries have been synthesised and characterised. They are thermally stable with high molecular weight, porous nature and rod like morphology. The conductivity of one of the solid polymer electrolytes prepared from P3 with 40 wt % of LiTFSI was 2.3×10^{-3} S cm^{-1} at 30 °C and 7.7×10^{-2} S cm^{-1} at 80 °C, and remaining all polymers (P1- P4) showed good conductivity at RT (~10^{-3} S cm^{-1}). The high conductivity achieved is explained by the porous nature of the polymers.

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FPC-13

Reduced Graphene Oxide (rGO) Embedded Flexible Solid Polymer ElectrolyteFilms

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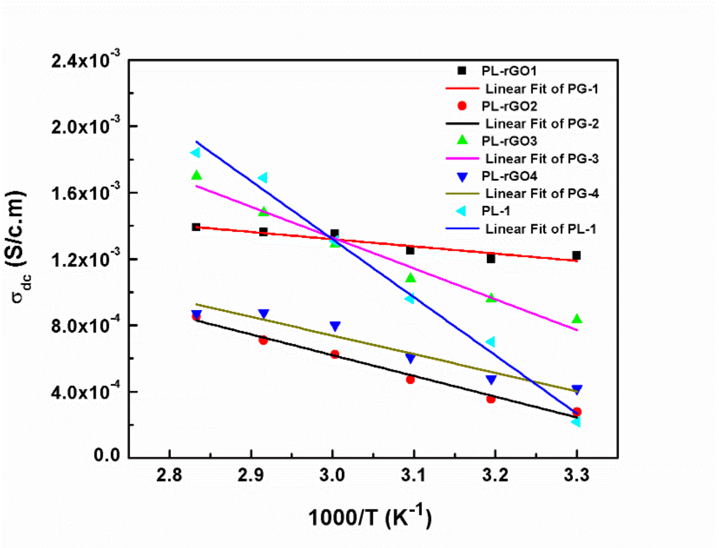
Abstract

Reduced graphene oxide (rGO) was synthesized from graphite by modified Hummers method. The rGOis embedded with Polystyrene sulfonic acid/Lithium phosphate to obtain PL-rGOsolid polymer electrolyte films. The electrical properties of Polystyrene sulfonic acid/Lithium phosphate/reduced graphene oxide composites were analyzed, which is an essential property to obtain the performance, reliability and lifetime of battery with respect to temperature. The mass and charge transfer process that takes place at the interface of electrode and electrolyte was obtained by Impedance analyser. The Nyquist plots were plotted in the frequency range 1 Hz- 35 MHz at different temperatures (30-200 ^{O}C). The ionic conductivity of PL-rGO polymer electrolyte is $1.4x10^{-3}$ S/c.m has been observed for the composition $PSSA/Li_3PO_4/rGO$::50:45:05wt%. The conductivity is found to increase with increase in temperature. The temperature dependent conductivity of the PL-rGO follows the Arrhenius relationship which shows hopping of the ions in the polymer matrix.



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FPC-15

Synthesis, Characterization of electrospun PEO/Cobalt oxide nanofibers and its photocatalytic activity

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Abstract

One dimensional cobalt oxide nanofibres with high photocatalytic activity were fabricated using the electrospinning method via a poly ethylene oxide (PEO)/Cobalt precursor based system. Cobalt oxide is a p type semiconductor with both direct and indirect band gaps and acts as a multifunctional material for catalytic activity. Optimum electrospinning parameters were investigated and the formation of Co_3O_4 nanofibers was confirmed with scanning electron microscopy (SEM) and energy dispersive X-ray (EDX) mapping. Furthermore, the crystalline lattice structure and surface roughness of fabricated nanofibers were evaluated using X-ray Diffraction (XRD) and Fourier Transform infrared (FT-IR) spectra. The dye degradation efficacy of Cobalt oxide/ PEO nanofibres was examined by using UV-Visible spectroscopy. Fabricated PEO/Co_3O_4 nanofibres exhibited excellent photocatalytic degradation activity against widely used model reactive dye, Reactive Methylene Blue (MB). Recently Co_3O_4 nanoparticles have gained a great deal of attention in dye waste removal from industrial effluents due to their exceptional adsorption ability and photocatalytic activity. Thus in this work the fabricated electrospun PEO/Co_3O_4 nanofibres degraded the reactive dye under UV-Visible irradiation.

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FPC-16

Rheological and Visco-elastic Performance Evaluation of SBC Electrospun nanofiber/Epoxy Composites: Experimental data Vs Theoretical Models

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Abstract

Electrospun nanofiber/epoxy composites are an advanced class of structural composite materials that provide superior specific mechanical properties. These fiber reinforced composites are benefitted from high aspect ratio and high surface area reinforcements[1-2]. In this work, the nanofibers of styrene butadiene copolymer were prepared from electrospinning technique and these fibers are incorporated in epoxy matrix and composites were developed. The tensile strength and modulus of reinforced composites were observed to increase. The dynamic mechanical properties of these composite materials were tested and a two-fold increase in storage modulus was observed. The experimental data was further compared with the known theoretical models. The fracture toughness of the composites displayed a tremendous improvement more than 100%, compared to unfilled epoxy systems. The rheological properties (strain sweep and frequency sweep) were experimentally determined and the results are fitted to the theoretical flow models. The thermal analysis of these composites was also performed and the thermal stability of the composites was investigated.

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Bio Composites from Styrene Butadiene Rubberand Chicken feather fiber

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Abstract

Fiber reinforced rubber composites are of immense importance both in the industrial field and in the area of research and development. The properties like tensile strength, elasticity, ductility, impact strength, abrasion resistance etc. of rubber can be improved by the incorporation of fibrous fillers. Short fibers obtained from agricultural resources are usually of lower density than inorganic fibers, environmentally friendly and relatively easy to obtain. Researchers have got momentum on the utilization of natural and biofibers as reinforcing agents in polymeric matrices for making composites for wide range of applications [1-2]. Chicken feathers are easily accessible fiber resource generated by poultry industry. The feathers are made of keratin, which contains ordered α-helix or β-sheet structures and some disordered structures. Chicken feathers possess unique properties which could be used advantageously in a number of applications. Use of chicken feathers as reinforcing agents for polymers has been tried by various researchers [4]. Chicken feather fiber was used as reinforcing agent in styrene butadiene rubber (SBR). Fibers of almost similar length and diameter were mixed into SBR using a Two Roll Mixing Mill. The mechanical and thermal properties of the composites were analysed as a function of fiber loading. The results indicate that feather fiber improves the mechanical properties and glass transition temperature of the rubber. Scanning electron microscopy revealed some interaction between the rubbers and feather fiber.

Key words*: Composites ,SBR, chicken feather*

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Effect of Pristine and Phytic acid Functionalized Boron Nitride Nanosheets (BNNSs) on Poly(L-lactic acid) Properties: Structure and Thermal Properties

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Abstract

Poly-L-lactic acid (PLLA) has received considerable interest in recent years because of its biodegradability, prominent applications[1] and polymorphism with six crystalline forms (α,α', α", β, γ, and ε). Each crystalline form was found to have unique sets of properties and therefore can be used for different applications. In the present work, we have prepared highly dispersed nanocomposites based on PLLA and pristine/phytic acid functionalized boron nitride nanosheets (BNNSs) - by solvent blending method. Characterization of PLLA nanocomposites was done based on the investigations on polymorphism, crystallization kinetics, thermal stability and thermal conductivity. In the presence of fillers PLLA crystallization was enhanced, optimum loading for pristine BNNSs was observed to be 0.5 wt.% with increased loading properties were retarded.The X-ray diffraction data showed that the presence of lower loadings of pristine BNNSs (0.5 wt%) readily favored the formation of ordered α-form in the melt crystallized samples. However with phytic acid modification, the rate of crystallization increased with increase in filler loading upto 20 wt.%. Also in the presence of surface modified filler, PLLA favored thermodynamically stable α form irrespective of filler loading percentage. This may be due to better dispersion of modified filler because of positive interaction between PLLA and phytic acid.

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FPC-19

Remote Functionalized Dual Distinct Solid State Sensor for VOCs

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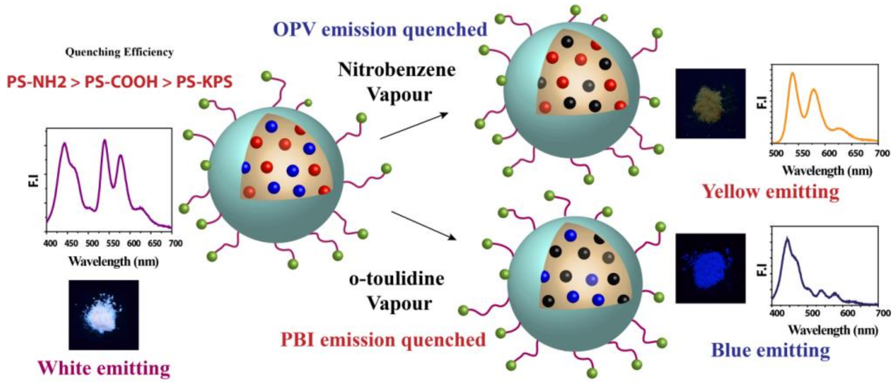
Abstract

Miniemulsion polymerization method was used to develop solid state emitting, distinctly dual vapour sensors with high quantum yield. Selective functionalization was done to decorate the polystyrene nanobeads having both perylene bisimide (PBI) and oligo (p-phenylene vinylene) (OPV) fluorophores with carboxy and amine functionality. White light emitting nanobeads on coming in contact with vapours of electron deficient nitroaromatics quenched OPV emission and exhibited yellow under UV lamp while exposure to amine vapours quashed PBI emission selectively and one observes blue emission under UV lamp. Such a wide range of color tuning from white to either blue or yellow from the same sensor makes it a true dual analyte sensor with two distinct outputs. Control of surface functionality (-COOH, -NH2 and neutral) on the nanobeads further enhanced the sensing efficiency. Real time, device based application has been demonstrated using free standing film. The fabricated film is capable for efficient detection of fast analyte exchange from dilute solution and it can be reused upto 8 cycles.



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FPC-21

Zwitterionic Poly(Vinylidene Fluoride) Graft Polymer With Unexpected Strong Blue Fluorescence

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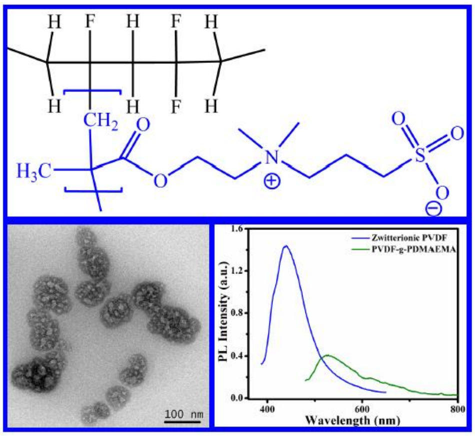
Abstract

Recently, many fluorescent polymers have been synthesized and extensively investigated due to their potential applications but it is a great challenge to prepare a new luminescent polymer from non-fluorescence polymer or without incorporating of any fluorophore moiety. The monomer *N*,*N*-dimethylaminoethyl methacrylate (DMAEMA) is grafted on PVDF backbone directly by atom transfer radical polymerization (ATRP). Then the amine groups of the graft polymer is reacted with 1,3 propane sultone to make a water soluble PVDF based zwitterionic polymer. ^{1}H NMR, DLS, and TEM study has been applied to investigate the structures and morphologies of the resultant polymer. TEM study shows vesicular aggregation of the zwitterionic polymer where PVDF helps to form this well defined self aggregation structure. Fluorescent study shows that the as-prepared zwitterionic graft polymer has strong blue fluorescence property. The precursor polymer shows very low emission where as the zwitterionc polymer shows strong blue emission with 8 fold increases in quantum yield. Theoretical study shows lone pair of the sulphate groups of zwitterionic pendent chains plays the key role to show the emission property of the polymer. The transition of lone pair (n to π* transition) from the sulphate group to the neighbouring carbonyl units of the grafted chains with in the vesicular aggregated structure causes the emission. Therefore, this study opens up a versatile platform to prepare PVDF based fluorescent polymers by post polymerization modification, which gives a new way to design fluorescent materials without incorporating of any fluorophore moiety for various applications.



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FPC-22

Self-Assembled Vesicles of Polystyrene-Clay Nanocomposite for Therapeutics

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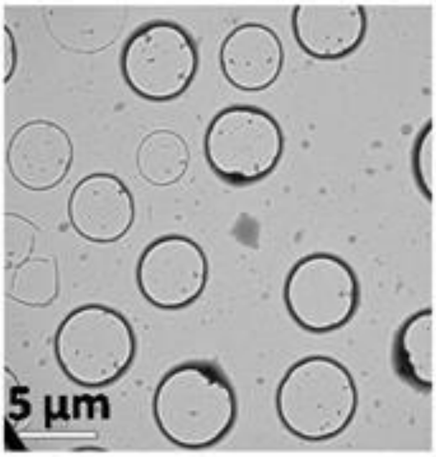
Abstract

Controlled delivery of drugs utilizing nano/micro structures using facile synthetic strategies are getting increased attention in therapeutics recently. In this context stable vesicles compared to liposomes in micro dimensions can be obtained by self-assembly by incorporating layered silicatetactoids in compatible polymers by suitable functionalization and tailoring the amphiphilicity. Polystyrene clay nanocomposite (PCN) particles, which exhibited concentration dependent self-assembly property in THF were synthesized by in situ intercalative polymerization of styrene with vinyl-grafted amino functionalized kaolinite. Microvesicles of diameter of 4.0-5.0 µm and average membrane thickness of 350 nm were produced from a solution concentration of 2.5 mg mL$^{-1.}$ The size of the vesicle showed an increase with increasing molecular weight. The particle possessed a sandwich structure consisting of PS-grafted intercalated clay tactoid at the core and PS chains growing from the tactoid surface, exposing the amino groups on the alumina layers. Curcumine encapsulated vesicles showed pH dependent release properties showing prospects for applications in therapeutics.



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FPC-23

Designing of Smart nanogels of Tragacanth Gum for anticancer drug delivery

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Abstract

Polymeric nanostructured materials have been playing an increasingly important role to revolutionize the diagnosis and treatment of diseases. Polymeric nanostructured materials including micelles, polymersomes, nanoparticles, nanocapsules, nanogels, nanofibers, dendrimers, brush polymers and nanocomposites, can be prepared by various methods. Smart materials transmit and respond to stimuli against external factors by producing a useful effect. The smart polymeric materials respond with a considerable change in their properties to small changes in their environment such as pH, temperature, humidity and light.

Tragacanth Gum (TG) is a polysaccharide which has excellent biocompatibility, hydrophilicity and functionality. TG was functionalised by grafting of itaconic acid using chemical initiation process. These smart hydrogels have been used for the immobilisation of anticancer drug. The investigation of the immobilised nanoparticle have been undertaken by the different techniques.

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FPC-24

Magnetically separable indolocarbazole based polymer - Ferrofluid hybrid system for efficient Cr(VI) removal

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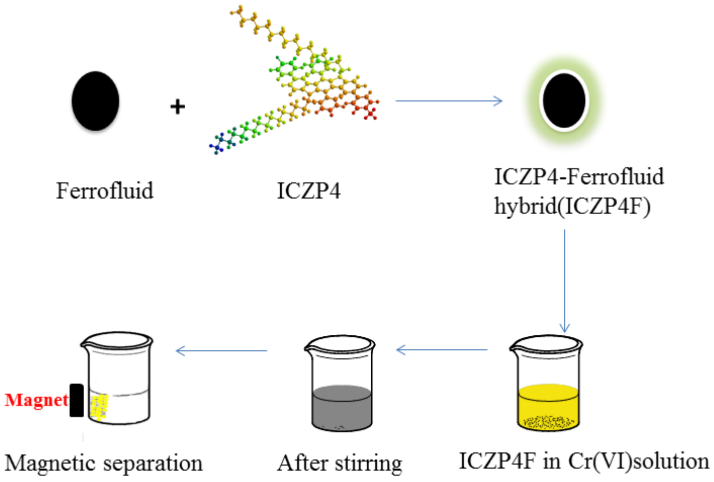
Abstract

A polyindolocarbazole-ferrofluid based magnetically separable composite has beendeveloped and characterized. Initially, the synthesis of a polyindolocarbazole based semiconducting polymer was done through Suzuki cross coupling reaction. The preparation of semiconducting magnetic polymer hybrid was achieved by mixing the newly synthesized semiconducting polymer with the magnetic ferrofluid. The characterization was done throughFTIR,^{1}H NMR,^{13}C NMR, GPC examinations. The hybrid material's (ICZP4F) characteristicswerefurther evaluatedby XRD, FTIR, SEM and magnetic susceptibility measurements. The magnetic hybrid materialhas been found to be a powerful adsorbent for toxic Cr(VI) ions in aqueous streams. The efficiency of the prepared hybrid was proved by the adsorptive removal and magnetic separation quickly within 11 min.The isotherm analysis indicates that the adsorption data impressively follow the Freundlichmodel. The adsorptive removal efficiency of the hybrid has beenexplainedby the synergistic effect between ICZP4 and the magnetite in ferrofliud.



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FPC-25

Surface-Patterned Polylactide/Schiff base/Zinc oxide Composite Membranes as a UV-light Shield

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Abstract

The present work highlights a novel way to develop ordered pores on polylactide (PLA) membranes. A breath figure formation (Figure 1) on the membrane surface, enriched with zinc oxide (ZnO) and a Schiff base (B) as additives, results in an interesting porous topography. Initially, hydrophilic ZnO has been found to be effectively dispersed in PLA - dichloromethane (PLA-DCM) solution in presence of the Schiff base. The polymer solution was later dried on a glass substrate in a humid atmosphere to generate porosity.

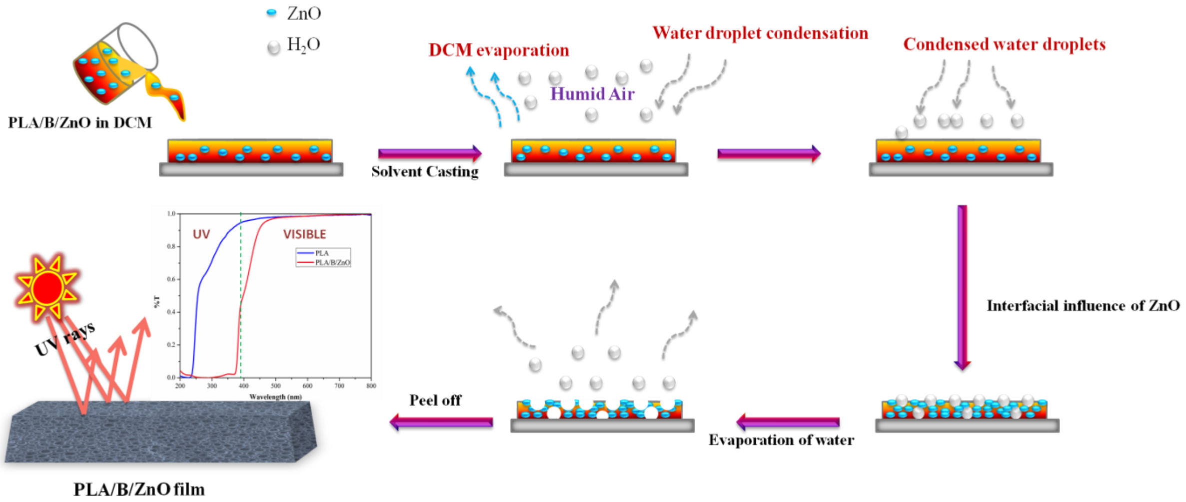

Figure 1. Breath figure patterning of polylactide membranes

The nitrogen atom in the Schiff base co-ordinates with the carbonyl group of PLA to plasticize the matrix for the effective dispersion of ZnO particles. An exciting feature exhibited by the newly developed composite membrane is its UV light screening with a perfect transparency towards visible light. The presence of ZnO and the porous texture causing multiple UV light reflection have been found to be responsible for the high impact UV shielding of the composite membranes.

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FPC-26

Synthesis, Characterization and BandgapTailoring of Poly (Methyl phenoxy) Phenylene/TiO_2Nanocomposites

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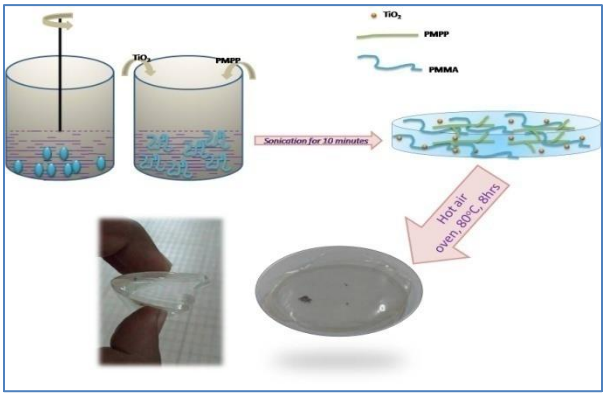
Abstract

Fabrication of conjugated polymer matrices and modification of their characteristics by the incorporation of suitable additives is an exciting area of research. In this work, we report the synthesis, characterization and bandgap tailoring of a polyphenyele derivative, poly (methyl phenoxy) phenylene*(PMPP)* using TiO_2 as an additive. Nickel catalyzed aromatic coupling has been adopted as the synthesis route for PMPP. Nano composites with 2%, 4%, and 6% loading of TiO_2have been developed. The composites are made into flexible films using a low weight percentage of PMMA as a partner. Absorption and emission characteristics of the systems were explored by UV-Visible and fluorescence spectroscopy. Thermal analysis confirmed the high temperature stability of the composites. The crystalline features of them have been confirmed from XRD and SEM techniques. The TiO_2 loading has been found to modulate the optical emission features of PMPP significantly.



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FPC-27

Synthesis of aromatic diimide containing bisphenols and their copolycarbonates

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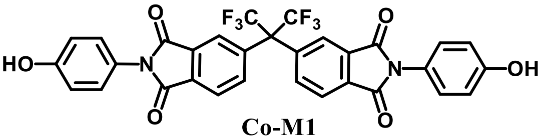
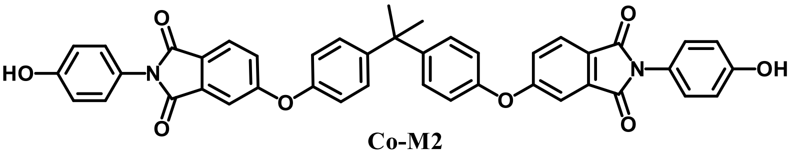
Abstract

A novel class of imide containing bisphenol A derivatives were synthesised using aromatic dianhydrides and 4-aminophenol by a simple solution condensation method. Different rigid (imide) and flexible (-C(CF_3)$_2$-, -C(CH_3)$_2$- and -O-) functional moieties were incorporated in the diimide comonomers. Aromatic bisphenol A copolycarbonates (Co-PCs) were prepared via melt-polycondenzation of bisphenol A with 5 and 10 mol percent of diimide containing bisphenol A (5,5'(perfluoropropane-2,2'-diyl)bis(2-(4-hydroxyphenyl)isoindoline-1,3-dione) (Co-M1) and 5,5'-(4,4'-(propane-2,2-diyl)bis(4,1-phenylene))bis(oxy)bis(2-(4-hydroxyphenyl)isoindoline-1,3-dion (Co-M2), and diphenylcarbonate (DPC).



Co-M1



Co-M2

The structures of polymers were characterized by FT-IR and NMR and thermal properties were measured by TG and DSC. BPA-PC homopolymers has a T_g of about 143° C. Co-PCs-1 and 2 with a 5 and 10 mol % incorporation of Co-M1, shows at T_g of 162 and 176 °C, respectively. Similarly, Co-M2 was incorporated (5 and 10 mol%), which shows a T_g of 153 and 159° C, respectively. Due to the incorporation of rigid (imide) and flexible (-C(CF_3)$_2$-, -C(CH_3)$_2$- and O) moieties in the polymer, the thermal stability of copolymers were enhanced by 20-30° C. High heat properties were achieved without loss of transparency, ductility and processability.

Keywords: Diimide; Copolycarbonates; Transparency; Ductility; Glass Transition Temperature:

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FPC-28

Multi-functionalization of Poly(vinylidene fluoride) Blend Membranes with pH- and Temperature-Responsive Permeation

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Abstract

A versatile approach for simultaneous immobilization and cross-linking of antifouling/low toxic polymers, e.g., poly(ethylenimine) (PEI),dextran (Dex), agarose (Agr), poly(ethylene glycol) (PEG), PEI−Dex, and PEI−PEG conjugates, and stimuli-responsivecopolymers on a porous membrane surface in mild reaction conditions is reported. A blend ultrafiltration membranes of poly(vinylidene fluoride) (PVDF), reactive copolymer e.g. poly(methyl methacrylate)-*co*-poly(chloromethylstyrene) and pore forming agent poly(vinylpyrrolidone) (PVP) was prepared and post-treated with the amine containing macromolecules. Sequentialnucleophilic substitution reaction between activated halide moieties of the copolymer and amine groups of different macromolecules readily provided series of modified membranes. The membrane was also treated with pH- and temperature-responsive poly(N,N-dimethyl amino ethyl methacrylate)-*b*-poly(N-isopropyl acrylamide) (PDMA-*b*-PNIPA) copolymer for the preparation of antifouling and stimuli-responsive membrane.Besides exhibiting good antifouling property, the membrane exhibited pH- and temperature-responsive permeation behaviour. The permeate flux of the membranes increases with either increasing pH or temperature or at a fixed temperature by increasing pH. The permeate fluxes show hysteresis during continuous heating and cooling cycles. Good reproducibility of each cycle of experiments was obtained. This indicates on-off switching of pore size with variation of temperature and pH. The membrane also showed pH-responsive permeates flux (42 $Lm^{-2}h^{-1}$ at pH 5 and 55 $Lm^{-2}h^{-1}$ at pH 7) during PEO filtration. Hence, this type of membrane can be used for tuneable filtration of macromolecules.[1] The modification of blend membrane with polyelectrolyte gave superhydrophilic and underwater superhydrophobic membrane for oil-water separation.[2]

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FPC-29

Phase Inversion Process for the Preparation of Ion Exchange Membrane

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Abstract

Ion-exchange membranes are wildly used in fuel cell, vanadium redox flow battery, electrodeionization, water purification and desalination. Ion exchange membranes (IEMs) are classified into two types depending on the charge (positive or negative) available on the membrane surface[1-5]. Cation exchange membrane (CEM) contains negative charge whereas anion exchange membrane contains positive charge on the membrane surface. Electrodialysis (ED) is a potential driven separation process used for separation of ionic species from aqueous solution, water desalination and purification. ED has some advantages over commonly used reverse osmosis process due to higher membrane life, low membrane fouling propensity and can be operated using solar power. IEMs are the heart of ED process. Good IEM should have high ion exchange capacity, high ionic conductivity and high transport number. Ion-exchange membranes are prepared by solution casting method. The membranes prepared by solution casting followed by drying are dense in nature. On the other hand, non-solvent induced phase inversion process are commonly used for the preparation of ultrafiltration membrane. The process is very fast and robust. A large quantity of membranes can be prepared in a very short time. We report the preparation of dense ion exchange membranes (CEM and AEM) from the compatible blend of polyvinylidene fluoride and reactive copolymer by non-solvent induced phase inversion process followed by post treatment. The parameters such as polymer concentration, solvent type, temperature of gelation bath, speed of roller of the casting chamber has been optimized to prepared dense membrane by phase inversion process. The membranes has been used for water desalination and purification (removal of fluoride, heavy metals) by ED process in domestic ED.

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FPC-30

Appling different testing methods to check compatibilization effect of ethoxy functionalized DevuleNR on SBR/DevuleNR/SiO2/Graphene oxide composites

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Abstract

The demand of styrene butadiene rubber (SBR) in tyre industry is growing day-by-day for reduced fuel consumption and consequently less CO_2 emission due to its low rolling resistance. SBR has inferior low temperature properties, tensile and tear properties whereas good aging and abrasion resistance property but natural rubber has outstanding tensile and tear strength. The fillers also play an important role for the product performance of the vulcanizate. Among the different fillers silica is eco-friendly widely used in rubber industry due to its petroleum-independence, outstanding reinforcement and low cost. However, the large number of hydroxyl group present on the surface of the silica makes it incompatible with the non polar rubber like NR, SBR etc., due to the agglomerate formation of silica particles. Moreover, the tensile, tear, and abrasion loss of the blend vulcanizates is further improved by silica-grapheme oxide (GO) dual phase filler along with lower rolling resistance without loss of wet skid resistance. It is reported in the literature that the GO-silica/SBR composite exhibited outstanding wear resistance and low rolling resistance which make it very competitive for "green tire" application. The in depth literature review clearly indicate that the dispersion of silica or GO into the non polar rubber matrix can only be achieved through functionalization of rubber or by addition of coupling agent.

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Controlled Growth of Polyaniline Chains from the Surface of Graphene Nano Sheets using 'Grafting from' Approach

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Abstract

A significant research efforts are devoted for the development of graphene/polyaniline (PANI) hybrid supercapacitor electrode fabrication where integration of capacitive performance of graphene nano sheet (GNS) and pseudo capacitance of PANI is accomplished.[1] Covalent attachment of PANI chains on GNS surface is acceptably the best way for extracting their maximum synergy.[2] In this respect, it is more acceptable strategy to grow PANI chains from GNS surface following a 'grafting from' strategy, as it allows retention of the structural sophistication of the GNS supports. However, it requires the growth of PANI chains in a controlled fashion. The literature reports show attempts for growth of PANI chains initiated from monomeric aniline moieties anchored on GNS surface.[3] However, given the mechanism of PANI, this strategy should result in the formation of significant amount of non–grafted chains from the aniline molecules present in the bulk during oxidative polymerization of aniline. In our previous report we have successfully demonstrated controlled growth of PANI chains from surface of carbon nanodots attached with *N*,*N'*-bis(4'-aminophenyl)-1,4-quinonediimine (APQD) a trimer of aniline in emaraldine state.[4] Here we apply the same strategy for explaining the general applicability of this strategy for growth of PANI chains initiated from the similar trimer moieties attached on graphene oxide nano sheets. The analysis of the prepared GNS/PANI materials through different instrumental techniques is presented. Interestingly, a similar attempt by initiating aniline polymerization from GNS surface tethered with aniline trimer (leucomeraldine form) moieties however does not give similar results.

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Exploring Novel Green Routes of Cross-Linking of Elastomers

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Abstract

Cross-linking is a crucial and important step in any rubber product manufacturing process. The requirement of the final products and economic aspects often govern the choice of crosslinking methods. Cross-linking enhances the elasticity of rubber through the formation of three-dimensional network structure and severely restricts the long-range motion of chain molecules. Unfortunately, the excellent properties of these cross-linked rubber compounds are associated with the practical impossibility of reprocessing these materials after their service life. The crosslinked rubber eventually becomes a less-valued material only suitable for non-technical applications, such as reclaimed rubbers. Therefore, recycling of conventionally crosslinked elastomer products is one of the major research interest at present. Here, we have explored multiple approaches to develop a recyclable elastomers without sacrificing required physical strength. For this purpose, molecular-recognition routes can prove to be a potential solutions for various recyclability problems those associated with elastomeric compounds. In the first approach, we present a study on chemical reactions between cis-1,4 polybutadiene(PBd)-graphene(G)- spontaneously instigated at 170 °C temperature. Several characterizations techniques, such as DSC, DMTA, and 1H–NMR study indeed showed the potential role of graphene as the cross-linking agent. We are also explore a relatively new approach, i.e. molecular recognition, which does not involve covalent bonding between two or more molecules. Incorporation of interactions, such as H- bonding, metal coordination, van der Waals forces or π-π interactions into the matrices enhance the initial attributes of sole elastomers. Development of alternative to conventional cross-linking techniques, preferably thermo-reversible cross-linking of general purpose elastomer is currently in the stage of infancy for commercial implementation.

FPC-34

Green synthesis of cellulose nanofibres (CNF) hybrid sponge and its applications

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Abstract

A sustainable and greener approach towards the environment has introduced different low-cost, non-toxic and biodegradable materials for the removal of an oil spill. Cellulose is worlds' lush natural biopolymer with the exception of this it conjointly offers a superb biocompatibility, lower density, substantial strength and mechanical characteristics, inexpensive in cost. By applying the physiochemical and mechanical techniques, cellulose structure explore to nanolevel i.e. cellulose nanofibres (CNFs) and even cellulose nanocrystals (CNCs). On the basis of functional modification of hydroxyl groups present on 2, 3, 6 positions of nanocellulose it's used in various outstanding application such as zero-dimension structure for drug delivery, spun in to 1- dimension fibers for enhance strength, cast in to 2 dimension films, composites for flexibility and molded in to 3 dimension aerogels and sponge for compressibility and porous material. With suitable functionalization and coating of this 3-dimensional sponge of nanocellulose from hydrophilic to the hydrophobic and oleophilic surface, we used it for the removal and recovery of oil from water resources. Additionally, the reusability of these materials after the recovery of oils has taken a step towards sustainability.

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FPC-35

Surface modification and biocompatibility improvement of muga (*Antheraeaassamensis*) silk fibroin by oxygen plasma

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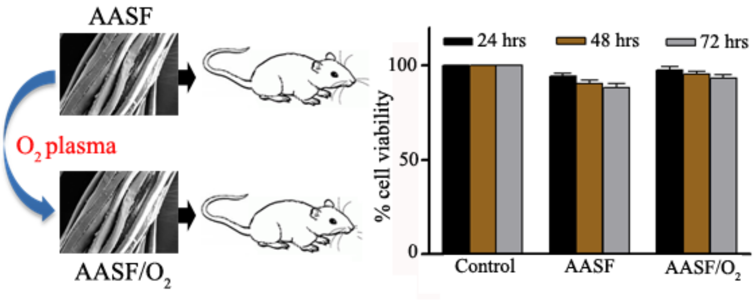
Abstract

Natural biopolymer such as muga (*Antheraeaassamensis*) silk fibroin (AASF) has recently drawn increasing research interest due to its ability to promote faster tissue growth and regeneration [1, 2]. Several studies have already been performed to investigate the surface modified silk fibroin as potential biomaterials, but most of them are achieved through wet chemical treatment [3]. In this work, surface functionalization of AASF has been carried out using low temperature oxygen (O_2) plasma (AASF/O_2) for improvement in its biocompatibility. The study further includes the effect of O_2 plasma treatment on surface morphology, surface chemistry and *in vivo* biocompatibility of AASF.O_2 plasma treatment induces surface hydrophilicity in AASF due to incorporation of polar functional groups onto the surface as revealed from X-ray photoelectron spectroscopy (XPS) analyses.Besides, O_2 plasma treatment facilitates formation of hydrogen bonds on the surface of AASF resulting in better mechanical behavior of the yarns.*In vitro* hemolysis assay and MTT cell viability results reveals improvement in biocompatibility of AASF over O_2 plasma treatment. From *in vivo* biocompatibility studies, it is observed that O_2 plasma treatment results in significant minimization of immunogenicity towards AASF without altering its biodegradability. The results demonstrate that AASF/O_2can be explored asmechanically robust potential non-immunogenic biomaterials in clinical and tissue engineering applications.



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FPC-36

Development of silk fibroin and zinc oxide Bionanocompositenanofibres

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Abstract

Bionanocomposite nanofibres comprising of *B. mori* Silk fibroin as natural component and Zinc oxide nanoparticle as an inorganic component were prepared using eletrospinning technique. The effect of incorporation of zinx oxide nanoparticles in the nanocomposite fibre was studied by uv-vis spectroscopy, optical microscopy and scanning electron microsopy. The thermal and antibacterialproperties of nanocomposite fibres were evaluated and compared with that of electrospun pure silk fibres.UV-VIS spectroscopy ananlysis of visible region showed reduction in the % Transmittance of nanofibrous mat containing Zno nanoparticleto about half of the pure SF mat, making it more translucent. Using optical microscopy and SEM analysis change in diameter of fibre from micrometer range to nanometer range is observed. Thermal analysis shows the shift in onset temperature and residual mass on incorporation of zno nanoparticle.This nanocomposite nanofibres have significant antimicrobial activity against *S. aureus* and*E.coli* bacteria.

Keywords: Bionanocomposite, Nanofibre, Silk fibroin, Zinc Oxide, Electrospinning

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FPC-37

Plant Nutrient Delivery through Foliar Route using Electrospun Nanofibers

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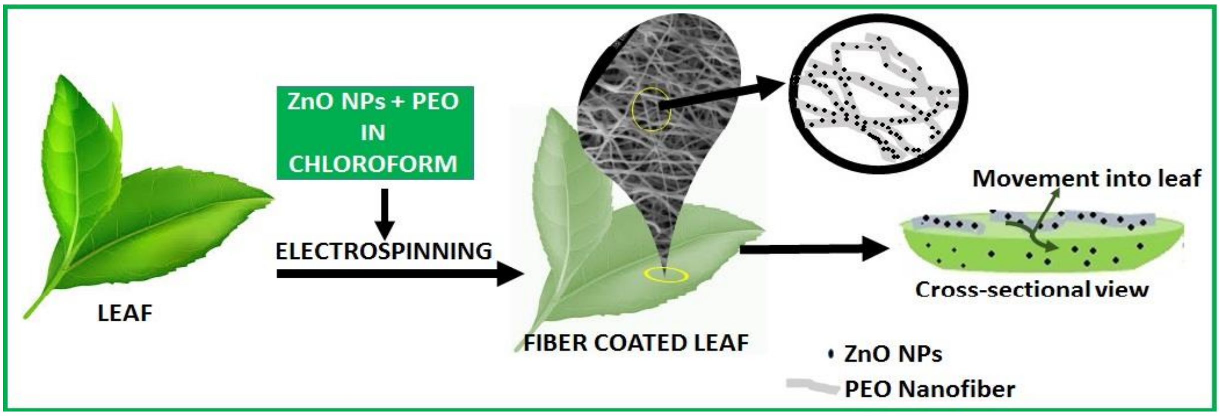
Abstract

Electrospun nanofibers have been applied to various fields but its application in agriculture is yet to be explored. Here nutrient incorporated polyethylene oxide (PEO) nanofibers have been used for sustainable agriculture through foliar application. A method where nutrients are supplied directly to the leaf when there is low accessibilityfrom the soil or the roots are not adequatelyactive. This would be an economic and environmentally desirable method to improve crop productivity. Zincis very important for the plantsas it forms an important constituent of enzymes and steps up productivity. Zinc oxide nanoparticles (ZnO NPs) have been delivered to the plant through the leaves viaemploying the PEO nanofibers which allows maximum dispersion. ThesynthesisedZnO NPs(ZnNO$_3$ with NaOH)were characterised and needle like nanostructures were observedfrom SEM studies. Smooth, uniform nanofibers of PEO were obtained on optimisation and about 1 wt % ZnO NPs were stirred with PEO and chloroform and electrospun into nanofibers. SEM images of the nanofibers confirmed ZnONPs incorporation. TGA studies showed an increase in the decomposition temperature of PEO and the water contact angle were also found to increase. These nanofibers were electrospun on the surface of the leaf to allow movement of nutrient zinc into the leaves. Other methods like solution or film coating may give agglomerated nanoparticles. Such usage, leads to economical use of the nutrient zinc, does not allow environment issues due to leaching and also provides for regulated consumptionof the nutrient.



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FPC-38

Effect of Long/Bulky Aromatic Side Chains on the properties of Polyimidesand nanocomposites of Polyimides with silica and Graphene oxide.

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Abstract

New kinds of diamine monomers were prepared with long and bulky aryl pendent groups and flexible linkages in the chain backbone as well as in the side chains**.**Diamine monomer structures were characterized by FT-IR, and ^{1}H-NMR. Polyimides were synthesized by reacting newly prepared diamines with dianhydrides BTDA or BPADA by two-step method and were characterized using NMR and FT-IR spectral techniques. Nanocomposites of polyimide were prepared from silicon-dioxide and graphene oxide nano particles by blendingthese fillers in to the polyamic acid by ultrasonification method followed by the thermal imidization method. Properties of polyimides and nanocomposites were studied using DSC, TGA, SEM, XRD, UTM etc. The resultant polyimides showed low T_g, fairly high thermal stability, improved elongation at break.Molecular weight of the polyimides are determined by Gel Permiation Chromatographic method. SEM analysis shows a uniform distribution of the nano filler in the polyimide matrix. TGA shows that the polyimide and nanocomposites have good thermal stability and LOI values of all polyimides and nanocomposites are above 28%. DSC analysis shows very low T_g values for neat polyimides and nanocomposites showed higher $T_g$than neat polyimides. The neat polyimides show good elongation at break but low tensile strength. The nanocomposites of polyimide show lower elongation at break but have improved tensile strength. The chemically imidised polyimides shows good solubility in solvents like DMF, DMAc, NMPand DMSO.

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[4 Tharakan, S.K;R,Sathyamoorthy;Radha,B;Sarojadevi M. *Polymer Composites*

FPC-39

Failure Analysis of Polymeric material using Analytical Pyrolysis

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Abstract

The failure of polymer and plastic materials often is caused by the inhomogeneous distribution of the used components inside the polymeric material or contaminations like particles, fibber's or inclusions may be the reason for its failure. In case of composite materials defect layers or a layer made from the wrong material will have a negative impact on the product properties. As such defects are often extremely small they are hard or even impossible to analyse by a macroscopic measurement. However, a successful failure analysis includes the chemical analysis of the faulty region in the sample.

In this paper, we present the application of analytical pyrolysis technology for a successful failure analysis by determining minute chemicals from faulty materials. Analytical pyrolysis consists of four different methods namely, evolved gas analysis (EGA), thermal desorption (TD), Pyrolysis (PY) and Heart-Cutting (HC). The sequence of the analytical approach is decided depending the data obtained from EGA. We present two examples (PVA and Rubber materials) to demonstrate how analytical pyrolysis is an useful tool for a successful failure analysis. A typical chromatogram obtained from a heart-cutting method is presented in Fig 1.

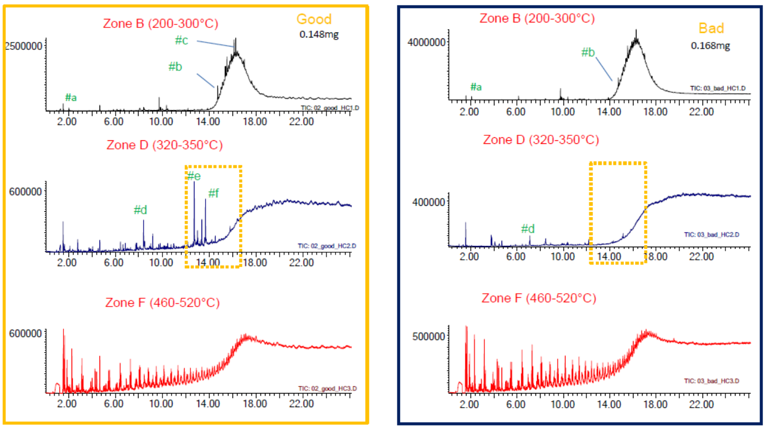

Fig 1 Heart-cut chromatogram of good and bad rubber from Diaphragm

FPC-40

Studies on High Heat Resistant Acrylic Adhesive

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Abstract

Acrylic copolymer was prepared by solution polymerisation technique using water as a solvent. The Cloisite 30B/Acrylic Copolymer nanocomposites with different loading of nanoclay (0.5-3.0%) were prepared by In-situ method. For compositional analysis fourier transform infrared spectroscopy (FTIR), Proton nuclear magnetic resonance (^{1}HNMR) and Isothermal thermal gravimetric analysis have been studied and results show that a suitable copolymer has been formed.

Different parameters like solid content, solubility, appearance, acid value and pH values were checked for each nanofilled copolymer.All compositions were checked for thermal stability by thermal gravimetric analysis (TGA) analysis and found that 50 % wt. at 398 °C for 2.0% filled Cloisite 30B/ Acrylic nanocomposite. Epoxy resin was added as tackifier with curing agent with acrylic system. Peel strength was checked for two substrate: corona treated metallised biaxially-oriented polypropylene (bopp)and nylon cloth. Peel strength was increasing with nanofiller loading upto 2.0%.

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FPC-41

Development of HTPB based Polymer Clay Nanocomposite as a New Binder System for Composite Propellant

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Abstract

HTPB is considered as a work horse polymeric binder for composite propellants because of its unique physico-chemical properties such as excellent solid loading capability and better shelf life than other binders. This research work reports the methods of preparation for HTPB-clay nanocomposites (HCN) and their mechanical and thermal properties for their functional utility in composite propellants as an improved binder system. These HCN's were prepared by dispersing nanoclays like closite 15A and closite Na+ (3% by wt) in the polymer matrix by high shear mixing. Process parameters like time, temperature and RPM, are optimized. After dispersion, dispersed clay platelets were trapped by curing of the polymer with isocyanates in presence of cure catalyst. Polyurethanes obtained by above said method were analyzed by small angle X-ray scattering (SAXS) and energy dispersive X-ray (EDX) spectroscopy. Elemental mapping using EDX suggested homogenous dispersion, while, SAXS analysis revealed partial exfoliation of clay platelets in polymer matrix. Tensile properties revealed that there is almost 17 % increase in tensile strength by inclusion of 3% closite Na+ while E-modulus increased exponentially (175%) with a 20% increase in elongation at break values. However, inclusion of closite 15 A (3% by wt) results in more or less similar tensile strength and elongation with an increase of E-modulus by 165%. Tensile properties for these nanocomposites were also determined at extremes of temperatures i.e. -40ºC and +55ºC to confirm their functional utility as operating temperature range for most of the missile systems lies in this range. These HCN's showed excellent low temperature strain capabilities and enhanced tensile strength and modulus at high temperatures also. Apart from improved tensile properties, HCN's showed better thermal stability over pristine HTPB.

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Nonlinear Absorption Studies in Functionalized Polymer

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Abstract

Electrospun nanofibers are being studied and developed because of their great potential in diverse domains of application such as optical sensors, tissue engineering etc. Functionalization of the surface and interior of these polymeric nanofibers with nanoparticles is an efficient fabrication method for a wide variety of nanoparticle-embedded materials. The aim is to compare the third order nonlinear absorption coefficient of the Au nanoparticles incorporated nanofibers with the casted films of CAN/PVA Au nanocomposites. Linear optical studies and morphological analysis of the prepared samples confirmed the incorporation of Au nanoparticles into the matrix. Open aperture Z-scan measurements were carried out at 532 nm and the samples were exposed to a 5 ns laser pulse. The nanofibers with Au nanoparticles exhibited higher two photon absorption coefficient than its nanocomposite solution. This enhancement is correlated with the morphology of nanofibers and electric field enhancement of Au nanoparticles into the polymer matrix. Optical limiting performance of the prepared nanocomposites and nanofibers show a better result than the film of CAN/PVA blend and CAN/PVA nanofiber mat due to the nonlinear absorption of the nanoparticles in resonant regime, thus making it suitable for optical limiting applications.

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Mechanical and Thermal Properties of Synthesized Polysilsesquioxane Powder Reinforced Epoxy Adhesive

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Abstract

Epoxy resin is the most commercially used polymer matrix for advanced composites field due to its chemical and mechanical properties. polymethylsilsesquioxane (PMS) and Poly (methyl/vinyl)silsesquioxane (PVS) powder was synthesized by hydrolytic condensation of organosilane precursor in aqueous phase. The synthesized Polysilsesquioxane (PS) powder were characterized by Fourier Transform Infrared Spectroscopy (FTIR) , Scanning Electron Microscopy (SEM) and the particle size of the PS powder was corroborated by imaje j software from the SEM images. The epoxy composites adhesives were developed using PS powder with different loading (1-4 phr). Tensile and compressive strength of the adhesive formulation were studied using the Universal Testing Machine. It was observed that the mechanical properties of the composites shows an increase on increasing the filler loading. Among all adhesive systems, PVS (4 phr) loaded epoxy composite (EPV-4) showed 65.4% enhancement than the neat epoxy system. Adhesive strength of the epoxy composites on mild steel substrate were investigated by conducting lap shear test and EPV-4 exhibited higher adhesive strength on mild steel adherent. Surface morphology of the epoxy composites and the fillers were visualized from the SEM images and the thermal conductivity of EPV-4 revealed 43% higher than as compared to neat epoxy composite.

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FPC-45

Isolation and Characterization of Chitin and Chitosan from Fresh Water Prawn Shells

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Abstract

Chitin and chitosan were prepared from exoskeleton of fresh water prawns found in Nepal employing standard experimental procedures. The chemical structure and degree of deacetylation (DD) in chitin and chitosan were studied through FTIR spectroscopy, XRD analysis complemented with titration methods as well as ash and moisture content measurements. In particular, the deacetylationprocess was monitored by variation of reaction time. It could be inferred that the chitin could be deacetylated to a considerable degree. The distinction between chitin and chitosan could be made through the nature of absorption bands in the frequency region corresponding to O-H, N-H stretching and amide group vibrations. It was found that the value of DD leveled off after a certain time indicating that the DD could be adjusted *via* reaction time control. Furthermore, targeting at antibacterial packaging material applications, the biodegradable blends with commercially available co-polyester were prepared and their mechanical properties were evaluated.

Keywords: *Chitin, Chitosan, FTIR spectroscopy, XRD, Biodegradable Blends*

FPC-47

Poly-Norbornene coupled Rhodamine-B derivative as an excellent Fe(III) ion chemodosimeter in semi-aqueous medium: a colorimetric and fluorimetric approach

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Abstract

Having significant role in cellular metabolism and enzymatic catalysis, iron is the most vital transition metal in case of both plant and human body [1]. Excess proportion of Fe(III) can cause harm to the lipids, nucleic acids and proteins, while deficiency of it can hamper oxygen transportation process and causes liver, kidney damage etc.[2]. Keeping these factors in knowledge we have designed a Norbornene coupled Rhodamine B derivative (**NR**) and its polymer (**PNR**) which can detect Fe(III) in 1:1 Acetonitrile/Water medium by changing the color from colorless to pink in naked eye and emission from non-fluorescent to reddish-yellow under UV light. Sensing behavior of NR has been investigated utilizing both UV-vis and fluorescence spectroscopic methods. Job's plot has been exploited to establish the binding stoichiometry between NR and Fe(III) as 2:3 which is further supported by ^{1}H NMR spectroscopy study and theoretical calculations. The association constant is found to be 4.9 x 10^5 M^{-1} using Benensi-Hildebrand method which implies strong binding of Fe(III) with **NR**. After thorough study of sensing behavior of NR we have synthesized its homopolymer(**PNR**)for "In-field" sensing application, which also exhibited similar response against Fe(III).Whole process has been demonstrated in Figure 1.

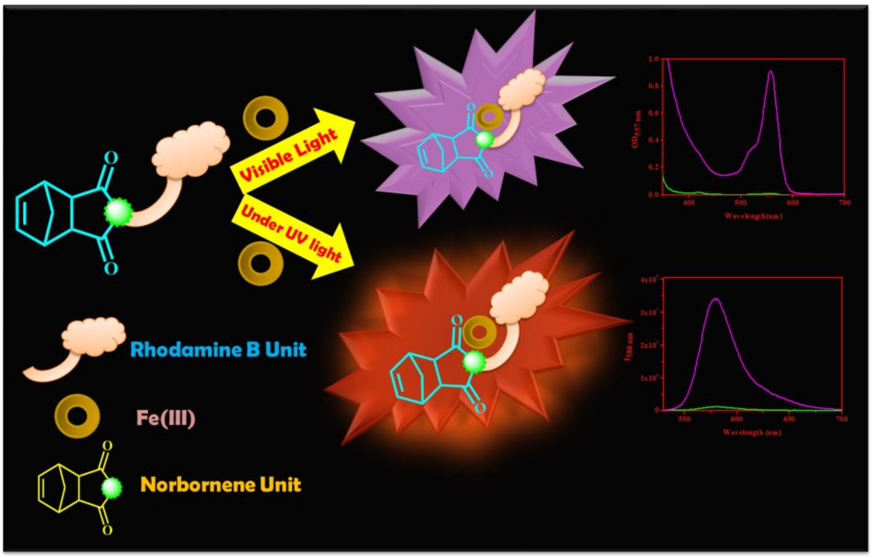

Figure 1: Cartoon representation of overall sensing phenomenon.

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FPC-49

Cross-linked Chitosan-Aminopropylsilane Graphene Oxide Adsorbent for Selective Removal of Pb(II) in Aqueous Medium

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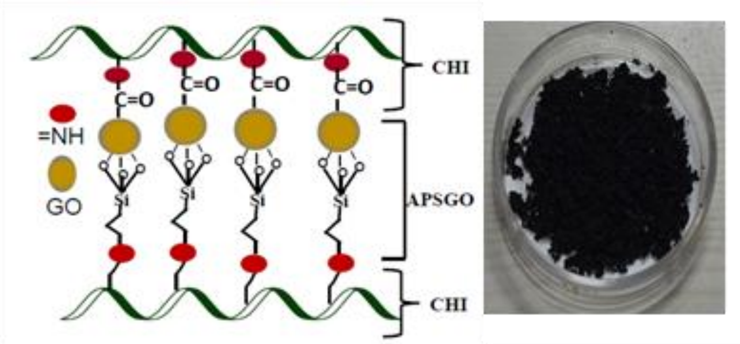
Abstract

Using graphene oxide (GO) and 3-amino-propyltrimethoxysilane (APTMS), aminopropylsilane graphene oxide (APSGO) was synthesized by condensation reaction. Cross-linked chitosan (CHI)-APSGO was prepared by acid-catalysed sol-gel process using glutaraldehyde as cross-linking agent. Prepared adsorbent was designed to exhibit high surface concentration of active-sites (-NH$_2$/=NH), and low swelling properties (due to incorporation of silica and formal cross-linking). The spherical and rough surface morphology of the adsorbent was altered after Pb(II) adsorption (SEM images). Cross-linked CHI-APSGO adsorbent showed selective adsorption for Pb(II) in may be due to larger hydrated radius of Pb(II) in compare with other metal ions (Cu^{2+}, Ni^{2+}, and Cr^{3+}). Effect of equilibrium time, temperature, pH, adsorbent dose and adsorbate concentration were investigated for selective removal of Pb(II) from aqueous solution, in batch process. Equilibrium adsorption followed the Langmuir and Freundlich isotherms, while different thermodynamic parameters (ΔG°, ΔH° and ΔS°) were confirmed the endothermic and spontaneous adsorption process. The adsorption capacity of CHI-APSGO adsorbent (112 mg g^{-1} at pH: 5.0) was superior to other adsorbents reported in literature. Desorption studies also revealed effective utilization of developed adsorbent for selective removal of Pb(II) from wastewater.



Specific cross-linked CHI-APSGO adsorbent with unique structura features for the selective removal Pb(II) from the aqueous media.

FPC-50

Effect of Mixing Strategy on Mechanical, Electrical, and Electromagnetic Shielding Effectiveness Performance of Chlorinated Polyethylene-Carbon NanofiberNanocomposites

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Abstract

Chlorinated polyethylene (CPE) filled with carbon nanofiber (CNF) nanocomposites were prepared using two different techniques such as melt mixing and solution cum melt mixing. A better dispersion of CNFs in nanocomposite was achieved by solution cum melt mixing compared to only melt mixing process. Nanocomposites prepared by solution cum melt mixing process showed higher mechanical properties, electrical conductivity (σ), and electromagnetic interference shielding effectiveness (EMI SE) compared to that of melt mixing process. 1 wt% CNFs filled nanocomposites prepared by the solution followed by melt mixing showed 124% higher tensile strength whereas at the same percentage of CNFs, melt processed nanocomposite exhibited 58% higher in tensile strength compared to neat CPE. The EMI SE and σ of both types of nanocomposites were increased with increasing CNFs loading. At 10 wt% CNFs loading, solution cum melt processed nanocomposite showed EMI SE 24 dB; whereas at the same wt% of CNFs loading, melt processed nanocomposite showed 22 dB.

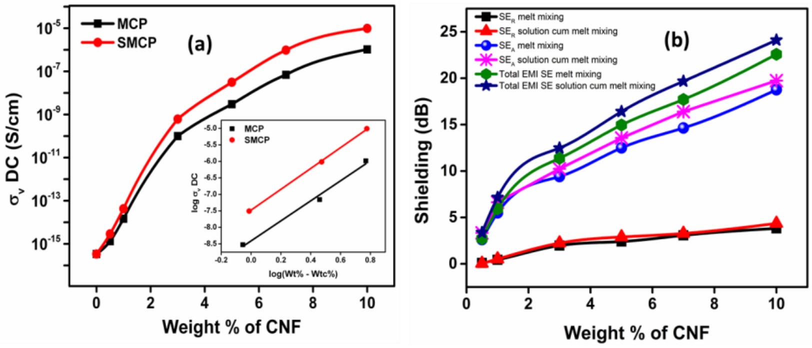

Figure: (a) DC conductivity of melt and solution cum melt mixed nanocomposites vs CNFs loading and (b) total EMI shielding, SE_R, and SE_A vs CNFs loading at 8.2 GHz frequency

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FPC-51

Synthesis of modified gum ghatti grafted acrylonitrile copolymer for adsorption of Mehtylene blue dye: Kinetics, Isotherm and thermodynamic studies

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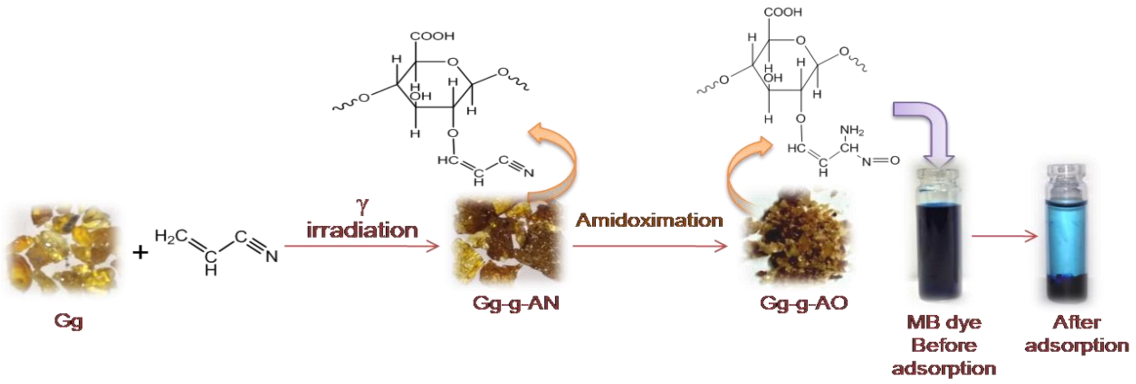
Abstract

Gum ghatti grafted acrylonitrile (Gg-g-An) copolymer was synthesized by gamma irradiation method. The structure of the Gg-g-An was characterized by FTIR, XRD and FESEM. The amidoximation of Gg-g-An was carried out in alkaline condition using hydroxylamine hydrochloride at 50^0C. The conversion of amidoximation (Gg-g-AO) was confirmed by FTIR. Adsorption of Methylene Blue dye (MB) as a function of effects of pH, amount of adsorbent, contact time, dye concentration and temperature were optimized by synthesized Gg-g-AO. The removal percentage of adsorbent to MB reached to 94.7 % at 50 mg/L. In order to investigate the adsorption mechanisms, kinetics models and isotherm models were employed to analyze the equilibrium data. The characteristic parameters and correlation coefficients for each model were determined. The adsorption kinetics was well described by the pseudo-second order model (r^2=0.998) and Langmuir adsorption isotherm (r^2=0.980). The calculated thermodynamic data demonstrates that adsorption is spontaneous and enhanced at higher temperatures. The findings of this study revealed that Gg-g-AO is a potential adsorbent for cationic dye pollution remediation.

Key Words: Graft copolmer, gum ghatti, kinetics, isotherm, thermodynamic studies



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FPC-53

Multi-functional properties of naturally derived ilmenite nanoparticles for Protective clothing

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Abstract

The study describes that thehydrophobic, UV-shielding and fire resistance properties of cotton fabric coated with $FeTiO_3$(FT) nanocompositesintercalated with Thermoplastic polyurethane (TPU). In this investigation, FT nanoparticleswere prepared using the acid extraction method. The prepared nanomaterials were characterized using some comprehensive analysis. The novel strategies were opted in this research including the design of TPU blended with silane functionalized FT based nanocomposite coated on cotton fabrics. Here, the colloidal TPU was prepared using the sol-gel method, mixed with thefunctionalized FT nanoparticles by shear mixture.Un-coated cotton fabrics were separately soaked with the prepared polymeric solutions with and without particles followed by Rocker shaker method. The surface morphology of the coated and uncoated cotton fabrics was analyzed using scanning electron microscopy (SEM) and confirmed the presence of nanoparticles on the surface of the fabric by energy dispersive X-ray spectroscopy (EDS). The structural, wettability and thermal analysis of the coated and uncoated fabrics was performed byFourier transform Infrared with Attenuated Total Reflectance Spectroscopy (FTIR-ATR), surface wettability and thermogravimetric (TGA) analysisrespectively. The physical interlinking between polymer and fillers was also responsible for risethe flammability property (LOI) than TPU.The FT nanoparticles coated cotton fabrics were exhibited a strong UVblocking ability on the cotton fabric surface. Furthermore, the coated cotton fabric also achieved outstanding washing durability after ten water laundering cycle. The nanocomposites coated fabrics could be recommended as the remarkable efficient for UV blocking applications.

Keywords: Thermoplastic Polyurethane, UVblocking, rocker shaker, $FeTiO_3$ nanoparticles, Surface wettability

FPC-54

Ultra Low Dielectric Constant Aerogels of Syndiotactic Polystyrene with Nanoporous Channels (ε) and Cavities (δ)

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Abstract

Syndiotactic polystyrene (sPS) is known to be crystallized into nanoporous-crystalline forms, where the density is lower than the corresponding amorphous phase. Recently, Guerra and co-workers reported the formation of nanoporous-crystalline sPS aerogelsby supercrtical carbon dioxide extraction procedures. In our work, nanoporous-crystalline sPS aerogels were prepared by a meticulously designed preparation route, which is simple, cost-effective, easily scalable and environmentally friendly compared to that of supercrtical carbon dioxide extraction.Briefly, the sPS gel was prepared using a solvent or a solvent mixture and subjected to successive steps of solvent exchange using non-solvents like ethanol and water. Such obtained hydrogels were subjected to freeze-drying to obtain aerogels as shown in Figure. In our recent paper, it has been showed that the δ aerogels exhibited the lowest ever dielectric constant of any polymer aerogel ($k = 1.03 \pm 0.02$), which is very close to the air. Herein, we systematically investigated the role of crystalline phase of aerogel on properties like dielectric constant, thermal conductivity, hydrophobicity, etc.

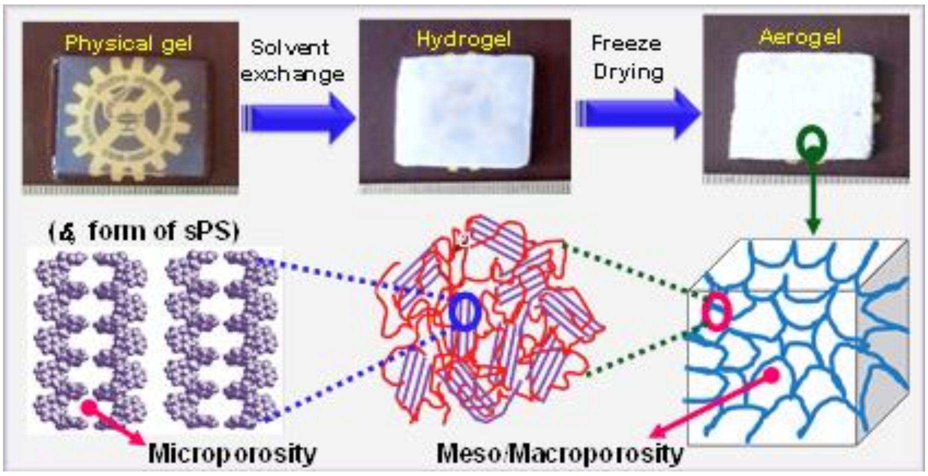

Figure 1. Photographs and schematic representation of the different stages involved in the preparation of sPS aerogel possessing macroporosity, mesoporosity and ordered microporosity.

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A selective ratiometric choromogenic fluoride chemodosimeter by 2,4-dinitrophenylhydrazine derivative in semi-aqueous medium and its mode of interaction.

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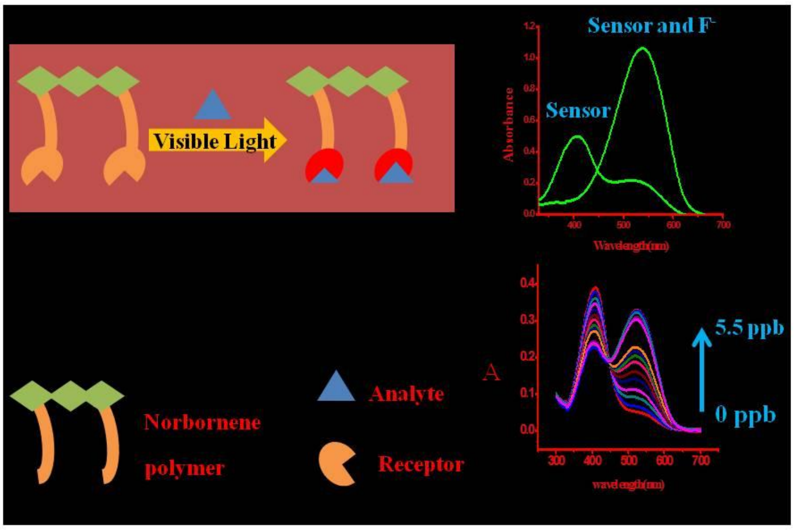
Abstract

Colorimetric anion sensors are very useful to detect the response by naked eye. Two novel highly selective 2,4-dinitrophenylhydrazine based colorimetric probes were designed, synthesized and employed as a selective ratiometric optical chemodosimeter for fluoride through naked eye. The anion recognition properties were investigated via pattern of color change as well as changes in absorbance signal. Sensor molecules were characterised by ^{1}H-NMR,^{13}C-NMR, MASS and FT-IR spectroscopy. Selectivity towards fluoride anion was attributed to the capability of hydrogen bonding interaction of N-H bond, which was detemined by ^{1}H-NMR and UV-vis spectroscopic titration as well as Density Functional Theory calculation. The association constant was calculated using Benesi-Hildebrand equation by UV-vis analysis. Job's plot analysis was reveled the existance of 1:1 complex formation of fluoride anion with sensor molecule. Same colorimetric response and selectivity properties were shown by norbornene based homopolymer towards fluoride anion.



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FPC-57

Internally Functionalized Porous Crosslinked Polymers using Thermally Cleavable Porogens

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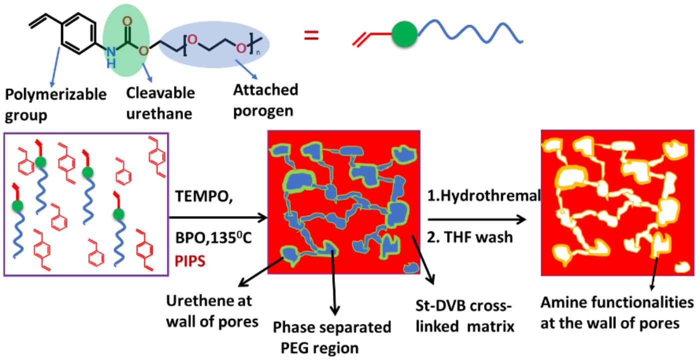
Abstract

Porous polymers with functional groups lining the pores walls are of special interest because of their potential application in gas storage and separation,as catalyst support, water-purification membranes, and other applications.[1] While in most cases, functional groups are incorporated by post-polymerization modification, a strategy to install functional groups directly during the process of pore-formation would be highly desirable. Typically, porous polymers are prepared by the use of porogens that serve as *space-holders* during the polymerization process, and are removed subsequently. Polymerization Induced Phase Separation technique[2] (PIPS) is an interesting process that leads to the phase-separation of the porogen during the polymerization process. In the present study, we have designed a *polymerizable porogen*, wherein the space-holding segment that microphase separates is linked to the polymerizable fragement via a *thermally labile urethane linkage*; thermal treatment and removal of the porogen segment leads to porous crosslinked polymers bearing amine groups on the inner walls of the pores.



Schematic of the design for generating amine functionalized porous matrices

Our specific design invloves the synthesis of a molecule bearing a styrenic unit that is linked to a water-soluble PEG segment via a thermally labile urethane linkage; polymerization of this polymerizable porogen (PP) in presence of divinylbenzene (DVB) by Nitroxy-mediated controlled radical polymerization leads to the formation of a crosslinked matrix. During polymerization, the hydrophilic PEG units undergo microphase separation to form PEG-rich domains within the hydrophobic crosslinked polystyrenic matrix; the key feature of this design is that, during this process, the urethane linkages become located at theinterface of PEG and PS domains. Hydrothermal treatment (@165°C) of these cross-linked matrices leads to the cleavage and transformation of urethane linkages to amines, that line the internal walls of the matrix; PEG-OH that is liberated in the process is removed along with the water (see schematic). In the presentation, various factors that influence the pore-size, internal surface area and functional group density will be highlighted; furthermore, altenative strategies to directly install other types of functional groups will be discussed.

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FPC-59

Enhancement in Structural, Mechanical and Gas Barrier Properties of Poly(ethylene terephthalate)/Indian Clay Nanohybrid

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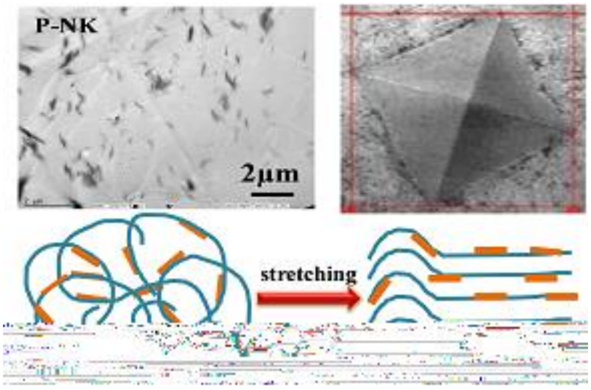
Abstract

Thermoplastic and amorphous poly(ethylene terephthalate)/clay nanohybrids have been prepared via solution route. Indian origin organically modified nanoclay have been used as a filler in different concentrations to enhance the properties. A significant level of dispersion and intercalation of nanoclay in the polymer matrix occurs due to strong interaction between nanoclay and polymer matrix. The nanohybrids have been tested for thermal stability and exhibit higher glass transition temperature. The Young's modulus has increased significantly (66%). Halpin Tsai and Hui-Shia models have been fitted well to explain the nature of stiffness [1]. Vicker hardness test has shown considerable improvement in hardness (16%) in nanohybrids as compared to pure PET and the hardness values are nicely predicted using the modified rule of mixture model. The effect of uniaxial stretching on the structural development is explored through small angle X-ray scattering and wide angle XRD. The nanoclay has induced short range ordering in nanohybrids upon stretching as compared to pristine PET. Debye Bueche model has been used to calculate the blob size which has increased in stretched samples. Nanoclay has induced high barrier for gas permeation in nanohybrids in comparison to pure PET. Oxygen transmission rate has also been found to decrease up to 38% for using meager amount of nanoclay. The experimental permeability data has been fitted with different models for aspect ratio as a fitting parameter and the prediction of barrier properties has been found suitable for its real applications [2].



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FPC-60

Thermoresponsive Shape Memory Polymer Nanocomposite for Self-Expanding Stent Application

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Abstract

The nanocomposite of polyurethane has been synthesized through in-situ polymerization of aliphatic diisocyanate, ester polyol and chain extender in presence of two-dimensional nano clay (30B). Polymerization within the platelet galleries helps to intercalate, generate diverse nanostructure and improved nano to macro scale self-assembly leading to the significant enhancement in toughness and thermal stability of the nanohybrid in comparison to pure polyurethane. Nanohybrid exhibits significant improvement in shape memory phenomena (91% recovery) at the physiological temperature suits them for many biomedical applications. Structural alteration, studied through temperature dependent small angle neutron scattering and X-ray diffraction, along with unique crystallization behavior have been extensively revealed the special shape memory behavior of this nanohybrid understanding the molecular flipping in presence nanoplatelets. In-vivo study on albino rats exhibits the potential of nanohybrid as self-tightening suture in keyhole surgery by closing the wound lips appropriately through the recovery of the programmed shape at physiological temperature. Further, the improved biodegradable nature along with the rapid self-expanding ability of the nanohybrid at 37 °C make it appropriate for many biomedical applications including a self-expanding stent for occlusion recovery due to its tough and flexible nature.

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FPC-61

A Water-Soluble Tryptophan Based Dual-Action Polymeric Probe for Turn-On Sensing, Bioimaging and Removal of Mercury(II) Ions; Chemosensor for Hydrogen Sulphate Ions

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Abstract

At present, selective recognition and sensing of both cations and anions by a single fluorescent receptors have attracted a considerable research interest in terms of their potential environmental and biological applications. In this context, a new tryptophan-dithiocarbamate based fluorescence polymeric probe was synthesized and has been targeted with a view for sensing both cation and anion in aqueous media.Upon addition of various metal ions, the probe afforded an irreversible change only with Hg^{2+} ions in aqueous media with a five-fold enhancement of the fluorescence (Φ = 0.055→0.250)attributed to photo-induced electron transfer (PET) process. Intracellular detection of Hg^{2+} ions was achieved in human breast cancer cell line, MDA-MB-468 using the synthesized macromolecular probe. Moreover, this unique design has an unprecedented detection sensitivity of 300 parts per trillion (ppt) for Hg^{2+} ions, the most effectivewater-soluble amino acid-based polymeric sensor reported till so far. Hg^{2+} ions gets trapped when it passed through a column containing polymeric probe with 94% removal capacity as verified using ICP-OES instrument.In addition, the probe can also be able detect parts per million (ppm) level of hydrogen sulphate anion (HSO_4^-) among various anions with high selectivity in aqueous medium, induced by the hydrogen bonding interactions of polymeric probe with the anion. Even though our synthesized polymeric probe possesses two separate binding site for HSO_4^- and Hg^{2+} ions, it has been shown that the presence of the cation influences the binding of the anion.

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FPC-62

Modification of MMT clay by Polyphosphoric acid for water purification

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Abstract

Fresh Water being the most vital requirement for sustaining life on earth is being depleted day by day due to anthropological activity. According to the World Bank estimation, organic pollutants are prominent and 17−20% share of polluted water comes from of thetextile and dyeing industries[1]. In our work the removal of organic dye pollutants from is studied using montmorillonite clay (MMT) and a modified MMT and its composite with Poly vinyl alcohol (PVA) usingMethylene Blueas model dye.MMT was modified using Polyphoshoric acid,an olegomer of phosphoric acid by a simple method.The polyphosphoric acid modified (PMMT) obtained was characterized using FTIR, TGA XRD,FESEM, and TEM. It was found that the interlayer distance and the surface area of MMT was increased tremendously in PMMT, which was confirmed by XRD analysis. The 2θ angle changes from 7.29 to 6.02 and the inter space distance increases from 1.21nm to 1.46 nm[2]. The BET surface area is found to be 545.53m²/g. The dye adsorption studies were carried out at different concentrations of Methylene Blue by UV analysis. PMMT is showing better dye adsorption because it has an acidic nature, high inter layer distance between the planes and high surface area and hence highly effective and a low cost adsorbent for cationic dyes[3]. A thin film composite of MMT and PMMT with Poly vinyl alcohol were aslo prepared and the dye adsorption properties were studied. The PVA-PMMT composite shows better adsorption properties.

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Epoxy-Polydimethylsiloxane-Zinc Oxide Nanocomposite Coatings for Protective Applications

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Abstract

Epoxy-polydimethylsiloxane-zinc oxide coatings were fabricated successfully to improvise the coating properties like superior mechanical strength, increased thermal stability and corrosion inhibition property. The synthesis of the nanocomposite coating was confirmed by FTIR and XRD analysis. The aim is to tune the surface properties of epoxy-polydimethylsiloxane composite coatings in order to obtain hydrophobic and corrosion-resistant protective surfaces to cater marine applications. The compatibility of the blend components was investigated usingFESEM and TEM analysis. The mechanical, thermal and hydrophobic properties of the synthesized coatings were evaluated by tensile, DSC, TGA and WCA tests, respectively. The corrosion behavior of the coatings was evaluated as per ASTM G102 using potentiodynamic polarization curves in 3.5 wt. % NaCl solution.A significant amount of reduction in the corrosion rate of the designed nanocomposite coating was observed providing barrier protection at various degrees to metallic substrates.It is worthwhile to notice that the nano- filler based epoxy-polydimethylsiloxane coatings are reported to be the best of the thermoset class promoting excellent corrosion- resistant properties.

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FPC-64

Improvement of Hydrophilic Characteristics of Polypropylene

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Abstract

Polypropylene (PP) is a thermoplastic fastest growing polymer having excellent chemical Resistance, elasticity and toughness, fatigue resistance, insulation and transmissivity hence its use in numbers of application such as automobile, packaging, spare parts, consumer product, fibers, packaging etc. but at the same time PP has highly hydrophobic in the nature with very low surface energy result in poor printability, printability, dyeability which restricts its use in some specialty[1] application such as medical, filtration, fiber as reinforce material etc.

The melt blending of polypropylene (PP) and hydrophilic modifier having with polar group phenol ethoxylated phosphate ester at different weight ratio through melt extrusion process. The blended material is used for prepared film through compassion molding, which was characterized for FTIR, contact angle, DSC and morphology – SEM & EDX. The film prepared through blended material showed significant improvement in contact angle compared to as such pure homo PP sample indicated improvement in hydrphilicity. Blended modified PP is used for spin fiber through multifilament extruder. The fiber was used as reinforce agent in cement sheet, the adhesion of fiber with cement particle was studied through scanning electron microscope. The adhesion of cement particle with modified fiber was better compared to as such homo pp. The modified hydrophilic PP is simple and convenient process and easy operation, and may be applied for many industrial application

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Impact Properties of Polyurethane based Concrete System

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Abstract

Concrete is one of the popular construction material used all over the world. But over the last few decades, polymer concrete is being introduced in order to fulfil various constructional requirements (such as zero water absorption, quick setting time, earthquake resistance, impact barriers, high flexural strengths, chemical resistance, etc.) However, there has been relatively less published work available on the mechanical behaviour of Polymer Concrete.The objective of this project is to improve the commercially used Polymer based Concrete material, to make it suitable for applications like Industrial Flooring and thin section Precasts. The project, therefore, aims at evaluating the impact behaviour of Polymer based Concrete over Conventional Concrete, using destructive testing(drop weight impact test). The uniqueness of this work encompasses modification of impact strength using Polyurethane Emulsion in Polymer based Concrete applications wherein the system works as organic-inorganic interpentrating polymer network (IPN). The system consisted of Polyurethane resin, hardener, white cement, fine silica.The effect of PET fibers (Recron®3s) used as reinforcement on the system was also studied. Overall, eight formulations based on varying fibre quantity, filler particle size, polyurethane resin were studied. It was observed that the impact strength of polyurthane based concrete was significantly enhanced (up to 25 times)compared to Conventional Concrete. The material with modified resin and modified fillers, achieved strengths comparable with M40 mix design of Conventional Concrete.

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FPC-66

Thermoresponsive N-Heterocyclic Carbene capped Pd Nanoparticles

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Abstract

N-Heterocyclic Carbene (NHC) has been used as a versatile ligand for metal complexes in organometallic transformations.Being strong donor and poor π electron acceptor theyprovide stability to the NHC-Metal complexes/nanoparticles(NPs) and stable in air and moisture[1].Having phosphine as a ligand may lead to the decomposition in metal complex hence NHC has been used as a ligand instead of phosphines[2]. Even thoughNHC moiety provides stability to metal complexes, they lacked water solubility and recyclability hence NHC moieties were modified using polymers, silica, nanoparticles.Ghotbinejad et al. reported recyclable magnetic nanoparticles for Suzuki coupling reaction using DMF at 70 °C[3].Zhong carried out coupling reaction usingNHC-Pd complex and additivein water at rt to 100 °C[4]. Wang reported NHC-Microporous polymer-Pd NPs for Suzuki coupling reaction using Ethanol/Water mixture at 80 °C[5]. Based upon the literature reports it is noted that either mixture of solvents, high temperature or additive is requiredto perform the reaction.

To overcome these drawbacks, we synthesized Thermoresponsive NHC capped Pd nanoparticles which is incorporated withpoly(N-Isopropylacrylamide) moiety to possess for water solubility and recyclability by undergoing phase separation at Lower Critical Solution Temperature (LCST)&NHC to act as a capping agent for the Pd NPs. Using this catalyst Suzuki coupling reaction can be carried out in water medium at room temperature and the catalyst can be recovered by heating the reaction mixture to above LCST and be able to successively recyclable for few cycles with minimal loss of activity.

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FPC-67

Controlling Hydrophobicity On Leather Surface By Incorporating Various Carbon Nanomaterials Integrated With Acrylate Polymers

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Abstract

Leather auxiliary used for leather surface coating, leather finishing agents not only can protect the leather from damage but also can beautify the leather surface, thereby covering the shortage of artificial leathers[1]. Among the most promising systems, nanomaterials are currently attracting the worldwide interest of researchers to develop novel approaches in leather finishing and coatings[2].Lately, scientists have explored the potential of nanotechnology to alter physicomechanical, optical, electrical, and biological properties of various leather materials[3]. We synthesized Polymer(PMMA/PMAA) Nano(MWCNT / Fullerene) Conjugates through free radical polymerization with Chain Transfer Agent (CTA). The important usage of Carbon nanomaterial is to create surface roughness on the Leather surface and also to give extra stability to polymer matrix through strong interaction with the polymer chains.Small angle X-ray scattering, AFM roughness measurements suggests that a surface morphology with fractal dimension allows for the optimum coupling of roughness-induced superhydrophobicity and was confirmed by contact angle.Its thermal stability was confirmed by TGA and DSC thermogram. The possible interaction between the polymer and the Carbon nanomaterials was further confirmed by FT-IR and RAMAN spectroscopy. Surface morphology was confirmed by FE-SEM analysis. Confirmation of polymerization was studied using 1H NMR and its mass was obtained by MALDI. Above results supports and confirms the stability as well as superhydrophobic interaction between the polymers nano conjugates with Leather. Also Fullerene bonded Polymer conjugate gave a smooth coating on the surface of leather whereas MWCNT bonded Polymer conjugate showed improved hydrophobic properties on the surface. Further studies with these Polymer nano conjugates may open up ways for a clean and smooth coating finishes.

PNC coated on leather surfaces

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Thermal, Mechanical and Rheological Evaluation of Reactor Made PP/CNT Composites

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Abstract

Polymer nanocomposites are playing very important role in advanced material and composite industries. Carbon nanotubes (CNTs) and other natural resources based materials are suitable fillers for thermoplastic polymers due to their electrical and mechanical properties. Nanofillers/microfillers are used to reduce the cost of the new material and to enhance the properties for desired applications. It is well established study that the properties of different polymer-basednanocomposites strongly depend upon the dispersion of fillers. Polypropylene compatibility with nanofillers also can be improved through extrusion route by matrix modification and grafting it with reactive moieties, such as acrylic acid, acrylic esters, and maleic anhydride. Ziegler-Natta catalyst is the most used systems in industry for the production of polyolefin. The polypropylene (PP) nanocomposite was prepared by incorporating highly pure MWCNT by In-situ polymerization of propylene with Ziegler-Natta (ZN) catalyst at certain temperature and pressure. The mechanical rheological and thermal stability of reactor made PP/CNT nanocomposite increased in comparison with neat PP. SEM images shown better dispersion of carbon nanotube in polypropylene matrix.

The aim of this paper is to provide comprehensive study of reactor made PP/CNT nanocomposite preparation method and properties.

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FPC-69

Facile method for the reduction of graphene oxide and its composites with epoxy resins

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Abstract

Large scale preparation of graphene can be done by either chemical or thermal reduction of graphene oxide (GO). Compared with the chemical reduction route, thermal reduction offers high electrical conductivity and large surface area to the final product. This work repots a simple and low cost method for the thermal reduction of GO. GO was synthesized from graphite powder by Modified Hummer's method and was thermally treated at 400 ºC for 4 h in a muffle furnace resulting in a low density, fluffy material (RGO). Characterizations including XRD, FTIR, Raman analysis and TGA of GO and RGO revealed the intercalation of oxygen functionalities upon oxidation and restoration of graphitic network after thermal treatment. FESEM images shows the layered structure of RGO. TGA shows better thermal stability of RGO compared to GO. Epoxy/RGO nanocomposites containing various loadings (0-3 wt. %) of RGO were prepared and its mechanical properties such as tensile strength, Young's modulus and impact strength were improved. The DC and AC conductivity also increased with increased loadings of RGO.

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FPC-70

Study on mechanical,thermal and morphological properties of TPU/PBT Blends and TPU/PBT/MWCNT nano- composites

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Abstract

Polymer nanocomposites based on thermoplastic polyurethane elastomer, polybutylene tetrephathalate and multiwalled nanotubes (MWCNTs) were prepared. Between TPU and PBT, the effects of different percentage of carbon nanotubes content on the mechanical, thermal, and morphological properties of the nanocomposites were investigated. The tensile strength of the nanocomposite increased, while the elongation at break decreased with the amount of MWCNTs in the blend. Differential scanning calorimetry (DSC) results showed that the addition of MWCNTs reduces the degree of crystallinity and increases the melting temperature of the blend. Thermogravimetric analysis (TGA) studies of the TPU/PBT/MWCNTs nanocomposites exhibit a remarkable thermal stability much higher than that of the TPU/PBT blend. Further, scanning electron microscopy (SEM) showed that the added MWCNTs reduced the domain size of the dispersed phase in the blends.

Keywords : Thermoplastic blend; multiwalled Carbon nanotubes; Mechanical property; thermal property and nanocomposites

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FPC-71

Effect of Micro- and Nanoparticlesof Ceramics on Thermal and Mechancial Properties of High Performance Polymeric Composites

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Abstract

High-performance polymeric materials have been increasingly demanded by many cutting-edge fields like printed circuit boards/electronic substrates, tribological, biomedical, and aerospace industries. In present work, high-performance polymeric composites based on polyetherketone (PEK) as a matrix and hexagonal boron nitride (h-BN) powder (both micro- and nanosized particles) as reinforcements were fabricated using planetary ball mill followed by hot pressing. The effect of micro- and nanoparticles of h-BN on crystallization, thermal stability, dimensional stability and mechancial properties were studied. Field emission scanning electron microscopy showeduniform dispersion of micro- and nanoparticles of h-BN in the PEK matrix.Thermal stability and the dimensional stability of both micro- and nanocomposites were found to increase with increasing h-BN particles compared to that of pure PEK. The Vickers microhardness and storage modulus of the composites were also found to increasesignificantly with increasing h-BN particles.

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FPC-72

TriphenylamineAppended derivatives: Electropolymerization, Electrochromic and Electrofluorochromicbehaviours

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Abstract

Triphenylamine containing two derivatives (Benz-3TPA and Benz-3CNTPA) have been designed and prepared with good yield to have polymeric film using electropolymerization and to check electrochromic properties. Through the oxidative electrochemical polymerization on ITO surface, both the derivatives form polymers (p-Benz-3TPA and p-Benz-3CNTPA) that have been verified with the help of UV-Vis, fluorescence studies. Electrochromic (EC) and electrofluorochromic (EFC) properties have been checked with Cyclic Voltammetryand spectroelectrochemical techniques. These two polymer films haveexhibited stable reversible multi-color electrochromic changes with high coloration efficiency and contrast ratioupon electro-oxidation. These electrochromic polymers have not only produced EC properties with high opticalcontrast ($\Delta T\%=65–71\%$) but also exhibited high contrast ratio ($I_{on}/I_{off}=179$, I_{on}=fluorescence on (neutralstate) and I_{off}=fluorescence off (oxidized state)) EFC properties at low working voltage. Both the polymers reveal excellent electro-switching stability even after 100thcycles. Solid state electrochromic devices (ECD) usingboth the polymers have been fabricated and its color and fluorescent state are simultaneously switched by anapplied potential, making the polymer a unique candidate for electrochromicapplications in future.

Fig. 1Absorption studies at various voltage: (a) p-Benz-3TPA and (b) p-Benz-3CNTPA thin films on the ITO-coated glass substrate in 0.1 M TBAP/ACN solution

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Mechanical and Crystallization studies of Borassus Cellullose Nanofibers Reinforced PLA Nanocomposites

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Abstract

Nanocomposites consisting ofborassus cellulose nanofibers (CNFs) and Polylactic acid (PLA) were prepared with a goal of making green nanocomposites. Borassus fruit fibers were treated with alkali to remove lignin and hemicelluloses. Films of ~70 micronthickness with varying ratios of PLA and fiber were prepared using a solvent casting method followed by drying. Scanning Electron Microscopy (SEM) showed uniform distribution of CNFs in the polymer matrix. Microstructures, mechanical and thermal properties of the nanocomposites were studied. The tensile strength and Young's modulus were found to increase with the incorporation of fiber in the PLA matrix. Differential Scanning Calorimetry (DSC) revealed that the presence of CNFs accelerates the crystallization rate of PLA. The crystal morphologyof neat PLA and the PLA/CNF composites during isothermal crystallization was studied using a Polarized Optical Microscopy. The crystal nucleation rate was slow for the neat PLA and only a few large crystallites could be observed. By contrast, the incorporated CNFs accelerated the PLA's crystallization and the crystal nucleus density increased dramatically with an increased CNF content. These results suggest that CNFs can improve physical properties of PLA based composites. The developed PLA/CNF bio-nanocomposite films could extend the application of PLA as a new biomaterial for food packaging application.

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Polyanilne/rGO composite as photocatalyst for the pollutant organic dyes

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Abstract

The hazardous and non-biodegradable dyes discharged from the different industries are the major contaminants in wastewater and the removal of these dyes are essential to change it into usable water. Out of several methods for the removal of these organic compouds and dyes, the photocatalytic degradation attracts great interest. It has been proved that the composites of conjugate polymers with carbon nanomaterials can efficiently degrade the dyes under UV and visible illumination [1-3]. In this work we are evaluating the suitability of Polyaniline/rGO (Pani/rGO) compositeas a photocatayst for the dye degradaation. The Pani/rGO composite is synthesized by the in-situ polymerisation of aniline in the presence of reduced graphene oxide (rGO) using toluene sulphonic acid as dopant and ammonium persulphate as oxidant. GO synthesised through modified hummers method, is reduced via hydrothermal reduction reaction. Based on the prilimainary analyses the aniline to GO ratios selected for the hybrid preparation are as 5:0.1, 5:0.2, 5:0.3and 5:0.4 and 5:0.5. The hybrids are characterised by X-ray diffraction (XRD), field emmision scanning electron microscopy(FESEM), ultraviolet-visible spectroscopy(UV-Vis), fourier transform inftra red spectroscopy (FTIR) analyses. Photocatalytic activities of Pani/rGO hybrids are analysed by the degradation of methylene blue dye under UV illumination. The photocatalytic activity of the hybrid is better than polyaniline alone and this may be due to the reduction in recombination time of excited electrons as it is tranferred through rGO in the hydrids.

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Newer Polyesters containing Pendent Biphenyl Moiety: Synthesis, Characterization, Thermal behaviour and Effects of methyl substitution

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Abstract

Aromatic polyesters are counted as high performance engineering materials in electronic and automobile applications due to its excellent thermal stability, résistance to chemicals and good mechanical properties. Most of the aromatic polyesters are difficult to process because of its rigidity which reflects its limited solubility and high melting or high glass transition temperature (Tg). The development of newer aromatic polyesters with better organic solubility without loss of its thermal stability is major research interest now days.

In this context, we are synthesized the three new diol monomers, 4,4'-[1-(4-biphenylyl)ethylidene] bisphenol (BBP), 4,4'-[1-(4-biphenylyl)- ethylidene]-bis,3-methyphenol (O-BBP) and 4,4'-[1-(4-biphenylyl)ethylidene]bis,3,5-dimethyphenol (DM-BBP). The synthesized monomers are well characterized by FTIR, ^{1}H-NMR, ^{13}C-NMR, and elemental analysis. These monomers are used for synthesis of newer polyesters containing pendent biphenyl moiety using terephthaloyl chloride (TPC) as other monomer through phase-transfer catalyzed interfacial polycondensation technique. The number average molecular weights (Mn) of polyesters are found in the range of 10,213 to 35,112 g/mol with inherent viscosities in-between 0.50 to 0.71 dl/g. The synthesized polyesters are highly organo-soluble and dissolved in solvents like dichloromethane, tetrahydrofuran, chloroform, and 1-methyl-2-pyrrolidinone. Polyesters showed the Tg inbetween 243°- 273°C and T_{10} ranging from 328°- 423°C. Results of thermal analysis are indicated that the unsymmetric methyl substitution in O-BBP based polyester found low Tg, low viscous and heavy mol wt. material while other polyesters shows normal trend due to symmetrical structure.

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FPC-78

Synthesis and characterization of polyamides containing pendant naphthalene acetamide moiety

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Abstract

A new aromatic diamine viz., N-(3',5'-diaminophenyl)-2-(naphthalene-2"-yl) acetamide (2-DAPNA) was synthesized starting from naphthalene and 3,5-dinitro benzoic acid. It was characterized by FT-IR, ^{1}H- and ^{13}C NMR spectroscopy and mass spectrometry. A series of new aromatic polyamides containing pendant naphthalene acetamide moiety was prepared by Yamazaki's phosphorylation polycondensation of 2-DAPNA with five commercially available aromatic diacids viz., Biphenyl-4, 4'-dicarboxylic acid, Naphthalene-2, 6-dicarboxylic acid, 4, 4'-Oxydibenzoic acid, 4, 4'-Sulfonyldibenzoic acid, and 4, 4'-(Perfluoropropane-2, 2-diyl) dibenzoic acid. Inherent viscosities of these polyamides were in the range 0.44–0.85 dL/g in N, N-dimethylacetamide at 30 ± 0.1°C. pendant naphthalene acetamide moiety into polyamides led to an enhanced solubility of these polyamides N, N-dimethylacetamide (DMAC), N-methyl-2-pyrrolidinone (NMP), Dimethylformamide (DMF) and Dimethyl sulfoxide (DMSO) at room temperature. The polyamides could be solution-cast into tough, flexible and transparent films from their DMAC solution. Wide angle X-ray diffraction patterns exhibited broad halo at ($2\theta = \sim$15-25°) indicating that these polyamides are essentially amorphous in nature, which is reflected in enhance solubility of these polyamides in polar aprotic amide type solvents. The glass transition temperatures observed for these polyamides were in range 168–246°C thses aromatic polyamide with pendant bulky group shows increase segmental motion at lower temperature because of the lose packing of polyamide chain. The temperature of 10% weight loss (T_{10}) and char yields at 900°C of these polyamide in nitrogen were in the range 465-638°C and more than 58% respectively determined by TGA indicating the good thermal stability. These soluble thermally stable aromatic polyamide may have potential application as coating material at elivated temperature, R.O. membranes for desalination/gas seperation and in aero-space industry.

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FPC-79

Investigation and Polymerization Behaviour of Structurally different Benzoxazine Monomers

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Abstract

Polybenzoxazine were one of the thermosetting polymer which have been successfully synthesized from ß-naphthol, paraformaldehyde, and four different types of diamines : tetraphenyl thiophene polybenzoxazine (TPPBOX), oxydiamine diphenyl ether polybenzoxazine (ODPBOX), sulphonyldiamine polybenzoxzine (SDPBOX),benzoic acid polybenzoxazine (BDBOX) using solventless method. Synthesised benzoxazine and polybenzoxazine charecterised by IR,^{1}HNMR spectroscopically and thermogravimetrically. Thermal curing of benzoxazines to give polybenzoxazines having excellent thermal stability. The percentage of char yield at 900ºC is about 45% indicates high thermal stability. The polybenzoxazine (TPPBOX) contains heterocyclic moiety which shows high thermal stability.

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Robust Omniphobic Coatings

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Abstract

A functional acrylic polymer is synthesized by free radical polymerization followed by blending with functional siloxane oligomers. A multilayer coating approach involving the acrylic siloxane polymer and inorganic particles is used to prepare structured Cassie Baxter surfaces. The polymers and the coatings are chemically and physically characterized using NMR, FTIR,GPC and DSC. Correlation between the robustness of the omniphobic property and the surface morphologyisstudied using microscopy (SEM) and surface energy measurements. By optimizing cross-linking density and surface morphology, mechanically robust oil and water repellent coating systems are prepared with contact angle hysteresis<10°. These coatings have potential use as self-cleaning coatings for a variety of substrates.

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FPC-83

Exfoliation of layered titanate using pH-responsive graft copolymer and its application towards photocatalytic degradation of cationic/anionic dyes

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Abstract

Recently, in authors' laboratory, a novel composite has been fabricated by *in-situ* exfoliation of layered titanate using a *pH*-responsive graft copolymer. The graft has been developed by grafting of DEAEMA on dextrin. The *pH* has been varied to obtain the fully exfoliated layered titanate based composite. The ^1H and ^{13}C NMR, TGA, XRD and HRTEM analyses have been carried out to confirm the exfoliation. The composite, which consists of fully exfoliated titanate nanosheet in presence of cationically functionalized dextrin exhibits excellent photocatalytic degradation capability towards anionic/cationic dyes.

FPC-84

Synthesis and Characterization of Processable Heat resistant Poly(amide-imide)s containing bulky Tetraphenylfuran moiety

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Abstract

The main objective of this work is to study the structure–property relationships of highperformance polymers with thermal stability, solubility and viscosity. Hence, a series of novel poly(amide-imide)s (PAIs) was synthesized from a tetraphenylfuran-thiazole[1] containing diimide-diacid (TPFThDIDA) monomer with commercially available various aromatic diamines by using Yamazaki's direct phosphorylation reaction[2-3]. The resulting PAIs were obtained in quantitative yields and inherent viscosities were in the range of 0.86–0.96 dL/g. The introduction of the heterocyclic thiazole ring unit on the properties of these PAIs was studied by comparison with the corresponding polymers containing tetraphenylfuran groups. The PAIs exhibited excellent solubility and good thermal stability. PAIs showed glass-transition temperatures in the range of 267°C–302°C.

Thermogravimetric analysis of the PAIs indicated a 10% weight loss (T10) in the temperature range of 609–736 °C and char yields at 900 ^{0}C under nitrogen atmosphere in the range of 73–80% depending on the diamine monomer used for the synthesis PAIs.[4-5] The LOI of all poly(amide-imide)s were more than 40, thus such type polymers of can act as flame-retardant materials.

Keywords: Tetraphenylfuran, Poly(amide-imide)s, TGA, DSC, Heat resistant

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FPC-85

Development of PU Coating with Environment Friendly Route

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Abstract

With a worldwide volume of 14-16 million tons/year, polyurethane (PU) is 6thin total global polymer productionand one of the most important polymer family in our everyday life with applications as thermoplastics or thermosets materials[1-3].Polyurethanes are characterized by use of toxic isocyanates which has prompted researchers todevelop alternative polyurethane technologies without use of toxic isocyanates, which has led to the emergence of what is called as Non-Isocyanate Polyurethane (NIPU), the relatively non-hazardous counterpart of the isocyanate polyurethanes.NIPUpolymers have beenapproached predominantly fromtwokeydirections:(1) reaction of a polyfunctional cyclic carbonate with a polyfunctional amine to delivera thermoset poly(β-hydroxy-urethane), (2) derivatization of the hydroxyl functions of an otherwise thermoplastic prepolymer into corresponding poly(carbamate) by reaction with urea, followed by curing with a polyfunctional aldehyde to provide a cross-linked thermoset.

All of these approaches have some or otherinherent limitations such as slow curing, use of formaldehyde that is equally toxic like the isocyanates if not more, weak cross-links like acetals and hemi-acetal bonds etc., which beat the expectations of a robust, tough and chemical resistant yet less hazardous polyurethane material.The present work combines various teachings of the NIPU art and utilizes the hitherto un-attended and apparetly unreactive secondary hydroxyl groups of the β-hydroxy-urethane moieties to react with urea, overcome many of the weaknesses and design a two-pack thermoset coating material with increased urethane density along with good mechanical, flow and surface properties and a favorable curing kinetics, quite suitable for both decorative and industrial surface finishes.

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FPC-86

Modified chitosan/TiO_2NPs-CDs based composite: An efficient photocatalyst

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Abstract

Recently, a hybrid composite material has been developed via *in-situ* deposition of TiO_2 NPs and C dots on the surface of poly (vinyl imidazole) crosslinked chitosan [cl-Ch-p(VI)/TiO_2NPs-CDs] under microwave irradiation. The fabricated composite material has been found to be an efficient photocatalyst towards the degradation of toxic organic compounds in presence of sunlight. The physical and structural properties of hybrid composite have been characterized using various techniques. The LC-MS analysis predicts that the degraded products are organic molecules with lower mass.

FPC-87

Surface Modified Nanocellulose for Functional Coatings

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Abstract

Functionalized nanocellulose obtained from waste has gained enormous interest due to its biodegradability and non-toxicity and potential to replace various plastic non-biodegradable materials. Due to the presence of multiple hydroxyl groups, it can be easily functionalized to realize the desired properties. Nanocellulose can be applied as an aerogel, transparent thin films, hydrogel as well as a coating. Nanocellulose by nature is hydrophilic and doesnot have any anti-microbial, magnetic, fluorescence property on its own. Cellulose has been functionalized by quaternary ammoniumsilanes for nonleachingantimicrobial effect but does not have efficient antibacterial property. Bioderived small molecules which do not have any toxic effect can be used to covalently link to cellulose to enhance its property. In this report, nanocellulose has been covalently linked with vanillin Schiff base and eugenol. The modification protocol was optimized and characterized using FTIR, ^{13}C-CP/MAS solid-state NMR and was evaluated for antibacterialproperties against *S.Aureus* and *E. Coli.*Eugenol modified nanocellulose has shown better efficacy against both the cultures compared to the vanillin Schiff-base modified nanocellulose.

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Polymer Surface Engineering with Metallic Nanomaterials for Interlocked Interfaces

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Abstract

Polymer surface treatments have been developed as processing tools for various applications. The interfacial interlocking with engineered surfaces could be a reliable solution for improving interfacial adhesion between immiscible polymers. Herein, we focus on surface engineering and surface-pore-assisted robust mechanically interlocking mechanism. To explore interlocking and nano-stitching adhesion behaviours, metal-based nanomaterials of two different dimensions such as spherical and long nanowires were employed. A limited amount of surface was allowed to dissolve by a solvent, and nanomaterials were embedded on polycarbonate surface through a directional melt crystallization process. The solvent was allowed to crystallize along a temperature gradient which is perpendiculae to the surface. As a result, surface perpendicular pores of well-defined patterns with different pore depth were prepared. The pore depth has a direct relation with the allowed surface dissolution. The various morphologies and contents of nanomaterials were successfully prepared, and confirmed under SEM. The respective metal nanomaterials were thoroughly embedded to each pore-wall with distribution gradient in depth direction and top surfaces has maximum metal content. The surfaces pores and embedded nanomaterials increased the contact angle of polycarbonates to 157 degree. The load-displacement results showed efficiently prepared polycarbonate surfaces and interfacial adhesion with poly(dimethyl siloxane) improved by embedded spherical and long shaped metal nanowires. This novel processing technique with embedding nanomaterials could open new application windows for many other applications such as stretchable electronics, softsensor, and microfabrication.

Keywords: interface, nanomaterial, adhesion, crystallization, surface engineering

FPC-89

Synthesis and characterisation of a new trifunctional epoxy-hexagonal boron nitride composite for electronic device packaging

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Abstract:

Epoxy resins widely applied industrially for surface coating, adhesive, composites, laminates, pottings, encapsulant for semiconductor, and insulating material for electric devices. A new epoxy monomer is synthesized using a resole obtained from reaction of formaldehyde with p-cresol. The epoxy monomer has been characterized by FT-IR, H-NMR, mass spectral analyses along with epoxy values. The curing characteristics of the monomer is studied by curing with different amines such as DDM, IPDA and TDDA. The thermal, mechanical and thermal conductivities of the epoxy/hexa gonal boron nitride composites was investigated. Based on the studied properties it is found that the new polymer is useful for encapsulation of electronic circuit boards.

Figure 1. Graphical representation of epoxy/hexa gonal boron nitride composite

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Novel conjugated polymers FunctionalPolychalcones

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Abstract

Conjugated polymers have gained prominent attention due to their potential application in the field of PLEDs, FETs and sensors. On comparison with inorganic optoelectronic materials and small-molecule organic semiconductors, conjugated polymers are advantageous due their low cost in production, light weight in handling, and good flexibility while processing, enabling printing of large-scale roll-to-roll printed electronics.[1]

One of the main objectives in design of conjugated polymer is to modulate the band gap. Various molecular designs approaches variety of problems, for example, introducing bulky side chains increased not only the ease of solution processability but also avoided intermolecular aggregation leading to high charge carrier mobility.[2]However it is also desirable to keep the manufacturing cost of conjugated polymer as minimal as possible whilst retaining the optoelectronic properties. In this context, we have explored polychalcones[3,4] as a novel polymer with tuneable optoelectronic properties which can be easily prepared following an inexpensive route.

Initial attempts were focussed on carbonyl based conjugated polymers wherein the carbonyl group can be used as functionalizable handle. Series of polymer with varying functionalization were prepared. UV-Vis and fluorescence studies were made both and solution and solid state. The emission charactericts varies as a function of functionalization. The prepared polymers were further characterized by CV in solution. The results will be presented.

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FPC-92

Synthesis, characterization and electrical conductivity of new fluorinated poly(ether-azomethines)s bearing triptycene moiety

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Abstract

A new series of triptycene-containing poly(ether-azomethine)s were synthesised from 1,4-bis(4-amino-2-trifluoromethylphenoxy), 2, 3-benzotriptycene (4a) with commercially available aromatic dialdehydes viz., terephthaldehyde (TPA), isophthaldehyde (IPA), and varying molar mixture of TPA and IPA accordingly, The chemical structures of the new diamine was elucidated by FTIR, ^{1}H NMR and ^{13}C NMR and HRMS spectrometry, whereas the polymers were characterized by FTIR and ^{1}H NMR spectroscopy. Their physicochemical properties of polymers were examined by their inherent viscosity which was found in the range 0.51-0.66 dL/g, organosolubility were checked in various common protic and aprotic solvents. Poly(ether-azomethine)s thermal properties were studied by thermo gravimetric analysis, T_{10} was found in the range of 497-530 °C, glass transition temeparture (T_g) were determined by differential scanning calorimetry showed in between 233 and 275 °C. Polymers were also characterized by UV-Visible spectroscopy and Wide angle X-ray diffraction. We have studied and interpreted the electrical conductivity of each polymer measured by the two probe method and the results indicate that the electrical conductivity of polymers lies in range 0.019–0.051 mScm^{-1} indicating its semiconducting nature.

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FPC-93

Synthesis and Characterisation of new processable poly(ether-amide)s containing naphthyl moiety

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Abstract

New diacid monomer 2,2-Bis (p-methyl carboxyphenoxy) -1,1-binaphthyl (IV) was prepared through reaction of 2-naphthol with iron (III) chloride to 1,1-bis-2-naphthol (I) followed by reaction with 4-fluoroacetophenone to get diacetyl 1,1-bis -2-napthol (II) which on Conrad Wilgerodt reaction with Kindler variation using Sulphur and morpholine gave 1,1-bis-2-napthol thioacetomorpholide (III) and finally new diacid (IV) monomer was obtained by base catalyzed hydrolysis of intermediate (III) in ethanol. The structure of diacid was confirmed by ^{1}H NMR, ^{13}C NMR, FT-IR and Mass Spectra.

A new series of poly(ether-amide)s were synthesized by using direct Yamazaki's phosphorylation polycondensation method from new diacid (IV) monomer with different commercial diamines such as ODA, MDA, SDA, pPDA andmPDA. Inherent viscosities of polymers were in the range 0.40 to 0.91 dL/g indicating moderate molecular weight built-up. These poly(ether-amide)s exhibited excellent solubility in various polar aprotic solvents, also showed good solubility in pyridine and cresol. The T_i and T_{10} of polymers werein the range of 340 - 404 ºC and 437 to 498 ºC respectively and the char yield was in the range 62 to 65 % at 900 ºC. X-ray diffraction pattern showed ether linkage and methylene spacer would disturb the chain regularity and packing, leading to amorphous nature. The structure-property relationship of naphthyl containing poly(ether-amide)s was studied in the view of potential applications as thermally stable and processable polymers.

Keywords: Structure-property relationship,Poly(ether-amide)s, Thermally stable, TGA

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FPC-94

Polymer graphene composites for energy storage

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Abstract

Graphene is a preferred choice of carbon material inporous electrode materials for energy storage devices due to its excellent mechanical and electrical properties.Among the various types of graphene electrodes, 3D graphene structures have recently gained prominence due to high super capacitance, high surface area, and fast ion transport. A challenge in using graphene in porous electrodes is the difficulty in graphene exfoliation. Most methods available cureently are either expensive or require solvents and surfactants that are toxic and hard to remove. This work describes an inexpensive and easy way to exfoliate graphite that uses graphene as a surfactant to stabilize high-energy interfaces between water and an oil. The graphite spreads at the interface into graphene sheets and forms stable water-in-oil emulsions. The oil in this system can be a monomer that can be polymerized, resulting in 3D polymer/graphene composites. These composites are conductive and have a 3D porous structure which makes them a suitable electrode material for energy storage.

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Studies on the effect of crosslinking agents on the mechanical properties of Semi- IPN Blends from Natural Rubber and Polyacrylamide.

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Abstract

The aim of polymer blending is to develop products with unique properties that cannot be attained from individual constituents. The performance of a polymer blend is determined by various factors,

including the nature of the individual components, type of crosslinking agent, processing parameters, and, to a certain extent, the application for which it is intended. In the present study, semi-interpenetrating polymeric network (IPN) blends of natural rubber and polyacrylamide were made using glutaraldehyde (GA) & NN-Methylene- bis -acrylamide(MBA) as crosslinking agents. The mechanical performances like Tensile strength, elongation at break and modulus of these systems have been studied using Universal Testing Machiene. The ratio of the constituents and the type of crosslinking agents are varied and the effect of each blend ratio on the properties was also studied in detail. It was observed that the tensile strength of the IPN blend increases with increase in the amount of polyacrylamide in the uncured system(NR/PAAm). The same trend was observed in the systems cured with MBA(NR/PAAm/MBA). But in blends with glutaraldehyde (NR/PAAm/GA) with increase in polyacrlamide, the tensile strength increases to a limit and then starts to decrease. It was noticed that there is an effective reduction in the elongation with the addition of both crosslinking agets. The modulus values are also increased with MBA. But a different trend was observed with GA. Improvement in tensile strength and modulus, and reduction in elongation at break are clear evidences for the significant enhancement of plasticity in NR/PAAm systems from the formation of semi-IPN by curing with MBA than GA.

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FPC-96

Effect of Resin Modification on the Various Properties of Carbon Paper as Anode for Li-ion Batteries

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Abstract

Carbon materials of various types have been extensively used as negative electrode materials for rechargeable Li-ion batteries because of their consistent performance and potentialities. The high aspect ratio of carbon fibers helps in the formation of a non-woven mat, utilizing the well-known papermaking technique which is further impregnated with resin and pyrolyzed. Carbon fiber based composites are basically carbon carbon composites in which fibers acts as reinforcement and the polymer resin is the matrix[1,2].Carbon paper composite have thus been used as free standing electrode material for the li-ion batteries.

Phenolic resin was used in the present study which in turn was modified by replacing it partially with pitch because of the graphitic properties of the later at high temperatures. Different concentrations of pitch and phenolic resin were used for the sample preparation of composite papers. Phenolic resin is known to impart the desired strength into composites and its modification using pitch will add to the variability majorly in that aspect.

The effect of pitch incorporation was remarkably visible through the enhanced electrical, mechanical and structural properties which were characterized using varied techniques. The charge-discharge characteristics for the Li-ion coin cells have been studied and analyzed at different rates and the mechanism of Li insertion-deinsertion has been proposed which is further correlated to the anode structure. Moreover, the samples were tested as anode for li-ion batteries the results of which will be discussed in detail in the conference.

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FPC-97

Effect of Intermolecular Interaction on Thermal and Dielectric Behaviour of Polyvinyl Alcohol – Mesoporous Silica Composites

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Abstract

The influence of mesoporous silica (MSiO$_2$) particleson thermal behaviour and dynamic relaxation behaviour of polyvinyl alcohol (PVA) based MSiO$_2$ composites was investigated using vibrational spectroscopy and braodband dielectric spectroscopic analysis.Vibrational spectroscopy revealed the formation of strong intermolecular interaction (H-bonds) between the PVA polymer chains and –OH functional groups ofMSiO$_2$ particles[1]in PVA-MSiO$_2$ composties. This has resulted in a significant variation in the transition temperatures, i.e, glass transition temperature (T_g) and melting temperature (T_m). Broadband dielectric spectroscopic (BDS) analysis was performed in the temperature range between -20 ºC and 150 ºC to understand the effect of MSiO$_2$ concentration on various dielectric relaxation signature of PVA chains.The experimental data were fitted with theoretical models to relate the shift in the relaxation frequencies corresponding to various relaxations of the PVA chains. Activation energy was calculatedfor various relaxation frequencies viaArehenious equation and Vogel – Tamann – Flucher (VTF) equation in PVA-MSiO$_2$ composite (see Figure 1).[2] ,[3]Figure 1 shows that E_a for -relaxation is increased from ~64.6 kJ/mol for pure PVA to ~110.9 kJ/mol in PVA-MSiO$_2$ composite of 5 wt% MSiO$_2$ concentration. The change in the relaxation frequencies was correlated to the variation in the extent of intra-chain H-bonding of PVA and interchain H-bonding between PVA and MSiO$_2$ particles.

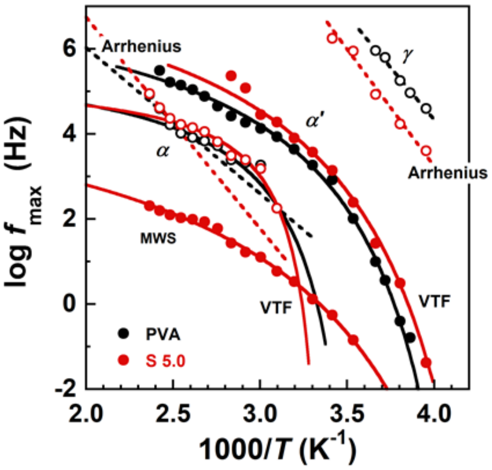

Figure 1: Activation energy calculation plot of PVA and S 5.0 fitted with Vogel – Tamann – Flucher equation (solid line) and Arrhenius equation (dashed line) for different relaxations.

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FPC-98

Synthesis and characterization of poly (ether-imide)s containing cardo cyclohexylidene moiety

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Abstract

A novel aromatic diamine viz .,1,1 bis [4-(4'-benzyl amine oxy) phenyl] cyclohexane (BBAPC) was synthesized from phenol and cyclohexanone in five steps and it was characterized by FT-IR, ^{1}H and ^{13}C NMR spectroscopy. A series of new aromatic polyimides having high temperature resistance and excellent mechanical strength, containing flexible linkages such as ether, amide and P. Cardo cyclohexylidene moiety was prepared by polycondensation of BBAPC with five commercial dianhydrides viz., 3,3',4,4' benzophenone tetracharboxylic dianhydride, Pyromelitic dianhydride, Hexafluoroisopropylidene diphthalic anhydride, Oxydiphthalic anhydride and Biphenyl tetracarboxylic dianhydride using a standard two step process with thermal imidization of precursor (PAA). Inherent viscosities of these precursor (PAA) were in the range 0.38 to 0.58 dL/g in N-methyl-2-pyrrolidinone at 30 + 0.1°C. The introduction of amide linkages and cardo cyclohexylidene moiety into polyimides led to an enhanced solubility in N, N-dimethyl acetamide (DMAC), N-methyl-2-pyrrolidinone (NMP), Dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO) at room temperature. The polymides could be solution-cast into tough, flexible transparent film from thermal imidization of precursor polyamic acid. X-ray diffraction pattern of poly (ether-amide-imide)s indicating that the poly (ether-imide)s are partially crystalline in nature which is reflected in enhance solubilityof these polymers in polar aprotic amide type solvents. The glass transition temperatures observed for these polyimides were in the range 157 – 196 °C. The temperature of 10 % weight loss (T_{10}) and char yields at 900 °C of these polyimides in nitrogen were in the range 302-441 °C and more than 25% respectively determined by TGA indicating good thermally stability. These soluble thermally stable aromatic poly (ether-imide)s may have potential applications as coating material at elevated temperature and in aerospace industry.

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FPC-99

Poly(vinylidene fluoride) reactive blend membrane with hierarchical morphology for Separation of oil-water emulsions

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Abstract

Reactive poly(vinylidene fluoride) (PVDF)/poly[(methyl methacrylate)-*co*-(vinylvbenzyl chloride)] blend memmbrane with hirarchical surface morphology was prepared by the non-solvent induced phase inversion process. The surface morphology was induced by the use of high molecular weight poly(vinylpyrrolidone) (PVP) as additive (Figure 1). The reactive nature of the membrane surface allowed facile hydrophilization with hydrophilic polymers such as polyethyleneimine (PEI) and other amine functional polymers. The modified membrane showed superhydrophilic behaviour and underwater olephobic behaviour.The modified membrane exhibited good separation efficacy of both surfactant-free and surfactant-stabilized oil-water emulsions at low applied pressure. A permeate water flux of about 250 $\mathrm{Lm^{-2}h^{-1}}$(pressure 0.35 bar) with >99% rejection of oil and flux recovery ratio of >99% were obtained with the modified membranes during separationof oil-water emulsion.[1]Small domestic module prepared with the modified membrane also showed good oil-water separation efficacy. The detailed characterizations and the mechanism of formation of hirarachical surface morphology was systematically studied. This membrane also showed good antifouling property during concentration protien.[2] This work was extended to prepare pH- and temperature-reponsive membranes. Furthermore amphiphilic surface modification was also possible by the modification of raective blend membarne for separation of both oil-in-water or water-in-oil emulsions.

Keywords: Hierarchical globular morphology; High molecular weight poly(vinylpyrrolidone); Superhydrophilic/underwater oleophobic; Oil-water emulsion separation, Scalable process.

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Figure 1. SEM and AFM images of blend membrane showing globular surface morphology.

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FPC-100

Polymer supported Core Shell Nanoparticles as catalysts

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Abstract

A series of transition metal-loaded (Zr, Ti, Y) core-shell nanoparticles synthesized by sol-gel method, which further supported on polymer and evaluated for the acid catalyzed reactions. These materials were prepared by the impregnation method. The detailed discussion of the properties with experimental parameters has been carried out. The various characterization techniques for the core-shell nanostructure have also been discussed. Their physical and chemical properties have been addressed and then characterized by Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES), Fourier Transformed In-frared Spectroscopy (FTIR), High-Resolution Transmission Electron Microscopy (HRTEM), and X-ray Diffraction (XRD). All the prepared materials acted as efficient catalysts.

Keywords: core-shell nanoparticles, polymer supported, sol-gel, acid catalyzed reactions

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FPC-101

Nano ZrO_2 embedded cellulose incorporated poly ethylmethaacrylate/polyvinyl alcohol nanocomposite as a super capacitor

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Abstract

A simplistic *in situ* polymerization technique is used to fabricate polymeric nanocomposite film of PEMA/PVA/C@ ZrO_2. The thickness of the PEMA/PVA/C@ ZrO_2 nanocomposite films mainly depend on the polymerization of the ethylmethaacrylate and concentrations of the PVA. Phase analysis, microstructure, and chemical composition are examined through X-ray diffraction (XRD), Fourier transform Infrared Spectroscopy (FTIR), field emission scanning electron microscopy (FESEM),X-ray phoelectron spectroscopy (XPS) and high resolution transmission electron microscopy (HRTEM). The surface and nano-tribological characteristics of the polymeric nanocomposite films are investigated by atomic force microscopy (AFM). Dielectric properties of the polymeric nanocomposite films are studied as a function of frequency and temperature in the range of 100 Hz-3 MHz and 313-373K, respectively. The incorporation of ZrO_2 filler into PEMA/PVA/C remarkably improved the dielectric constant and suppressed the loss. Dielectric loss peaks are explained in terms of dielectric relaxation. The conducting behaviour of the nanocomposite film is ascribed to hopping mechanism. The chemical resistance, thermal, and biodegradable properties of the polymeric nanocomposite films are studied. The oxygen barrier property of the nanocomposite film is reduced by five folds due to the synergistic combination of nano ZrO_2 and PEMA/PVA/C can be used as an appropriate candidate for high frequency capacitor application.

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FPC-102

Conducting Polymer Guest in Porous Coordination Polymer Host

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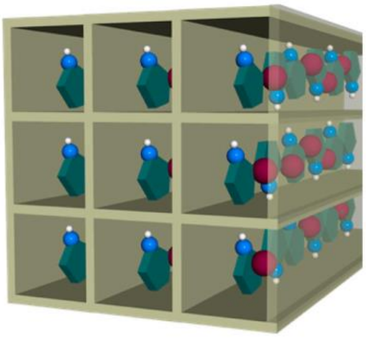
Abstract

Metal-Organic Frameworks (MOFs), in general, are not electrically conducting due to the insulating nature of the organic linkers and poor orbital overlap between the metal ion and the heteroatom of the linker.[1]Herein, we have demonstrated a Cd-based fluorescent MOF to host pyrrole monomers which were then assembled into polymer chains. Polypyrrole chains inside the nanochannels of MOF are confined in such a way that the non-covalent $\pi\cdots\pi$/N-H$\cdots\pi$ interaction lead to the formation of percolating conducting paths resulting in theelectrical conductivity enhancement by ~9 orders of magnitude.[2]Further, Hall-effect measurements revealed the composite to be an n-type semiconductor with magnificently high-carrier density (η) of $\sim 1.5 \times 10^{17}$ cm^{-3} and mobility (μ) of ~ 8.15 cm^2 V^{-1} s^{-1}.Also, the florescence of the pristine MOF was almost retained in the composite in the form of associated exciplex-type emission. Such observation on MOF-conducting polymer system will direct the rational designing of such materials for optoelectronic applications.



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Anthracene-Resorcinol Derived Covalent Organic Framework as Flexible White Light Emitter

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Abstract

The ordered polymeric structure of Covalent Organic Framework (COF) facilitates the selective incorporation of electronically active segments which can be tuned to function cooperatively. This designability inspires developing COF-based single-source white-light emitters, required in next-generation solid-state lighting. We have developed a new crystalline COF exhibiting white light emission. The keto-enol tautomers present in the COF gives rise to dual emission, which can be tuned by the O-donor and N-donor solvents. Importantly, when suspended in a solid polymer matrix this dual emission is retained as both tautomers coexist. A mere 0.32 wt% loading of the COF in PMMA gives a solvent-free film with intense white light emission (CIE coordinates (0.35,0.36)). From steady-state and time-resolved studies, the mechanism of the white-light emission has been unambiguously assigned to fluorescence, with the mixture of blue, red and green emission from a single source COF unit.Electroluminescence property obtained by dopping COF fluorophore into polymer matrix led us to go one step ahead of easy processibility of COF for optical device making and future LED application.

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FPC-104

Nanocomposite of Coordination Polymer and Conducting Polymer

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Abstract

Coordination polymers, in the last decade, have gathered immense attention in the domain of electronic and energy storage devices which is barred by their poor electrical conductivity and moderate stability.One of the approaches,to address this issue, is to assemble conducting polymer chains inside the voids of the coordination polymers leading to a fixed interpenetrating network, extending the conjugated path effectively for electrons to delocalize. In this line, one of the representative examples is UiO-66hosting polyaniline (PANI) chains which enhanced the electrical conductivity of the composite as well as rendered the composite to be exceptionally supercapacitive in nature.[1]Though, the nanocomposites of coordination polymers and conducting polymers are shown to be promising for commendable performance, the concern is regarding the overall stability of the composite. In that pursuit, we hosted thiophene based monomers inside UiO-66, followed by polymerization which indeed enhanced the electrical conductivity of the composite from insulator range to semiconductor range(~10^{-3} S·cm^{-1}). Further, our preliminary investigations on all solid-state supercapacitor derived of such conducting nanocomposite reveal interesting capacity values as well as cycling stability.

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FPC-105

Synthesis of new co-polymers via ring-opening metathesis polymerization (ROMP) of cyclic olefins with oxanorbornene containing pendent sulfur moiety

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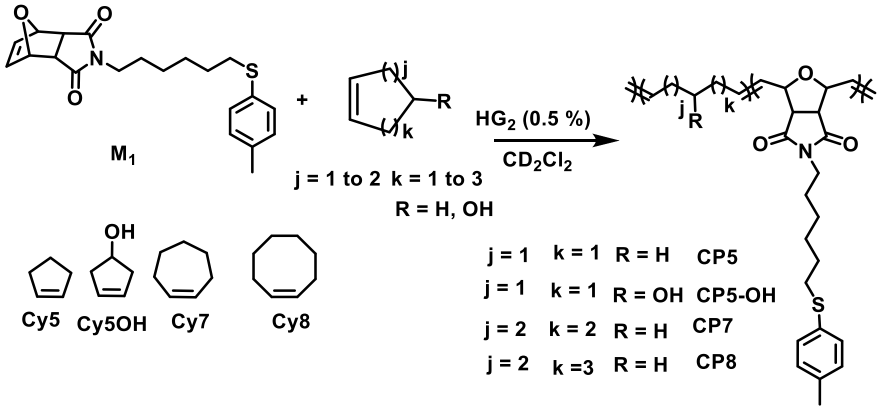
Abstract

The realm of ring opening metathesis polymerization (ROMP) has become an effective method for preparing a wide range of functional polymers and copolymers, owingto its high functional group tolerance and chemical robustness.[1]Compared with free radical polymerization, ROMP can control over the content of functionalities and their distribution along the polymer back bone.ROMP copolymerization of olefins with polar comonomers by using transition metal catalysts is another predominant approach to obtain different polyolefins.[1]Till to date there are many reports documenting the ROMP of norbornene and its derivatives,[2] as well as ROMP of low-strain monocyclic olefins with five-,six-, seven- and eight membered rings and its derivatives.[3] However, copolymerization of monocyclic olefins with bicyclic olefins are rare in literature due to its difference in reactivity. In this work, oxanorbornylene monomer containing pendent sulfur unit (**M_1**) was used in copolymerization with different cycloolefins by using 2nd generation Hoveyda-Grubbs Ru catalyst (**HG2**). Systematic ^{1}H NMR kinetics were conducted to know the reactivity of each monomers. We have also investigated the effect of temperature on conversion of each monomer in to co polymer.



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FPC-106

Studies on hydroxyl terminated polycaprolactone-butadiene-polycaprolactone block copolymer based nitrate ester plasticized composite propellant

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Abstract

Conventional composite propellant based on HTPB/AP/Al has reached a plateau in terms of energetics. In an attempt to enhance the range of rockets/missiles, development of hydroxyl terminated polycaprolactone-butadiene-polycaprolactone block copolymer (HTBCP) as potential binder system was carried out [1]. HTBCP was plasticized with nitro glycerine in plasticizer/polymer ratio of 0.5 and solid ingredients like AP/Al/nitramine were incorporated in propellant composition.The performance of the propellant was compared with the HTPB/DOA/Al/Nitramine based propellant. Various physical, mechanical, ballistic and sensitivity parameters were evaluated and compared. Various rocket performance parameters of both compositions were first theoretically predicted by the NASA CEC-71 program followed by processing of these propellants in vertical planetary mixer. Strand Burning rates were determined in pressure range of 3–11 MPa by acoustic emission technique [2]. Approximately 2% gain in standard I_{sp} was observed in Ballistic Evaluation Motor (BEM) firing. In addition, 5% enhancement of density was also observed in HTBCP based propellant composition. Mechanical properties, friction and impact sensitivities of compositions were also evaluated and found to be in acceptable limits [3-4]. Study reveals that HTBCP based propellant are superior in terms of ballistic parameters viz. characteristic velocity (C*) and specific impulse (I_{sp}) and also provides higher density values as compared to HTPB based propellant without compromising safety criterion.

Abbreviations:

HTPB-Hydroxyl Terminated Polybutadiene, AP-Ammonium Perchlorate, Al-Aluminium, DOA-Dioctyl Adipate

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FPC-108

Comparative Evaluation of Conventional and Contemporary Flame Retardants Behavior in Coir Fiber- HDPE Composites

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Abstract

High density polyethylene composite with improved flame resistance containing macro-sized coir fibers as reinforcing agent was prepared using novel flame retardants such as triphenylphosphate and ammoniumpolyphosphate and the properties were compared with conventional flame retardants based on polyvinylchloride. Optimized 20% coir fiber with alkali treatment time of 5h and 5% concentration were loaded in all flame retardant composites. Limiting oxygen index (LOI) and thermal degradation characteristics of composites were evaluated. The LOI value registered improvement in flame retardancy with 30, 35 and 45% respectively for triphenylphosphate, ammoniumpolyphosphate and polyvinylchloride composites. Flame retardant composites showed early stage degradation nearly at 250 °C with high residual mass for all the systems. Residual char mass of conventional system were found remarkable and it could be correlated with LOI value obtained.

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FPC-109

Knitting the Macrocycles through Aromatic Linkerstowards the Generationof Task-specific Porous Organic Frameworks

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Abstract

Resorcin[n]arenes are an important class of macrocycles possessingconformational flexibility, functional tunability, and excellent guest recognition properties.[1] They have been employed for sensing, catalysis, chiral discrimination, and drug delivery in the solution phase.[2] In contrast, these macrocycles in the solid state have not gained much attention as sorbents due to the guest inaccessible zero-dimensional (0D) discrete pores having no apparent pore connectivity.[3] Connecting the 0D porous cavitands using organic linkers may lead to a new generation porous organic frameworks (POFs) where interconnected pores are easily accessible to the fluids.Herein, we corroborated the concept of linking 0D discrete pores by connecting resorcin[4]arene core through different task-specific linkers to obtain a series of POFs.The surface areas of the POFs were increased up to 8-fold than that of the resorcin[4]arene monomer (156 m^{2}g^{-1} to 1229 m^{2}g^{-1}).Utilizing three different reactive sites of the resorcin[4]arene core and tuning the linker size, and functionality,we developeda series oftask-specific POFs (CLX-OH, CLX-Az-OH, CLX-F) exhibiting excellent performance towards metal-free carbon dioxide fixation, organic micropollutantsseparation from water, and gas adsorption. Thus, '*connecting the dots*' (0D pores) opens upan interesting field of research wherewe can address many unresolved problems like water desalination and energy storage in near future.

Figure 1. Connecting macrocyclic core with different organic linkers leading to task-specific porous organic frameworks (POFs).

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FPC-110

Micromechanical Modeling of Sisal/Polylactic acid (PLA) Biodegradable Composite

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Abstract

Industries are looking for sustainable green material where natural fiber reinforced biopolymer composites can be an option in present scenario. In the present study, a representative volume element (RVE) based micromechanical model implemented to evaluate mechanical properties of sisal fiber reinforced PLA composites. The 3D model of RVE prepared using finite element analysis software ANSYS 18 in unit cell. RVE modeled with periodic square packed array and hexagonal packed array which assumes the perfect bonding between fiber and matrix. Effect of fiber weight fraction from 10 % to 50% on longitudinal modulus, transverse modulus and shear modulus of Sisal/PLA composites have been studied. The tensile properties of Sisal/PLA composites evaluated using different analytical method and compared with RVE model. It shows the good agreement between them. This study will empowers to understand mechanical behavior of green composite material.

Keywords

Green composites, Micromechanical modeling, Representative Volume Element (RVE), Sisal fiber, PLA

Figure: Meshed Model of RVE for Sisal/PLA

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Thermal, Tensile and Electrical properties of HBPI/GO nanocomposites

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Abstract

A series of hyperbranched polyimide/graphene oxide (HBPI/GO) nanocomposites were successfully prepared by in situ polymerization of TAPOPOB, PMDA and GO by varying the percentage of GO (0.5, 1, 3 and 5 wt %). The GO was synthesized using modified Hummer's method. All the nanocomposites exhibit good thermal stability (T5% - 489-510 oC) compared to pure HBPI. The Tg values were in the range of 257-270 oC. Well dispersion of GO into HBPI matrix was explained using SEM and TEM analysis. The GO forms the bond with HBPI and enhances the mechanical properties. They have high dielectric constant in the range of 3.2 to 4.7 at 1 MHz and also good mechanical properties with tensile strength of 89 to 112 MPa, elongation at break 5.7 to 7.5%. The LOI values are in the range of 39-41 indicates that the HBPI/GO nanocomposites can be also used in high flame retardency applications.

Keywords: hyperbranched polyimides, graphene oxide, nanocomposites, thermal and electrical properties

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FPC-112

Kinetics and isotherm studies for the adsorption of brilliant green dye onto polyaniline/polyethylene glycol/Ag doped ZnO polymeric nanocomposite

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Abstract

A novel polymeric nanocomposite constituting polyaniline/polyethylene glycol (PAPE) and Ag doped ZnO (AZO) (1, 3 and 5% Ag) were synthesized by chemical oxidative polymerization for the removal of brilliant green (BG) dye. The PAPE/AZO nanocomposites were characterized FTIR, XRD and SEM analyses. The composition of nanocomposites was identified by elemental analysis. The dye removal performance of the PAPE/AZO was assessed by the adsorption studies of BG dye in various parameters such as contact time, pH, concentration of the dye and adsorbent dosage. The residual concentration of the dye was analyzed by UV-Visible spectrophotometer indicating a maximum dye removal of 99.63 %. The results were compared with isotherm models and found to be well fitted with the Langmuir isotherm model which may be due to the monolayer adsorption of dye molecules on the surface of the nanocomposite. The maximum adsorption capacity was determined to be 94.46 mg g^{-1}. Kinetic studies revealed that the PAPE/AZO follows pseudo second order kinetic model representing a chemisorption process. From the studies, it is considered that the PAPE/AZO can be used as a viable adsorbent for the extraction of BG dye from aqueous solutions.

Keywords: Polyaniline; Ag-ZnO; brilliant green; adsorption; kinetics; isotherms

Effect of non-covalent modification of hybrid nanofiller on morphology and electrical conductivity of Polyamide 6 basedhybrid nanocomposites

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Abstract

Polyamide 6 (PA6) based hybrid nanocomposites of expanded graphite (EG) and multi-walled carbon nanotubes (MWCNTs) were prepared via melt-mixing technique. In order to achieve improved dispersion of hybrid nano-filler (EG/MWCNT) in PA6 phase, a non-covalent organic modifier (lithium salt of 6-aminohexanoic acid; Li-AHA) was utilized. Morphologicalinvestigation of EG/MWCNTs hybrid filler in the presence of Li-AHA showedthe intercalation of MWCNTs into partially exfoliated EG, whereasunmodified EG/MWCNTs hybrid mixture exhibited a separate identity in themixture [1,2]. Further, selected area electron diffraction pattern of theLi-AHA modified hybrid composite depicted few-layer 'graphene-like'structure of exfoliated EG corresponding to the hybrid mixture in the PA6matrix. The refined'network-like' structure of the EG/MWCNTs hybrid mixture [3] led to anelectrical percolation threshold at ~1 wt% in the PA6 matrix, whereasunmodified hybrid based PA6 composite showed a percolation of ~3 wt% ofthe hybrid filler. Li-AHA mediated intercalation of the MWCNTs into thepartially exfoliated EG established a refined network-likestructure in PA6 phase with improved interfacial interaction.

Key Words: Non covalent modification, Hybrid nanocomposite, Electrical conductivity

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FPC-116

Synthesis and Characterization of linear Polyamides containing Benzoxazine moieties in the main chain

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Abstract

High molecular weight polyamides containing thermally curable benzoxazine units in the main chain have been synthesized. For these purpose,Thediacid monomer was synthesized through Mannich reaction of 4, 4'-isopropylidene diphenol (Bisphenol A), formaldehyde, and 4-aminobenzoic acid. Polycondensation of benzoxazinediacid with various diamine using Yamazaki condensation yields poly(amide-benzoxazine)s. The structure of the precursor diacid monomer and resulting products were confirmed by IR,NMR, and Mass spectroscopy. Thermal properties of polymerswerestudied by TGA and DSC. XRD data showed all polymers were amorphous in nature. Inherent viscosities were in the range of 0.24-0.41 dL/g. No weight loss below 250^{o}C,that indicatesmoderately high thermal stability.

Keywords: Benzoxazinediacids, Thermal stability.

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FPC-118

Swelling and Diffusion Characteristics of Polymeric nanocomposite films composed of Sodium alginate & TiO_2

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Abstract

Polymeric nanocomposite films have been made from a hydrophilicnatural polymer, sodium alginate (SA) and $TiO_2$by using $CaCl_2$ as crosslinker. Films have been preparedwith varying amounts of nanoparticles, polymer composition, crosslinking agent& by varying crosslinking time. The effect of these parameters, the preparation conditions and the pH ofthe medium on the swelling behavior of these gel films has been investigated.Dynamic swelling studies have been carried out and the kinetic parameters forthe swelling process have been evaluated. The influence of film characteristicsand pH of the medium on the permeability behavior of the films has been studied. The results revealed pH sensitivity of the filmstowards swelling. Based on the results, possible mechanismsof water transport through the films have been proposed.

Keywords: Nanocomposites, diffusion, kinetics, pH sensitivity, swelling.

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FPC-119

Synthesis, Characterization and Photocatalytic application of polypyrrole-CdS nanocomposite for photocatalytic degradation of dye

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Abstract

Polypyrrole/CdS (PC) nanocomposites have been synthesized with different mass fractions of CdS via in-situ polymerization of polypyrrole. Characterizations of the synthesized products were done by various techniques such as fourier transform infrared spectroscopy (FTIR) to study the functional groups, X-ray diffraction (XRD) for nature of the materials and thermo gravimetric analysis (TGA) to check the stability of the materials against temperature. Electron microscopy was used to study the surface morphology, size and shape of the particles. Cyclic Voltammetry have been used to study the electrochemical behaviour of the nanocomposites. Incorporation of CdS nanoparticle enhances the photocatalytic. Photocatalytic activity of the material was tested by monitoring the degradation of Rhodamine B dye by using the synthesized material as an effective catalyst in the presence of visible light source and the generated reactive species i.e. e^-, h^+ and OH^- was attributed for the photodegradation of the dye. The recombination rate of the reactive species generated upon irradiation was confirmed by PL intensities.

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FPC-121

Self-powered nanogenerators from bio-waste polymer hybrid

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Abstract

Complex synthesis techniques, biocompatibility, biodegradability and toxicity are the major challanges in development for self-powered piezoelectric nanogenerators for biomedical applications. Here, we report a novel bio-waste hybrid for self-powered nanogenerator by using abundantly available natural self-aligned collagen fibrous fish scale as an efficient energy harvester. Fish scale, a bio-waste, consist of type I collagen reinforced by apatite exhibit anisotropy and piezoelectricity in meager quantity. Fish scale induces the electroactive phase over its surface through synergism. Structure and morphology confirm the uniform distribution of scale particle in PVDF matrix and γ-phase formation in presence of the filler. Energy harvesting performance of the bio-waste based hybrid device exhibit voltage of 22 V and high energy density of 28.5 $\mu W/cm^2$, considerably higher value than the existing waste based device. Different modes of human motion is sufficient to generate energy from the bio-waste hybrid like twisting, bending, walking, foot tapping and finger pressing etc.

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FPC-122

Studies on thermal degradation behavior of magnetic particle loaded poly lactic acid

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Abstract

Biodegradable polymers such as Poly lactic acid(PLA), Poly vinyl alcohol(PVA), Chitosan, Cellulose are now a days utilized in different field of application specially in packaging. Different reinforcement substances like carbon fiber, graphene, clay are incorporated in the above polymer matrixes to prepare composite having improved property. Degradation behavior of the composites need to be studied to understand environmental impact of the polymeric composites as well as to investigate provision of conversion into value added product. Thermal degradation behavior of polymer indicate thermal stability and possibility of reprocessing of the polymer. In view of the literature that metal oxide has catalytic effect on degradation of PLA, in this work detailed thermal investigation of different magnetic nanoparticle loaded PLA was carried out. Model free and model fitting approaches are taken for multiple heating rate data fitting. Catalytic effect of iron oxide decorated graphene oxide also investigated at different loading. Isothermal TGA-FTIR also investigated to understand the impact on product formation. Impact of filler loading on PLA degradation also investigated throughly. It is found that iron oxide loaded filler has increased the depolymerization rate of PLA, thus increased the PLA degradation.

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FPC-123

Blown films of Poly lactic acid: Characterization and property

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Abstract

The present investigation accounts the modification and characterization of Poly lactic acid (PLA) based blown films using biofillersi.e. chitosan (CS), gum arabic (GA), functionalized CS (MCS), functionalized GA (MGA), and further usage of a cross linking agent i.e. dicumyl peroxide (DCP) with MCS (DMCS), and MGA (DMGA). The FTIR analysis gives the evidence of forming functional biofillers MCS and MGA through grafting mechanism of oligomer lactic acid (OLLA) with CS and GA, giving a new peak at 1539 and 1755 cm^{-1}, respectively. The used biofillers help in providing tailored properties to the developed blown films due to chain interactions, level of compatibility and loading percentage between matrix and reinforcements. The formulated biocomposites show improved properties over blow up ratio, mechanical, thermal, and thermomechanical properties of PLA.Moreover, the migration ratio of fillers in formulated biocomposites are within permissible limit confirming safe use of packaging material. In this sense, the used biofillers can overcome the shortcomings of PLA, for providing a single step method of developing an inflexible food packaging material.

FPC-124

Thermal behavior of Poly (lactic acid)/Silk based Microcellular Foams

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Abstract

This investigation mainly focuses on the thermal behavior of the fabricated poly (lactic acid) (PLA)/Silk Nano Disc (SND) based microcellular composite foams (Figure 1 (A) and 1(B)).Thermal stability of the fabricated PLA and PLA/SND based foams are thoroughly analysed with the help of isothermal thermogravimetric analysis. It is observed that SND improves thermal stability of the fabricated PLA based foams. Thermal degradation behavior of the prepared foams is also thoroughly investigated with the help of different well established "model-free" and "modelistic" techniques such as Flynn Wall Ozawa (FWO), Kissinger-Akahira-Sinouse (KAS), Kissinger, Friedman and Criado method. Degradation kinetic studies has been performed at dynamic heating rates (5˚C/min, 10˚C/min, 15˚C/min and 20˚C/min)using thermogravimetricanalyser (TGA).The activation energy (E_a) values of the fabricated foams has been calculated and an increase in E_a is observed with nanofiller loading. Different plots of activation energy with conversion will be discussed in the presentation.The mechanism of degradation of the fabricated foams are investigated in this study by using Criado plots. This investigation provides useful information of the thermal stability and mechanism of degradation of the fabricated PLA and PLA/SND based foams for their potential applications in different biomedical and commodity areas.

Figure 1 (A) Fabricated PLA/SND based microcellular foam. (B) Nanofiller in the PLA foam matrix.

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Surface modified carbon fiber based electrospun PVA nanofiber for advanced application

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Abstract

Electrospinning is a widely used and accepted method for nanofiber production. Carbon nanotube based PVA composites[1] have been used for conductive textile application whereas electrospun pristine CNT/PVA nanofiber[2] has compatibility issues between the filler and the polymer matrix. In our studies, we have taken the "grafting to" approach to graft PVA on to surface modified[3] carbon fiber to increase the filler-matrix compatibility and spinnability of the polymer solution. The electrospun conductive nanofiber is then studied using four probe method for conductivity, contact angle studies, FTIR studies, XRD and FESEM. The surface modified CF/PVA electrospunnanofibers can find application in flexible elctronics[4] and sensor based applications.

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Blending poly(butylene succinate) with poly(lactic acid) and the effect of modified chitosan as Studied by Synchrotron X-Ray Scattering and DSC

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Abstract

Structure and properties of poly(l-lactic acid) (PLA) and poly-(butylene succinate) (PBS) blends were studied with various composition and with addition of modified chitosan (MCH) to the blend system. Synchroton small angle X-ray scattering (SAXS) and differential scanning calorimetery (DSC) was used to study the structure and morphology of the blends, which reveals the increase in crystallinity of the blends with increase in the PBS percentage in the blends. SAXS result for neat PLA and neat PBS exhibits a scattering peak at $q=0.35nm^{-1}$ and $0.61nm^{-1}$ respectively, with corresponding crystal long period of 17.5nm and 5nm. While PLA/PBS blend showed two scattering peak and the scattering intensity increases with PBS content, which indicates the presence of dual lamellar structure in the blends. However, with addition of modified chitosan in the blend system it was observed that there is a decrease in the scattering intensity. The long period and average lamellar thickness for PLA increases with an increasing in PBS component and decrease with increase in the MCH content in the blends.

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FPC-127

PLA/Functionalized Gum (fG) film: Elucidation of degaradtion kinetic parameters and mechanism

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Abstract

A series of PLA/functionalized gum (fG) film in presence of dicumyl peroxide (DCP) are facilely fabricated using reactive extrusion process at 180°C. The non isothermal TG kinetics and release of volatile components are investigated using thermo gravimetric analysis (TGA) and coupled TGA–Fourier transform infrared spectroscopy (FTIR) techniques. TGA result shows that the DCP treated PLA/fG has higher thermal stability than PLA/fG. Moreover, the behaviors involved in the thermal decomposition of fG grafted PLA films in inert atmosphere are investigated by using the model free approach, i.e. Flynn Wall Ozawa (FWO) and Kissinger Akhaira Sunose (KAS) method to dynamical TGA data. The estimated average values of activation energy (E_a) determined using FWO are 158 (R^2~ 0.992), 148 (R^2~ 0.996), 118 (R^2~0.991), 155 (R^2~ 0.991) and 127 (R^2~ 0.994) respectively. The generalized mechanism suggested that mechanism for PLA, PLA-1fG follows ~A2 to R3, PLA-3fG proceed via ~A2 to A4 and in case of DCP treated PLA-fG, it shifts A2 to R2. Releases of the gaseous components are investigated by hyphenated TGA-FTIR such as CO2, CO, lactide or cyclic oligomer, acetaldehyde, water etc.

Keywords: PLA; Functionalized Gum, DCP, TGA kinetics.

Fig. Generalized mechanism plot for PLA.

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FPC-128

Nanocomposite ElectrospunNanofiber for High Perfoemance Application

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Abstract

In this work OLLA grafted Chitosan (OLLA-g-CH) a novel amphiphilicmaterial, dispersed into Poly-lactic Acid (PLA) matrix at different concentration (0.5% to 5%) and electrospun into nanofibers. The bionanofibers composite showed improvement in tensile strength of the nanofibers with increasing concentration of OLLA-g-CH. The modified biocomposite also tends to alter the wettability due to its amphiphilicnature.The change in the fiber diameter and dispersion of OLLA-g-CH within the PLA nanofiber matrix were examined under scanning electron microscopy. The nanofiber also shows enhanced thermal stability and crystallinity. The electrospun nanofiber with enhanced properties hold potential for engineering functional tissues or organs and smart pharmaceutical applications.

KEY WORDS: PLA, chitosan, amphiphilic

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Acknowledgements

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FPC-129

Morphology and Properties of Bio-Based Poly (Lactic acid) / Linear Low Density PolyethyleneBlends and their Microcrystalline Cellulose Reinforced Composites

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Abstract

The purpose of current work is to examine the influence of microcrystalline cellulose fibre on PLA/LLDPE polyblend and their characterization by the XRD, FTIR, FESEM, TEM, DSC, TGA, POM and UTM. All three constituents were taken in different loading and then extruded in the twin screw extruder via melt extrusion technique.

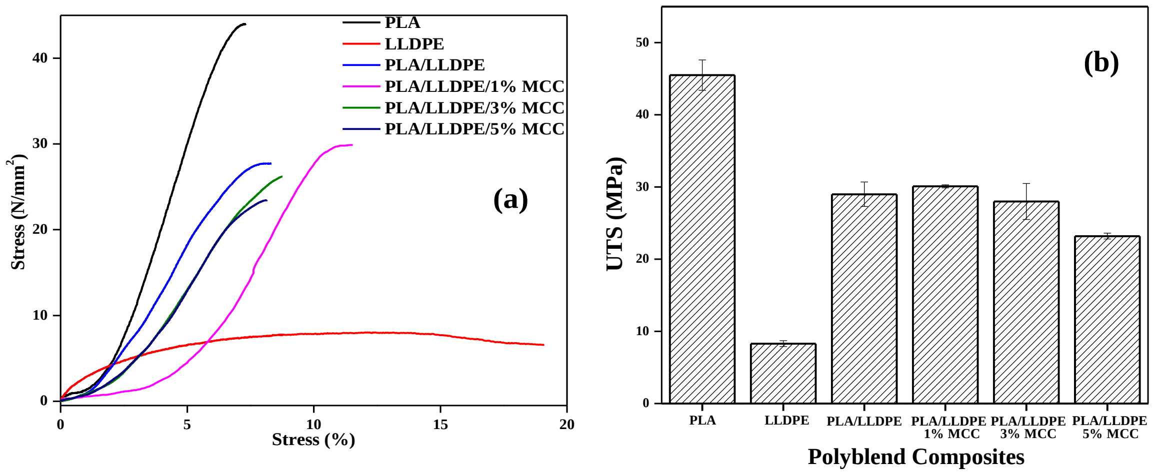

Fig. (a) Stress vs Strain curve and (b) UTS of PLA and its polyblend composite

The tensile strength and percentage elongation of PLA/LLDPE/1% MCC was reduced to 33.8% and increased to 43.9 % than pure PLA while both properties increased to 3.8 % and 2.6 % than PLA/LLDPE polyblend, respectively. The toughness of PLA/LLDPE/1% MCC was decreased to 144.6 J/m^3 from PLA (159.7 J/m^3). No change was observed in T_g of polyblend composite but the crystallization temperature was reduced by 5°C. This study showed noticeable changes in various properties of the polyblend composite like mechanical, morphological, and crystallinity were influenced by the orientation of fibre, composition, polymer miscibility and interaction at the edges among the matrix, disperse phase and filler.

Acknowledgements

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FPC-130

Fabrication and characterization of novel biocomposite of High Density Polyethylene/Poly (Lactic acid) Blendswith Microcrystalline Cellulose as Reinforcement material in food packaging application

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Abstract

High density polyethylene (HDPE) is the most popular synthetic polymer used in food packaging sector in the form of bottles, storage bags etc. The aim of this work is to minimize the global polution caused by this particular plastics by incorporating biopolymer (Poly lactic acid) (PLA). Miscibility, morphology, thermal behavior and mechanical properties of theHDPE/PLApolyblends and microcrystalline cellulose fiber (MCC) reinforced composites has been characterized. The Twin screw extruder followed by injection molding has been utilized for this melt blending. Various compositions of polymer blends has been taken along with constant MCC concentration for fabrication of biocomposites to obtain the desired properties.In this work, HDPE has been used as a matrix material in which PLA are in disperse phase and MCC fibers acted as fillers. The immiscible characteristics of both polymer blends has been stabilized by incorporation of fiber into the matrix and biodegradable nature of PLA has helped to improve the biodegradability of HDPE. The effect of MCC fiber on the morphology and mechanical properties of composites has also investigated.

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FPC-131

Iron oxide based nitrogen containing polymer nano-composite as a highly selective, quickly recoverable and reusable ammonia gas sensor

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Abstract

A facile, highly selective, quickly recoverable ammonia sensor was developed by using Polyaniline/Iron oxide (PANi/IO). The hybrid nanocomposite was synthesized by *in situ* chemical oxidative polymerization process of aniline in presence of hematite. The α-Fe_2O_3 nanoparticles were obtained by template (C.T.A.B.) assisted hydrothermal route at 200°C.The structural, morphological study and compositional analysis of PANi/α-Fe_2O_3 were performed by Diffuse Reflectance UV-Vis studies (UV-DRS), X-ray Powder Diffraction (XRD) analysis and Field Emission Scanning Electron microscopy(SEM).The particle hydrodynamic diameter measurements were performed by Diffraction Light Scattering (DLS). The gas sensing ability of this hybrid sensor was tested for chemical vapours like L.P.G., Chloroform, Methanol, Ethanol, Isopropanol, Acetone and Ammonia. Our investigation indicates that the newly synthesized PANi/α-Fe_2O_3 nanocomposites containing 10% by weight of α-Fe_2O_3 exhibited high selective sensing ability towards ammonia gas at room temperature.

Key words: hematite, *PANi*, nano composite, ammonia gas, sensor, selectivity

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FPC-132

Synthesis of bioactive 3, 4-dihydropyrimidine(DHPM) by Ultra-sonication method using polymer nanocomposite as reusable catalyst

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Abstract

Polymer nanocomposite was synthesized and well characterized by using FTIR, XRD, SEM techniques. Using polymer nanocomposite as a heterogeneous reusable catalyst new Green approach has been developed towards the synthesis of bioactive 3, 4-dihydropyrimidine (DHPM) under ultra-sonication method. A series of novel DHPM derivatives have been prepared with high yields, short reaction time and evaluated for their antifungal activity. The catalyst is reusable, easy to synthesize and work at moderate reaction conditions. Dihydropyrimidines derivatives have been characterized by NMR, IR and Mass spectroscopy. Synthesized compounds show promising antifungal activity.

Scheme

Keywords:

Ultra-sonication, green route, polymer nanocomposite catalyst, Solvent free, Antifungal

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FPC-133

Mechanical and Thermal Properties of Synthesized Polysilsesquioxane Powder Reinforced Epoxy Adhesive

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Abstract

Polymethylsilsesquioxane (PMS) and Poly (methyl/vinyl)silsesquioxane (PVS) powder was synthesized by hydrolytic condensation of organosilane precursor in aqueous phase. The synthesized Polysilsesquioxane (PS) powder were characterized by Fourier Transform Infrared Spectroscopy (FTIR) , Scanning Electron Microscopy (SEM) and the particle size of the PS powder was corroborated by imaje j software from the SEM images. The epoxy composites adhesives were developed using PS powder with different loading (1-4 phr). Tensile and compressive strength of the adhesive formulation were studied using the Universal Testing Machine. It was observed that the mechanical properties of the composites show an increase on increasing the filler loading. Among all adhesive systems, PVS (4 phr) loaded epoxy composite (EPV-4) showed 65.4% enhancement than the neat epoxy system. Adhesive strength of the epoxy composites on mild steel substrate were investigated by conducting lap shear test and EPV-4 exhibited higher adhesive strength on mild steel adherent. Surface morphology of the epoxy composites and the fillers were visualized from the SEM images and the thermal conductivity of EPV-4 revealed 43% increment as compared to neat epoxy composite.

FPC-134

Nonlinear Absorption Studies in Functionalized Polymer

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Abstract

Electrospun nanofibers are being studied and developed because of their great potential in diverse domains of application such as optical sensors, tissue engineering etc. Functionalization of the surface and interior of these polymeric nanofibers with nanoparticles is an efficient fabrication method for a wide variety of nanoparticle-embedded materials. The aim is to compare the third order nonlinear absorption coefficient of the Au nanoparticles incorporated nanofibers with the casted films of CAN/PVA Au nanocomposites. Linear optical studies and morphological analysis of the prepared samples confirmed the incorporation of Au nanoparticles into the matrix. Open aperture Z-scan measurements were carried out at 532 nm and the samples were exposed to a 5 ns laser pulse. The nanofibers with Au nanoparticles exhibited higher two photon absorption coefficient than its nanocomposite solution. This enhancement is correlated with the morphology of nanofibers and electric field enhancement of Au nanoparticles into the polymer matrix. Optical limiting performance of the prepared nanocomposites and nanofibers show a better result than the film of CAN/PVA blend and CAN/PVA nanofiber mat due to the nonlinear absorption of the nanoparticles in resonant regime, thus making it suitable for optical limiting applications.

Key words: Au Nanocomposites, Au Functionalised nanofibers, two photon absorption,

FPC-135

Polymer-ZnO Nanocomposites as Electrodes for Supercapacitor Applications

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Polyimides are thermally stable polymers with good chemical resistance that are often based on solid aromatic backbones. Polyimides are used as cathode materials for rechargeable lithium batteries. A polyimide is synthesized using 4, 4’ diphenyl diamine methane (DDM) and poly(styrene-*co*-maleic anhydrides) (SMA). The modified styrene-*co*-maleic anhydride is taken as the matrix into which ZnO nanoparticles are incorporated. This polyimide nanocomposite was characterized by spectral and thermal analysis. The surface morphology was studied using Scanning Electron Microscopy (SEM). Supercapacitor electrodes have been fabricated by using different composition of the Polymer Nanocomposite-Activated Carbon (AC)-Binder. Electrochemical properties of the fabricated composites has been studied using Electrochemical Impedance Spectroscopy, Cyclic Voltammetry (CV) and *Chronopotentiometry* (CP) techniques using 1 M KOH as the electrolyte. The cycling stability and the charge-discharge time were noted to establish its applicability as an efficient supercapacitor.

FPC-136

Semiconducting Properties of Modified Styrene-Maleic Anhydride Nanocomposites

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Abstract

Designing new semiconductor materials includes efficient tuning of electronic and optical band gaps and the charge-carrier transport properties of the material involved. Organic Polymers with extended pi-electron system serves as good candidates for building up a semiconducting material. Addition of heteroatoms to the matrix further provides the advantage of extra electronic mobility in the form of lone pair of electrons. The semiconducting properties experience a perceptible increase on the inclusion of nanoparticles. The semiconductor-electrolyte interface, the type of semiconductor and its charge-carrier densities can be studied in detail using the Mott-Schottky analysis. In the present work, a thiadiazole moiety is hooked on to styrene-maleic anhydride copolymer. The incorporation of ZnO nanoparticles were effectively carried out on the polymer matrix. Spectral and thermal analysis was carried out on the samples. Electrochemical impedance data and the subsequent linear fit were performed. The impedance analysis was useful in obtaining the Mott-Schottky plot and it helped in confirming the semiconducting nature of the nanocomposites and the type of semiconductor formulated.

FPC-137

Crystallization Behavior of Crystalline/Crystalline Polymer Mixtures under Confinement in Electrospun Nanofibers

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Abstract

The crystallization behaviour of polymers has been one of the most fascinating research area in polymer science for last several decades. With the advent of nanotechnology now focus has been shifting to understand the properties of materials in nano-dimensions and on crystallization study of polymers in nano-shaped materials. This is driven by the fact that any perturbation of crystallization behaviour in confinement may significantly alter the properties of the materials. Hence, an understanding of the polymer crystallization under nano-confinement is necessary for tailoring of the polymer properties when used in nanotechnology related applications. Study of polymer crystallization in electrospun nanofibers, in this respect, are interesting and provide knowledge about polymer crystallization in confined spaces. The electrospun nanofibers composed of an immiscible blend of an amorphous and a crystalline polymer, with the latter forming the dispersed phase in the fibers, could be used for studying the effect of confinement on the crystallization behavior. In this case, the limited radial dimension of the nanofibers may restrict the length scale of phase separation between the immiscible constituents, so as to generate the domains in nano-dimensions. In the present research, the crystallization behavior of polymers in polymer blend is systematically investigated by confining in electrospun nanofibers in order to gain vital fundamental understanding of confined crystallization in such materials. The effect of confinement on mixtures of crystalline/crystalline polymers is investigated which gives fundamental information on polymer crystallization behavior in confined conditions and structure-property relationship in electrospun nanofibers.

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Theme- APMP

APMP-01

Friction Stir Welding of Polymers a Review

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Abstract

Friction Stir Welding (FSW) is a modern welding process invented by The Welding Institute (TWI). In FSW a non consumable rotating tool is used to “Stir” metals and polymers along a butt joint. At Present, the process is applied exclusively in straight line welds. During FSW the tool probe of the rotating tool is plunged into a work piece or between two work pieces by a friction stir welding machine to produce the required joint. The resistant force is applied in to a softened portion which is softened by a frictional heat to form a region of plasticized material. Problems like solidification cracking, porosity and liquation cracking are eliminated due to its solid state nature. FSW benefits include reduction in fuel consumption in light weight aircraft, automotives and ship automation industries are numerous. This process is used for successfully for joining of similar and dissimilar like aluminium, magnesium and even polymers now-a-days.

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APMP-02

Polymer Based Network: An Ideal System for the Flexible Organic Light Emitting Diode (OLED)

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Abstract

Unlike conventional light emitting devices (LED), Organic LED (OLED) can provide flexibility. Such property will minimize the mechanical and electrical damage within the appliances. For the conventional LED, there is always leakage of electrical energy in the form of heat. As a consequence of this the quantum efficiency drops. The energy conversion from electrical to light is more prominent for OLED. To overcome the conventional drawback, efforts are in progress for the past few years to improve the efficiency for OLED. The optimum efficiency for OLED have reached at around 100 lumens per watt (lmW^{-1})[1–2]. There is steady improvement to increase the efficiency for OLED. Towards optimization of OLED appliances, we have developed an unique approach for the growth of soft material via photopolymerization[3–4]. To introduce flexibility[5] and to express the tunability, we have replaced the conventional low molecular composites as well as linear polymer with a compact polymer matrix. It is interesting that due to flexibility, the tunability in context to (i) energy emission over range and (ii) intensity could be achieved by the polymer matrix. We expect that the material to be an ideal OLED system as well as the energy source for various appliances, for example as photocatalyst.

Figure 1. Alignment of Chromophores in Flexible Polymer Matrix

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APMP-04

Processing of Ultra-High Molecular Weight Polyethylene(UHMWPE) into continuous oriented product

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Abstract

UHMWPE is a speciality linear polyethylene with exceptionally low coefficient of friction, extremely high impact resistance, abrasion, wear resistance and good long term mechanical properties. Such combination of properties makes it suitable for the preparation of stronger fiber and other oriented products suitable for diverseapplications. However, high molecular weight of UHMWPE results in extremely high melt viscosity and limits the polymer processability and thereby end use applications. Therefore, the conventional melt processing techniques like injection moulding, blow moulding cannot be used with UHMWPE and only compression molding or ram extrusion techniques used in molding of UHMWPE into finished articles. The present study describes aprocess for extrusion of an ultra-high molecular weight polyethylene (UHMWPE) in to continuous tape/profile [1]. The extrusion of UHMWPE powder (MW.3.5 million g/mole) was done by conveying and compacting the polymer in a single screw extruder unit without using the die in the temperature range 115-200°C. The elimination of the die-head as part of extruder helps in overcoming the processing limitations caused by very high reduced specific viscosity and flow resistance of the polymer melt. The high compression ratio (3.5) of extruder screw facilitates the compaction of polymer melt at distal end of extruder screw. The tensile strength (TS) and tensile modulus (TM) of extruded UHMWPE tape were found 0.048 GPa and 0.46 GPa, respectively which is very close to the compression molded sheet of commercialultrahigh molecular weight polyethylene(Relene 2504) (TS 0.0417 GPa, TM 0.51 GPa). The density of the extruded tape was obtained as 0.950 g/cm^3.

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APMP-06

Industry Scalable Polyurethane from Recyclable Waste Plastic

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Abstract

Waste plastic is hazardous to the living world and re-utilization is of high demand. 8 million metric tons of plastic wastes are going into ocean every year. In allover world, around 20000 plastic bottles are being purchased in every second and only one third of this is being reutilized to make polyester fiber in textile industry, application in coating industry being limited. As a company striving towards green and sustainability, Asian Paints Limited, has taken measures to reduce carbon footprint and utilize renewable sources. The current work focuses on converting nonstandard waste PET (from various sources) to a standardized glycolate-ester oligomer through process optimization having desired properties like hydroxyl value, molecular weight etc. The glycolate polyester oligomer was then converted to linear polyesters by reacting with polyacids like adipic, isophthalic etc. in a way reducing effective cycle time and avoiding glycol loss at higher temperature. This polyester can be tailor made by varying the glycols and polyacid resulting in varied properties suitable for different application. The polyester was also utilized in making polyurethane and polyurethane dispersions and characterized for various mechanical properties.

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APMP-07

Polyacrylonitrile Based Precursor for Carbon Fiber: Kinetics of Oxidative StabilizationReaction under Free Shrinkage in Isothermal Conditions

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Abstract

The thermal stabilization of polyacrylonitrile (PAN) fiber plays a critical role to impart infusibility in the fiber structure during its conversion to carbon fiber (CF) under oxidative environment. However, the PAN fiber shows a tendency to undergo a linear deformation (shrinkage) during the stabilization due to entropy recovery, cyclization, and dehydrogenation, etc.[1] These various reactions occur at different thermal regimes[2]. In the present investigation, the PAN fiber wasallowed to shrink freely aftersubjecting to alow tension (0.01 g per denier) at its free end (**Figure 1**). The PAN fiber wasexposed to five different temperatures viz. 200, 210, 220, 230, 240 °C for 6 hin theisothermal condition[3]. The structural changeduring the stabilization iscorrelated to the cumulative chemical shrinkage determined after excluding the physical shrinkage during the stabilization. The presentstudy may be useful to predict the rate of oxidative stabilization reaction for a batch of PAN fiber. This work also offers useful inputs aboutthe stabilization condition for producing stabilized PAN fibers with reduced skin-core homogeneity.

Figure 1: Experimental set up for shrinkage studies of PAN based precursor fiber

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APMP-08

Measurement of Anisotropic Modulus and Poisson Ratio of Reinforced Composites

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Abstract

Short glass fiber filled reinforced resins, are widely used for many structural applications, where determination of mechanical properties, especially strength and stiffness (E), are essential in ensuring performance of composite structures. The primary benefits of such composites are reduction in weight with adequate strength and elimination of secondary operations. Such reinforced composites, due to specific alignment of the reinforced filler in the flow direction, do not have an isotropic mechanical property and displays anisotropy. For a good Computer Aided Engineering (CAE) model, a knowledge of complete elastic stiffness and the true strain measurements (both, along longitudinal and lateral directions) are critical under loading conditions. While mechanical properties of such composites, are often modelled taking into consideration the resin and the filler attribute separately, experimental measurement of such properties increases reliability of CAE models, such as Autodesk Moldflow™, Abaqus™, LS-Dyna™, ANSYS™ etc.

A method was established for understanding glass fibre orientation in a given part, using a Scanning Electron Microscope, after which the directional dependent modulus and Poisson ratio were experimentally determined by Tensile tests. The results obtained from this method was, compared with theoretical values known in literature and was found to be in good agreement.

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Influence of Temperature on Properties of Polypropylene Foams Prepared by Single Step and Two Step Batch Foaming Process

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Abstract

This study reports the effect of temperature on morphological, mechanical and thermal characteristics of polypropylene (PP) foams prepared by two different methods of foaming at low saturation pressures. In the first method, involving single-step pressure-induced-foaming (PIF), the solid specimen is heated to different temperatures in a high-pressure vessel and then pressure is applied. On the other hand, in the second method, involving a two-step temperature-induced-foaming (TIF), the solid specimen is saturated with pressurized CO2 at room temperature for a specific period of time and then the CO2 laden specimen is immersed in hot glycerol bath at different temperatures for foaming. SEM micrographs of fractured foamed specimens were employed for measurement of cell-size distribution. The average cell sizes ranged between 3 – 310 µm in specimens obtained using PIF, while in case of foams prepared by TIF, the cell sizes ranged between 30 – 70 µm. The cell sizes obtained from TIF are significantly smaller and more uniform as compared to those from PIF foams. The density (0.393-0.186 g/cc) of PIF foams was seen to decrease with increasing temperature; in contrast, in case of TIF the density remains more or less unchanged around 0.43-0.47 g/cc with change in temperature. The uniaxial compression test at maximum strain showed a decrease in strength of both PIF and TIF foams with increase in temperature. The elastic modulus and collapse modulus of foams showed a decreasing trend with increase in cell size. The crystallinity of the foamed specimens was measured using differential scanning calorimetry. The thermal properties of both PIF and TIF foams exhibited improved thermal stability as compared to unfoamed PP matrix. The thermal stability of TIF foams also showed a decreasing trend with increase in cell.

Keywords: Pressure induced foaming, Temperature induced foaming, saturation temperature, foam density, cell size.

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APMP-10

High-Throughput Template-Free Continuous Flow Synthesis of Polyaniline Nanofibers

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Abstract

The scalability and high-throughput synthesis of conjugated polymer based nanofibers has always been a challenge for the chemists due to issues related to secondary nucleation and the resultant distortion in shape when synthesized via traditional batch processes. The generally adapted way of synthesis is by either employing very low concentrations of the monomer or by terminating the reaction at times much before secondary nucleation can actually commence. However, these batch methods are not economical and result in a throughput of only a few hundred milligrams per hour with poor space-time yield. In this work, we report the continuous flow synthesis of polyaniline nanofibers resulting in high throughput (17-30 $gL^{-1}h^{-1}$)_and space-time yield (140-450 $gL^{-1}h^{-1}$), which are a few orders higher than those when using batch processes. Moreover, the process also thereby becomes more scalable when performed through flow. These polyaniline nanofibers show a much higher surface area (35-46 m^2/g) as compared to traditional batch processes ($18 m^2/g$). It is also noteworthy that this method is generic in nature and, in principle, can be extended for the synthesis of other nanofibers based on conjugated polymers such as Polypyrrole, Polythiophenes, Poly(3,4-ethylenedioxythiophene) and their derivatives.

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APMP-12

Experimental Study on Abrasive Water Jet Machining of Sandwich Composites

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Abstract

Sandwich composites have advantage of having different skins which gives them different characteristics from either side. The core gives good damping and provides more thickness whereas skin provides strength. The present article focuses on study of kerf geometry in abrasive water jet machining of sandwich composite. Three process parameters of abrasive water jet machining namely jet pressure, traverse speed and stand-off distance (SOD) are considered.Kerf taper, Material Removal Rate (MRR) and roughness will studied by varying process parameters. Delamination and surface marks in machined samples is observed by using scanning electron microscope. Analysis of variance is performed in order to investigate the influence of input parameters on output. It is found that Increase in SOD and Traverse speed decreases Kerf taper angle and increases MRR.

Keywords

Abrasive water jet machining, Sandwich composite, delamination, kerf geometry, Material Removal Rate

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APMP-13

AWJM Performance Measurement of Sandwich Composites

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Abstract

Sandwich composites, wherein the skin and core fulfills the requirement of different properties, like in foam sandwich structure, foam is providing damping and skin provides rigidity to the structure. In this work a sandwich panels with foam core and glass/polyester skin is fabricated by vacuum infusion technique. Abrasive water-jet (AWJ) drilling of these materials is performed to study the effect of standoff distance (SOD), Water Jet Pressure (JP) and Traverse Rate (TR) on kerf taper and surface roughness and Material Removal Rate (MRR). The experiment is designed using Taguchi's L_9 orthogonal array. The ANOVA is done to study the influence of input parameters on output. It is found that SOD is the most influencing parameter on the kerf taper and surface roughness.

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APMP-14

Alleviation of Particulate matter bound Microbes by Natural polymer based Nanofiber

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Abstract

Particulate matter (PM) pollution is one of the most important issues that the world is confronting today because of the adverse health effects associated with it are attributed due to the presence of microorganisms in PM. Alleviation of PM bound microbes and protection of the environment is becoming a pivotal interest of sustainable development. Biodegradable natural polymer (Chitosan-Cs) based nano-fibers with nano-fillers (silver nanoparticles -AgNPs) capable of inhibiting growth of airborne microbes were prepared by Electro-spinning method. Biosynthesis of AgNPs was carried out with plant extracts and characterization of nanoparticles and prepared nano-fibers were accomplished by using different techniques (SEM, FTIR and XRD). SEM analysis revealed uniform distribution of spherical shaped AgNPs with an average size of 50 nm. FTIR and XRD studies confirmed the successful formation of AgNPs. Changes in the ratio of CS/PVA and AgNPs altered the fiber diameter effectively. The spectra of the prepared nano-fibers showed the presence of major characteristic peaks of both polymers. The individual peaks of AgNPs are absent in produced nano-fibers which explains the complete and successful blending of the polymers with each other and complete exfoliation of AgNPs in CS-PVA mixture. Antimicrobial activity assessed by disc diffusion method showed significant antibacterial properties of both CS-PVA and CS-PVA-AgNPs and maximum inhibition of bacterial growth has been found in the fibers with higher contents of Cs and AgNPS. Therefore, this produced fiber can be used to alleviate the microbes present in air and will thus be useful for the purpose of mitigating environmental contaminants.

APMP-15

Multimodal High Density Polyethylene with Ziegler-Natta Catalyst

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Abstract

Polyolefinsrepresent a class of large volume commodity plastics with annual production exceeding160 million tonnes in 2017.[1]The growing marketacceptance of these polymers is driven bycontinuous advances in catalyst and production technologies together with their versatility in diverse applications ranging from commodity products like carry bags to high added-value health care products. High-density polyethylene (HDPE)is commercially producedin gas phase and slurry technologies using Ziegler, Phillips and metallocene type catalyst systems.The processability of HDPE is generally enhanced by broadening the molecular weight distribution whilst the mechanical properties can be improved by selectively placing comonomer in the high molecular weight part of the molecular weight distribution. Such a comonomer distribution is known as a "reversed/inverse" comonomer distribution. Several approaches are currently used to produce polyethylene with reversed comonomer incorporation. These include concepts such as preparing multimodal PE in cascaded reactors[2], use of dual-site catalysts[3], catalyst blend approach, and use of binuclear catalysts etc.[4]

The presentation will coverseveral aspects of the production of multimodal HDPE in a cascade process using different catalyst systems. The inter-relation between catalyst, process and product together with the challenges encountered while bringing new products from laboratory scale to commercial plant will be discussed during the presentation.

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APMP-16

Fabrication of Stereo complex Poly (Lactic acid) (PLA) fibers reinforced withAmphiphilic Chitosan using Melt Spinning

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Abstract

Melt spinning of high molecular weight Poly (L-lactic acid) (PLLA) and Poly (D-lactic acid) (PDLA) in equal weight ratio fabricated with NanoAmphiphilic Chitosan was performed by laboratory scale fibre spinning machine. The blend obtained thereby has higher stereocomplex content with increase in melting point about 50°C more than Poly (Lactic acid) (PLA) without any formation of traces of homo crystallites which was confirmed by Differential Scanning Calorimetry (DSC). The effect of different weight % of MCH loading on PLLA/PDLA blend was investigated and formation of Amphiphilic chitosan that was synthesized via in situ condensation polymerization was confirmed by Fourier Transform infrared spectroscopy (FTIR) and Nuclear Magnetic Resonance Spectroscopy (NMR). The crystalline behaviour alongwith formation of α -form crystals of the blend fibre was confirmed by X-ray Diffraction (XRD) and how on significantly transformation of stereocomplexation structure of PLA takes place by annealing under tension was thereby studied to obtain the improved mechanical properties.

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APMP-17

Fabrication of stereo-complex poly (lactic acid)/hydroxyapatite (sc-PLA/HAP) bio-nanocomposite by melt-spinning

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Abstract

Poly (lactic acid) PLA, a biodegradable, bio-absorbable, non-toxic, environmental-friendly polymerfinds its application in areas of biomedical and food packaging. The stereocomplexation of PLAopens a new pathway for the discovery of new materials, also tunability of different properties in the field of biomedical research. The hydroxyapatite (HAP), received great attention due to its better osteoconductivity, biodegradability and enhanced mechanical properties. In this study, the X-Ray Diffraction(XRD) analysis ensures the formation of stereo-complex crystallites. The Fourier Transform Infrared Spectroscopy(FTIR)analysis proved the successful bond formation of the stereo-complex crystallites. The Differential Scanning Calorimetry (DSC) results also revealed the improved melting point of the crystallites around ~201 °C. Different techniques like solution casting, melt spinning and electro-spinning have been employed by researchers for the fabrication of the composite. The melt-spun sc-PLA/HAP nanocomposite is expected to have more surface-area to volume ratio with the introduction of new nano-structures applicable in the field of biomedical science.

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APMP-18

Comparison of various reactor designs for Lactic Acid oligomerization

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Abstract

Poly (lactide) PLA, is a biodegradable, renewable, environmental-friendly polymerand a natural alternative to petro based plastics. It has already found applications in food packaging and biomedical surgical devices. With the addition of different additives its various properties can be enhanced even more to increase its applicability and use. PLA can be formed by polymerization of lactide which can be formed by depolymerization of LA oligomer. Lactic acid oligomerization is the first step for PLA production. Various reactor designs have been studied in this work and compared for PLA oligomerization with their heat transfer and mass transfer areas calculated for optimal performance.

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