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# Conference Proceedings

## SPSI-MACRO-2023

17<sup>th</sup> International Conference on

**POLYMER SCIENCE AND TECHNOLOGY**

**DECEMBER 10 -13, 2023**

**Venue** | Indian Institute of Technology Guwahati



*17<sup>th</sup> International Conference  
on*

## **Polymer Science and Technology**



# **SPSI-MACRO-2023**

**December 10-13, 2023**

Organized by  
**Centre for Sustainable Polymers**  
Indian Institute of Technology Guwahati, India  
&  
The Society for Polymer Science, India



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Dated, the 7<sup>th</sup> December, 2023



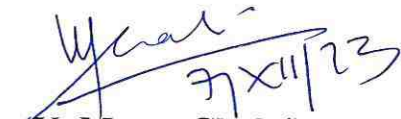
### **MESSAGE**

I am happy to learn that Centre for Sustainable Polymers (CSP), Indian Institute of Technology (IITG), is holding the 17<sup>th</sup> International Conference on Polymer Science and Technology, SPSI-MACRO 2023. It is highly appreciated to note that this event is organized with some of the finest minds.

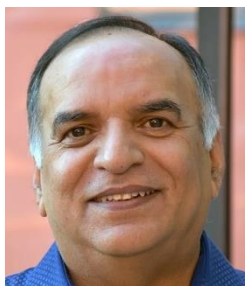
This conference will serve as catalysts for innovation, fostering collaboration and exchange of knowledge that propels the sector forward. I believe that this conference will provide an opportunity for eminent academicians, researchers, scientists, and policy makers to deliberate and discuss new advanced developments in the field of sustainable polymers.

I encourage each one of you to engage in this scientific meeting wholeheartedly, share your insights, and embrace this opportunity to learn, connect, and forge lasting networks.

I extend my heartiest congratulations to the organizers, sponsors, and every individual who has contributed to make this event a great success. May this conference be a fruitful and enriching experience for all.

  
(K. Moses Chalai)





**Prof. Rajeev Ahuja**  
Director  
Indian Institute of Technology Guwahati

**Message**

IIT Guwahati is hosting SPSI-MACRO-2023, one of the biggest conferences in the domain of Polymer Science and Technology. It is a matter of pride for the entire campus fraternity to welcome all the delegates to this auspicious event. Over the years, it has always been the tradition of this institution to support the culture of critical interdisciplinary deliberations amongst the scientific fraternity towards holistic technological advancement of the broader society.

Polymers, especially plastic materials, have revolutionized human lifestyle over the past century. However, these materials are raising serious ecological concerns caused due to the challenging waste management protocols at the end of the lifecycle. It is my belief that through rigorous scientific discussions and interactions between scientific, industrial and policy related stakeholders, the conference would be able to develop a roadmap towards an efficient plastic waste management strategy, by fostering a transition from conventional plastics to sustainable alternatives.

I wish all the very best to SPSI-MACRO 2023 towards a successful conference and welcome all the delegates to IIT Guwahati campus.

Officiating Director  
Indian Institute of Technology Guwahati



**Dr. S. Sivaram, FNA**  
Former President, SPSI  
Professor Emeritus and INSA Emeritus Scientist  
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### **Message**

I am very happy to note that IIT- Guwahati is hosting MACRO 2023, the 17<sup>th</sup> International Conference on Polymer Science and Technology (SPSI-MACRO-2023) from December 10-13, 2023. It is also gratifying to note that Tezpur University and CSIR-NEIST, Jorhat are co-hosting this event, thus, bringing together leading scientific institutions in the north-eastern part of India. The objective of this Conference is to provide a platform for scientists from India and overseas, from academia and industry as well as research students to meet and discuss recent fundamental understanding as well as technological advancement in polymer science. SPSI-MACRO-2023 conference is the seventeenth in the series of international conferences that are held in India every two years under the auspices of The Society for Polymer Science, India, the premier umbrella organization that brings together all practitioners of polymer science and technology in India. SPSI-MACRO-2023 has attracted many distinguished academic personalities, industrial leaders, and new entrepreneurs across the globe as speakers and participants.

I observe that many topics of contemporary interest in polymer science are the subject matter of this Conference. Polymer Science as a discipline is in the cusp of change. On the one hand, large volume polymers are demanding our attention from the point of view of sustainable consumption and addressing end-of-life issues. On the other hand, polymers and advanced materials are becoming critical “invisible” components of many applications, may it be in new energy systems, mobility, built environment, water, agriculture health, medicine, and wellness. Our society poses many challenges to polymer science as a discipline. The hallmarks of good polymer science that will serve the future are strong foundation in the fundamentals of the discipline, interdisciplinary understanding, applying systems thinking and integrating chemistry, physics, material science, biology, earth systems and engineering in our quest for solutions that will stand the test of time and benefit society without any unintended consequences.

I wish the Conference a grand success





**Dr. Anil Kumar**  
President, SPSI

### **Message**

It is my pleasure to welcome you all, on my personal behalf and on behalf of the Society for Polymer Science India (SPSI), for the 17<sup>th</sup> International Conference on "Polymer Science and Technology" (SPSI-MACRO 2023). This is being organized by the Guwahati Chapter of the SPSI. I congratulate the Guwahati chapter and the organizing committee for hosting this important activity.

SPSI was established in 1979 and has since played an essential role in general advancement of Science and Technology of Polymers in the country by providing a forum for the exchange of information amongst the members and persons attached to the Society. At present, SPSI has ten active chapters to help achieve the stated objectives of the Society.

After a couple of years of disruption due to the pandemic, we are back to normal "in-person" interactions. This is the second biannual "in-person" event, post-pandemic, of the SPSI after the Pune Chapter's successful completion of SPSI MACRO 2022. The organizing committee of SPSI-MACRO 2023 has done excellent work in bringing together so many of the best practitioners of polymer research in one place. This will provide an excellent opportunity for all the young researchers to interact and learn from the best in the field.

I am confident that SPSI-MACRO 2023 will be an excellent event to boost further growth of polymer research and education in India. I am sure all the participants will make the best use of their time interacting and discussing with others to develop new ideas and directions in polymer research.

I wish the SPSI-MACRO 2023 a huge success.

With warm regards

A blue ink signature of Anil Kumar, written in a cursive style.

Anil Kumar  
(President, SPSI)





**Dr. Vimal Katiyar**  
Chair, SPSI-MACRO-2023

### **Message**

Over the years SPSI-MACRO has established itself a prestigious platform to bring together the brightest minds in the field of polymer science and technology for the growth of research and innovation, towards the benefit of the society at large. We feel honoured to organize the 17<sup>th</sup> Edition of the International Conference on Polymer Science and Technology, SPSI-MACRO-2023 at IIT Guwahati, a serene and technologically vibrant campus in the north-east region of India. As a member of the IIT Guwahati family and a polymer science enthusiast, it is a matter of pride to welcome all the delegates to this meeting for sharing their intellectual and stimulating thoughts and experiences.

The conference has been categorized into 15 major focal themes with special emphasis on sustainable use of plastics. Beside hardcore scientific deliberations, special workshops for students and sessions for industry-academia interactions are also on the agenda to broaden the boundaries of our understanding and application towards polymers and related fields. We believe that the cross-pollination of ideas at this conference will lead to innovative solutions to some of the most pressing challenges of the current times with relation to polymer synthesis, product development, scale-up approaches, and plastic waste management especially of single use plastics.

Once again, on behalf of the organizing team, I welcome all the delegates from India and abroad. Your presence and contributions in SPSI-MACRO-2023 will undoubtedly enrich our discussions and enable the fraternity to thrive in advancing polymer science and technology to achieve the Sustainable Development Goals.

With Regards,



Vimal Katiyar  
(Chair, SPSI-MACRO 2023)

# **Award Lectures**

# **&**

# **Plenary Lectures**



**Dr. S. Sivaram Endowment Lecture****Recyclable and Degradable Polyethylene-Like Material Embedded by Catalytic Methods****Stefan Mecking***University of Konstanz, Germany**Corresponding author's Email: stefan.mecking@uni.kn***Abstract**

Plastics are key components of virtually any technology today. The excellent materials properties of polyethylene, the largest produced synthetic plastic, originate from a crystalline packing of the (linear) hydrocarbon chains. Their inert nature hinders chemical recycling, however, and also renders material lost to the environment persistent for many decades.

These problems can be alleviated by low densities of in-chain double bonds. As a direct approach to such polymers, a step-growth polymerization of long-chain monomers, obtained from natural oils, yields polyesters or polycarbonates with solid state structures and materials and processing properties similar to polyethylene (HDPE). At the same time, these materials can be closed-loop recycled under mild conditions via the low-density of in-chain functional groups [1]. The rates of degradation by microorganisms can be tuned over a wide range by the choice of monomers and repeat units [2,3]. Such HDPE-like materials can also be formed from mixtures of monomers with different length, as could potentially be sourced from biomass or plastic waste [3].

Non-alternating copolymerization of ethylene with carbon monoxide by state-of-the-art nickel(II) complexes provides access to polyethylenes with isolated keto groups in the chain (keto-PEs). Due to their high molecular weights, their properties are on par with HDPE, but the in-chain keto groups render the material photolytically degradable [4].

Ongoing studies address the understanding and advancement of this polymerization catalysis, materials for applications that particularly call for closed-loop recycling and biodegradability, and quantification of the latter by means of (catalytic) isotope labelling.

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## **Plenary Lecture I**

### **Equilibration of non-equilibrium polymer melt, implications on physical and mechanical properties**

**Sanjay Rastogi**

*King Abdullah University of Science and Technology, Chemistry, Physical Science and Engineering, Thuwal, Kingdom of Saudi Arabia*  
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#### **Abstract**

A single linear covalent bonded, long molecule having more than 1000 repeat units, because of its conformational restrictions result into free volume. This very basic concept is the folklore for the glass transition temperature in amorphous polymers, and the presence of physical network in a polymer melt. To recall, in a polymer melt having ensemble of chains, the free volume gets occupied with the formation of physical entanglement. Retrospectively, leading to bulk density of the polymer melt by several folds. The presence of physical entanglements is further facilitated by polymer synthesis, which has become basis of our understanding in chain dynamics. Here we will address scenarios, strongly influenced by polymer synthesis that show strong deviation from the anticipated entanglement formation and invoke non-equilibrium polymer melt, having implications on crystallization kinetics, crystal thickening, and mechanical properties of the resultant products.



**Prof. Santappa Award Lecture****An Overview of High-performance Polymers for Membrane-Based Applications****Susanta Banerjee***Materials Science Centre**Indian Institute of Technology Kharagpur**Kharagpur 721302, India**Corresponding author's Email: [susanta@matsc.iitkgp.ac.in](mailto:susanta@matsc.iitkgp.ac.in)***Abstract**

Polymers occupy a central role in the development of modern society. High-performance polymers are classes of polymer materials that are known to retain adequate mechanical, thermal, and chemical properties when subjected to harsh environments such as high temperature, high pressure, and corrosive chemicals. The development of these classes of polymers are crucial for many advanced applications, including their membrane-based applications. Polymeric membranes are selective materials and a rapidly growing field for several industrial applications, such as membranes for low-k applications, membrane separation of gas and liquid mixtures, water purification, and solid polyelectrolyte membranes in fuel cell applications. All these applications requires design and preparation of functional high-performance polymers that are processable and survive severe test conditions during their use in the form of thin films. Several aromatic polymers, e.g., poly (arylene ether)s, polyimides, polyaramids, polytriazoles, etc., has shown great promise in thess direction due to their excellent mechanical and thermal stabilities. However, the major drawback of these classes of polymers is their processing difficulty due to their infusible nature and insolubility in common organic solvents that restricts their processability by melt and solution processing techniques. The incorporation of fluorine polymers in the form of 3F (-CF<sub>3</sub>) and 6F [-C(CF<sub>3</sub>)<sub>2</sub>-] groups resulted in organo-soluble polymers. There has been a remarkable growth of research in semi-fluorinated polymers. It has been observed that incorporation of different fluorinated groups into the macromolecular chain not only increases the solubility but also improves many other polymer properties, e.g., reducing dielectric constant, increasing gas permeability, and also helping in the formation of phase segregated morphology that help in enhancing proton conductivity. The talk will cover different design approaches used to prepare different classes of fluorinated polymers in our group. The synthetic strategies, characterization, and detailed properties of the developed polymers with special emphasis on their membrane-based applications e.g., low-dielectric constant materials in microelectronics, membranes for gas separation, and proton exchange membrane properties will covered in this talk. This talk will address many of the practical problems that address the inherent trade-off between gas permeability and selectivity and likewise the membrane stability and proton conductivity

through manipulation of the fractional free volumes (FFV) and incorporating different structural elements in the membrane-forming polymers by macromolecular engineering.

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## Prof. Santappa Award Lecture

### Molecular Recognition Driven Controlled Supramolecular Polymerization

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#### Abstract

Co-existence of multiple pathways in supramolecular polymerization of a single building block has been recognized in many examples in the recent past. Despite significant recent development on this topic, it still remains a challenging task to identify generally applicable strategy to synthesize a supramolecular polymer with predictable internal order and mesoscopic structure. In this work, we have revealed pathway control in supramolecular polymerization of a carboxylic acid functionalized naphthalene-diimide-carboxylic-acid (NDI-1) monomer by a small amount of an organic base such as 4-dimethylaminopyridine (DMAP).<sup>1</sup> NDI-1 spontaneously self-assembles in decane to produce a mixture of aggregates (J- and H-aggregates) leading to the formation of mixture of short fibres and ill-defined particles (**Agg-1**, Scheme 1). With 100 % of DMAP, irrespective of cooling rate, only J-aggregate was noticed with entangled fibrillar morphology and gelation (**Agg-2**). Even with 10 mole % of DMAP, upon rapid cooling of a NDI-1 solution in decane, similar J-aggregation, morphology and gelation was evident (**Agg-2a**). When this same solution was slowly cooled, it produced predominant H-aggregate with 2D disc type morphology (**Agg-3**). Such 2D morphology and H-aggregate (**Agg-3**) was the only product when solutions were slowly cooled in presence of relatively less amount of DMAP (2.5 %). Such pathway control is attributed to H-bonding between DMAP and carboxylic acid group,<sup>2</sup> which eliminates the possibility of closed chain dimer formation but still may allow nucleation for open chain H-bonded pathway by H-bonding between the carbonyl oxygen of the complex and hydroxyl group of a free acid either in parallel or antiparallel fashion depending on the cooling rate and amount of DMAP (Scheme 1).<sup>2</sup> This presentation will describe such molecular recognition driven pathway control in supramolecular polymerization and copolymerization.<sup>3</sup>

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**Dr. K.H. Gharda Industrial Innovation Award Lecture****Natural silk-based high-strength porous materials for bone repair****Anuya Nisal & Team***Serigen-Mediproductions Pvt. Ltd.**Corresponding author's Email: anuya@serigenmed.com***Abstract****Journey of lab-to-market translation of a silk fibroin bone void filler**

Bone cavities may be formed due to accidents or may also be caused due to a tumor or an infection in the bone. Bone void fillers or bone grafts are materials that are used to fill and accelerate healing of defects or cavities formed in the bone. A variety of natural and synthetic materials (ceramics, polymers, metals) have been used as bone void fillers. While these materials have shown some effectiveness in bone void filling, these materials frequently cause post-surgical complications like secondary fractures. Thus, there is an active interest to develop novel bone void filling materials that overcome these limitations of existing materials. Silk fibroin, a natural polymer extracted from the *Bombyx mori* silkworm cocoon, has been explored as a promising material for bone void filling applications. In our study, we have demonstrated a patented protocol for producing silk fibroin microparticle scaffolds. These scaffolds have been designed to have appropriate pore size ( $> 100\mu\text{m}$ ), interconnected porosity, excellent dry compression modulus ( $> 100\text{MPa}$ ) and controlled rate of bioresorption. The scaffolds have been shown to be biocompatible as per ISO 10993, a global biocompatibility standard. The scaffolds show excellent differentiation of bone cells into an osteoblastic lineage as compared to any of the products used globally in this application. Further, the scaffolds have been implanted in a pilot clinical trial in patients and recovery for the patients has been phenomenal. The silk fibroin microparticle scaffolds are currently in second stage clinical trial in India, post which the product will be launched in the Indian market after securing appropriate regulatory approvals. The product is being commercialized by Serigen Mediproductions. Serigen is a CSIR-National Chemical Laboratory spin-off company supported by Venture Center.

## Plenary Lecture II

### Unleashing the Architectural Marvels: Advancing the Structural Landscape of Supramolecular Polymers

**Subi J George\***<sup>1</sup>

<sup>1</sup>New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR),  
Bangalore, India

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#### Abstract

Supramolecular polymers formed by the noncovalent association of monomers have evolved over the last two decades as the most promising candidates for the design of dynamic, adaptive, and recyclable materials. Study of dynamic and adaptive supramolecular polymers has now entered an era that demands assemblies with more structural and dynamic control. The synergy between structural and temporal control is important for the advent of supramolecular polymers to be employed as functional adaptive materials. Thus, taking cues from the biological self-assembly process, kinetically controlled seeded growth has been recently shown to provide length, dispersity, and sequence control on the primary structure of dynamic supramolecular polymers.<sup>[1]</sup> However, command over the molecular organization at all hierarchical levels for the modulation of higher-order structures of supramolecular polymers remains a formidable task. In this context, a surface-catalyzed secondary nucleation process, which plays an important role in the autocatalytic generation of amyloid fibrils and during the chiral crystallization of small monomers, offers exciting possibilities for topology control in synthetic macromolecular systems by introducing secondary growth pathways compared to the usual primary nucleation–elongation process. However, mechanistic insights into the molecular determinants and driving forces for the secondary nucleation event in synthetic systems are not yet realized. Recently, we have filled this dearth by showing an unprecedented molecular chirality control on the primary and secondary nucleation events in seed-induced supramolecular polymerization.<sup>[2]</sup> I will be discussing our recent attempts to use surface-catalyzed secondary nucleation process to modulate the topology of supramolecular polymers and to modulate the functional outcomes of supramolecular materials.<sup>[3,4]</sup>

#### References

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## Prof. Kishore Memorial Award Lecture

### Synthetic Strategies to Attain Polymer Functionalized Particles and Catalytic Porous Polymer Particles

Leena Nebhani

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#### Abstract

New strategies and techniques have been developed for the synthesis and structural tailoring of polymer functionalized particles. Nitron is a versatile compound widely used in organic synthesis for diverse reactions leading to complex molecules. The nitron functionalities are also proven efficient in polymer grafting techniques such as enhanced spin capturing polymerization (ESCP) and nitron mediated radical coupling reactions<sup>1</sup>. We have grafted nitron functionality over green silica derived from rice husk ash via co-condensation, and the potential of polymer grafting via ESCP using styrene and 1,3-dipolar cycloaddition using polystyrene macromonomer has been investigated<sup>2</sup>.

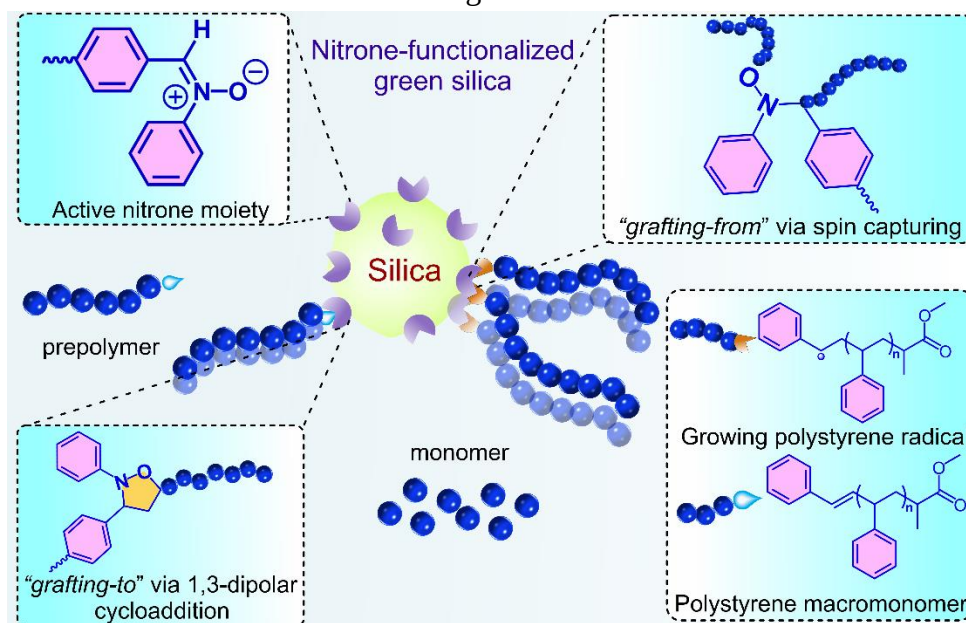


Figure. Surface nitrones on green silica for innovative polymer grafting<sup>2</sup>.

The immobilization of catalytic moieties as heterogeneous support is expected to be one of the most effective ways for the preparation of well-defined heterogeneous catalytic systems providing economic and environmental importance. We are working on porous microparticles prepared by copolymerizing 2-(methyl(pyridine-4-yl)amino)ethyl methacrylate based monomer with divinylbenzene, where the former acts as a catalytic moiety. Initially, the solvent



system has been optimized for the Baylis–Hillman reaction between 4-nitrobenzaldehyde and acrylonitrile using porous as well as nonporous microparticles comprising approximately 70% of the catalytic moiety<sup>3</sup>.

The molecular design flexibility of polybenzoxazine is currently being utilized by our research group to achieve a rational network that is suited for several intended applications. However, the permanent covalent crosslinks responsible for the interesting properties of thermosets hinder its reprocessability generating huge waste. Our research team is addressing this issue as well by incorporating dynamic covalent chemistry, such as imine, disulfide, etc. into the crosslinked network of polybenzoxazines, thereby producing a vitrimer for self-healing adhesives, coatings, and recyclable fibre reinforced composites. The modularity of various phenols and amines enables the design of functionalized monomer units with variable properties, including network flexibility, thermal and mechanical strength, optimal viscosity, dynamic linkages, and reprocessability. Carbonization is yet another feasible route for the reutilization of thermosets<sup>4</sup> which has motivated us to validate the heteroatom-enriched network of polybenzoxazine as a viable candidate for deriving inherently doped carbon structures suitable for energy storage applications.

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## Prof. Kishore Memorial Award Lecture

### Functional Peptide-Polymer Conjugates for Stereoselective Enhancement of Chiroptical properties

Asish Pal

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#### Abstract

Supramolecular assemblies are essential for specific biological functions and mandate precise control over the mesoscopic scale for higher functional efficiency. Reinforcement owing to inner stress formation is of supreme importance in life and is the basis for a lot of biomechanical pathways and muscle actuations. We demonstrate an elegant synthetic design of peptide-polymer conjugate network that exhibits multiple hierarchical control over its stiffening and exhibit non-linear mechanical behavior to match with the actinomyosin network and has features analogous to biopolymers ubiquitous in cells and tissues.

Homogeneously ordered macroscopic assemblies of chiral  $\pi$ -conjugated polymers into adaptive morphologies offer many opportunities in chiral photonics. The nanoscale engineering of such helical materials with controllable geometrical parameters provide access to enhanced chiroptical effect in the desired visible to near infrared range. Peptides offer a greener and easily functionalisable alternative as chiral precursors, with pure enantiomers being available commercially. We report diacetylene-peptide based chiral bolaamphiphiles that undergo topochemical polymerization to furnish chiral polydiacetylenes. Placing chiral polydiacetylene enantiomers in a confined system can give insights on the more superior role of either chiral end groups interaction or hydrogen bonding interactions, resulting in self-sorting of homochiral domains or co-assembly of heterochiral domains in the resulting composite. Tendency to self-sort or co-assemble also depends on the hard-soft segment ratio in the enantiomers. The chiroptical properties of these diacetylene systems can be further enhanced by mesophase formation upon annealing and plasmonic doping.

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## Dr. S.R. Palit Memorial Lecture

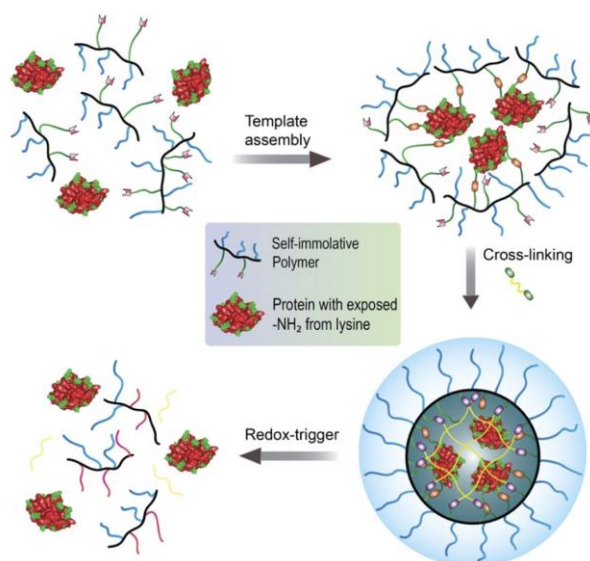
### Reactive Self-Assembly of Polymers and Proteins for Therapeutic Applications

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#### Abstract

Direct use of proteins, to address a specific deficiency, has the promise to mitigate the off-target effects of typical drug molecules. The show-stopper here is that these therapeutic proteins are not accessible for on-target delivery. Most current approaches are restricted to delivery of extracellular proteins (*e.g.* insulin). This leaves behind a rather large number of pathologically important intracellular proteins. We report a novel self-assembly protein shrink-wrapping strategy that addresses key shortcomings of prior approaches. Here, the protein itself acts as the template for the polymer to self-assemble around it. Because the protein is the central component in the self-assembly, protein loading is high. Moreover, the polymer is designed such that the assembly is non-toxic, not prone proteolytic degradation in serum conditions, but releases the protein cargo in the cytosol with complete retention of their structure and function. Complementary approaches taken in this regard will also be discussed.



## Plenary Lecture III

### Biodegradable Macromolecular Architectures for Biomedical Applications

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#### Abstract

Synthetic macromolecular architectures have been emerging as an integral part of biomedical-field for organ specific delivery of therapeutics molecules, in the development of diagnostic probes, and prevention of infectious diseases caused by microbes. Enzymatic-biodegradation of polymers into low molecular subunits under physiological conditions and its instant clearance is an essential structural-parameter required to be in-built to minimize toxicity and unwanted side effects while employing them in the biological system. Among the many available options, biodegradable block copolymers provide narrow molecular weight-control and also possesses unique ability to self-assemble into discrete compartmentalized nano-vectors that can carry substantial amount of cargoes (drug or genes) of specific function so that the target-specificity could be accomplished both in vitro and in vivo. In the last one-decade, our research group has developed large numbers of enzyme-degradable polycaprolactone core-shells, unimolecular micelles, linear and star-block polymers, and self-immolative nanocarriers and so on to address several fundamental problems in cancer research as well as for antimicrobial activity. Block copolymer structures were fine-tuned to programme the biodegradation by lysosomal-enzymes in the endo-lysosomal compartments at the intracellular levels to deliver clinical anticancer drugs against drug detoxification and also to achieve synergistic combination therapy to overcome the multi-drug resistance, etc. Fluorescent chromophores were tagged in the block copolymers to develop bio-FRET probes to get more insight into the cellular-action and real-time living-cell models were established to directly visualize and quantify the drug-action at in vitro by confocal microscope. Deep-tissue penetrable near infra-red biomarkers are employed to probe the action of the macromolecular carriers in cargo delivery to brain tissues. Tumor-models are currently developed to study the accumulation of the drugs and their action by live-animal biodistribution IVIS technology. The presentation will provide an overview on our group's contribution in the area of biodegradable macromolecular systems to address specific problems at the chemistry-biology interface.

## **Plenary Lecture IV**

### **Polycarbonate-based Copolymers as Effective and Attractive Substitutes for Polyolefins**

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CO<sub>2</sub>-based triblock copolymers, made of a central poly(propylene oxide-co-propylene carbonate) (PO-co-PC) block flanked by two polylactide<sup>1</sup> or poly(tosyl propylene urethane) outer blocks<sup>2</sup>, were obtained in one-pot :

- a) by CO<sub>2</sub>/PO copolymerization using a difunctional onium salt initiator in the presence of triethylborane,
- b) and then by ring-opening polymerization (ROP) of lactide or through copolymerization of p-tosyl isocyanate (TSI) with PO.

Upon varying the pressure of CO<sub>2</sub> during its copolymerization with propylene oxide (PO), the T<sub>g</sub> of the central block could be fine-tuned allowing the synthesis of poly(propylene oxide-co-propylene carbonate) with various carbonate versus ether contents.

These ABA triblock copolymers were then mechanically characterized; as their content in ether linkages progressively increased, a transition from brittle-to-ductile-to-elastomeric behavior could be seen.

Copolymers including two poly(tosyl propylene urethane) outer blocks showed higher toughness than commercial polyolefins. As for triblock copolymers flanked by two polylactide blocks, they outperformed the mechanical performances of both high density polyethylene (HDPE) and low density polyethylene (LDPE) by all accounts, their elasticity modulus, tensile strength, toughness and elongation at break being indeed superior to those of the polyolefins tested.

Besides exhibiting superior mechanical properties, these polycarbonate-based triblock copolymers were all degradable unlike polyolefins, which adds to their attractiveness.

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## Plenary Lecture V

### Strain-Induced Crystallization of Natural Rubber by Biaxial Elongation

Ruito Tanaka<sup>1</sup>, Tomohiro Yasui<sup>1</sup>, Yuji Kitamura<sup>2</sup>, Katsuhiko Tsunoda<sup>2</sup>, Hideaki Takagi<sup>3</sup>, Nobutaka Shimizu<sup>3</sup>, Noriyuki Igarashi<sup>3</sup>, Kenji Urayama<sup>4</sup>, Shinichi Sakurai\*<sup>1</sup>

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#### Abstract

Natural rubber (NR) is soft and simultaneously robust to meet requirements for exclusive safety of tires of aircrafts. Namely, they should not be broken when momentary stress is applied. Strain-induced crystallization (SIC) is considered to play an important role for the toughening of NR. To check the significance of SIC behaviours experimentally, we have thoroughly conducted wide-angle X-ray scattering (WAXS) measurements on NR specimens under the biaxially elongated states using some beamlines at Japanese synchrotron radiation facilities such as SPring-8 and Photon Factory of KEK. For this purpose, we have developed the specially-designed apparatus (**Fig. 1**), which enables biaxial elongation of the sheet specimen of vulcanized NR. The studies on SIC of NR by WAXS have an extremely long history since 100 years ago [1], and reliable crystalline lattice parameters have been reported by Nyburg as the orthorhombic lattice with  $a = 1.246$ ,  $b = 0.889$ , and  $c = 0.81$  nm [2]. Then, comparatively recently, have actively reported such studies by using the X-ray scattering technique [3-7]. In this presentation, we will show the diversity of the strain-induced crystallization (SIC) behaviors by conducting biaxial extension of NR in several manners including the planar deformation (equibiaxial and non-equibiaxial, as well as the hysteresis of the crystallization behaviors depending upon the ways of deformation of the specimen).

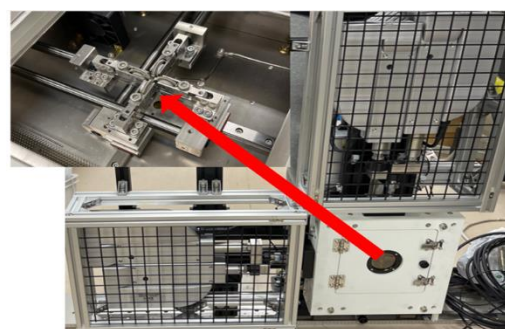


**Figure 1:** Apparatus for the measurement of the X-ray scattering of the NR sheet specimen subjected to the biaxial deformation. The stress measurement is simultaneously possible. Also, temperature-control up to 130°C is possible.

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## Plenary Lecture VI

### Two Structurally Different Polymers from a Monomer

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#### Abstract

The primary structure of a polymer has a huge influence on its properties. Tuning the primary structure of synthetic polymers necessitates the use of unique monomers for each polymer synthesis. But remarkably, nature often uses the same monomer to create structurally different polymers by varying regiochemistry, stereochemistry, etc. For example, cellulose and 1,3- $\beta$ -D-glucan are regioisomeric polymers of D-glucose, starch and cellulose are polymers of D-glucose differing in stereochemistry and *cis*-1,4-polyisoprene (natural rubber) and *trans*-1,4-polyisoprene (*Gutta-percha*) are polymers of isoprene differing in the stereochemistry of the olefin. This remarkable ability of nature to tune the stereochemistry and regiochemistry to create different polymers having different properties from a single monomer is a motivation for researchers to synthesize structurally different polymers from a common monomer. Hybrid monomers possessing functionalities that can react differently to form two types of linkages under different conditions have been explored for synthesizing two structurally different polymers from a monomer.<sup>1,2</sup> Also, the synthesis of different polymers differing in stereochemistry from a common monomer could be achieved by using different catalysts or reaction conditions.<sup>3</sup> To date, there is no report on the chemical synthesis of regioisomeric polymers from a monomer. Topochemical azide-alkyne cycloaddition (TAAC) polymerization has emerged as a reliable method to synthesize various crystalline polymers.<sup>4</sup> By using this chemistry, we have shown that a single monomer can be used to make two structurally different polymers via the marriage of topochemistry and polymorphism.<sup>5</sup> These results will be discussed.

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## **Keynote Lectures**



## Keynote Lecture-1

### Metal-catalyzed Synthesis of Ethylene Oligomers/Polymers and Their Applications

S. H. Chikkali\*<sup>1,2</sup>, R. S. Birajdar, and H. V. Pol

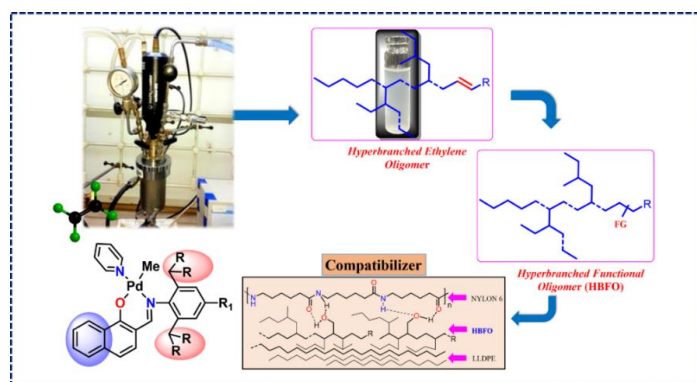
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#### Abstract

Metal catalyzed ethylene polymerization to polyethylene is known for decades.<sup>1</sup> The dimerization, trimerization or oligomerization of ethylene is traditionally practiced to produce higher alkenes. Such higher alkenes find applications in plastics, plasticizers, lubricants and surfactants. However, controlled dimerization, trimerization or oligomerization is not trivial, and is a highly challenging task. My lecture will present synthesis of two naphthoxy imine ligands, L1, and L2 with different steric and electronic features and corresponding Pd/Ni complexes. When exposed to ethylene pressure, Pd-catalyst produced hyperbranched ethylene oligomers, while Ni-complex produced polyethylene. The use of polar solvent, tetrahydrofuran, led to a remarkable 3 fold increase in oligomerization activity without compromising the branching and molecular weight. The resultant hyperbranched ethylene oligomers were selectively monofunctionalized using industrially practiced hydroformylation, ozonolysis, and epoxidation, almost quantitatively. The hydroxy functionalized ethylene oligomer was melt-compounded with LLDPE and Nylon-6 to produce a tough yet flexible blend with a higher strain-to-failure as compared to an un-compatibilized blend.<sup>2</sup>



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## Keynote Lecture-2

### Covalent Adaptive Network in Polymers using Dynamic Chemistry based on Furfuryl functionality

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#### Abstract

In this ‘Polymer Age’ polymers have been the most essential materials in human life. These are not only used in household and commodity materials, but they are also used in hi-tech as well as in strategic materials. In many cases, polymers, especially elastomers are crosslinked to improve their properties. The major disadvantages of these materials are their limited service life and poor recyclability leading to a large amount of wastes every day. Introduction of covalent adaptive network (CAN) into the polymer leads to its easy reprocessing, better recyclability and excellent self-healing characteristics. There are several approaches to incorporate CAN into the polymers, like via cycloaddition reaction based on Diels-Alder chemistry, Alder-ene reaction, metathesis reactions based di-sulfide exchange or boronic ester exchange reaction,  $\beta$ -hydroxy ester exchange reaction etc. Many of these reactions belong to the category of “Click” reactions, the name coined by Barry Sharpless. There are several CANs which are associated with furfuryl derivatives. Furfuryl has been a very useful chemical available in renewable resources like in molasses, barley, sugarcane bagasse etc. Since our initial work in 2007 with tailor-mode acrylates having furfuryl functionality, we have used furfuryl derivatives in different dynamic chemistry using bismaleimide or triazoline-dione (TAD) as a coupling agent. Different reactions like Cycloaddition reaction, electrophilic substitution (ES) reaction, Alder-ene reaction etc. were used in different polymers (like acrylates, polyurethanes etc) as well as in elastomers like, NBR, EVA-GMA, ENR etc. In this case, self-healing as well as reprocessing of these polymers were studied.

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### Keynote Lecture-3

## Speciality Enzymes for a Greener, Safer Bioeconomy: Its Challenges towards Biopolymer Interventions

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### Abstract

With a rapid growing global population and a severe changing climate in 21st century, human being faces serious environmental issues and shortages of food, energy, and other resources. Biotechnology is one of the key technology to solve these challenges. Enzyme technology, exiting in the center of biotechnology, obviously is expected as a promising technology to transform the conventional society to a new bioeconomy society.

Amano Enzyme, Japan, is one of the world-leading industrial enzyme manufacturers and a top in the Asia-Pacific region, having a long history of 124 years from its establishment and of 75 years of enzyme business from its foundation. Amano have set “**coexistence with nature**” as the corporate philosophy, which is derived from one of Japanese cultural concepts. In this context, we are concentrating not only enzyme screening from nature but also advanced biotechnology tools. This makes Amano a “**World No.1 Speciality Enzyme Producer**”, which is our corporate vision.

Development of enzymes to contribute to biobased economy solutions is our challenge. In this presentation, we will be showcasing the biopolymer based enzymatic modifications, which are beneficial to the food, energy, and healthcare industry. Few of the completed, ongoing works will be discussed, with collaboration outcome based and opportunities existing with a greener safer biobased economical motive.

## **Keynote Lecture-4**

### **Polymer-protein complexes and nanoparticles: Engineered polymers for biomedical applications**

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#### **Abstract**

Polymers are now being designed specifically for biomedical applications such as for scaffolds for tissue engineering and delivering drugs [1-3]. The talk will discuss two such applications. For one application, polymers were designed to enhance the stability of proteins and preserve the activity of enzymes in atypical conditions. Biophysical characterization related to the stabilization of horse radish peroxidase and lipase enzymes using methacrylate polymers will be discussed [1]. For the second application, polymers were designed to self-assemble into nanoparticles (NPs). The core-shell structure of these NPs was investigated using X-ray and neutron scattering [2]. The significance of the structure of the core of the NPs, with special reference to NPs with smectic hydrophobic core, will be presented. Adsorption behavior of NPs onto model surfaces was investigated using quartz crystal microbalance with dissipation. It was found that the particles deform and, in some instances disassemble, upon adsorption onto surfaces, depending on the structure of the NPs and the polarity and charge of the substrates [3]. The consequences of the particle deformation on the adsorption behavior, especially on the interaction of nanoparticles with proteins and cells when used in biomedical applications, will be discussed. These results are compared with more recent findings from our work on single chain NPs.

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## Keynote Lecture-5

### Diversified Functionalization of Polypeptide Scaffolds and Smart Materials Thereof

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#### Abstract

Pre/post-polymerization modifications are the powerful strategies for the generation of functional polypeptides with different attractive properties such as stimuli-responsive, amphiphilic, self-assembly, etc. In addition to these properties, the inherent biocompatibility and biodegradability of these functionalized polypeptides make them interesting bio-inspired materials for potential biological applications. The functionalization with hydrophilic segments also overcome the inherent solubility issue of hydrophobicity of polypeptide backbone for their use in biomedical applications including drug/gene delivery. Thus, the functionalization polypeptides with various hydrophilic segments is one of our major research focuses to introduce water solubility, stimuli-responsive properties, amphiphilicity for generation of nano-assemblies and their biological applications. A series of different synthetic strategies involving ring-opening polymerization (ROP), cationic ring-opening polymerization (CROP) and CuAAC/thiol-ene “click” reactions for functionalization of polypeptides will be discussed. Pseudopeptidic bio-inspired water-soluble poly(2-oxazoline)s are grafted to reactive polypeptides for stimuli-responsiveness and self-assembling capability to generate micellar/vesicular nanostructures for applications including encapsulation of dyes/drugs and their control release. Ionically functionalized polypeptides are also synthesized, which exhibit anion-induced thermo-responsiveness and photoresponsive behaviours as well as DNA-binding capability. The attachment of long allyl side-chain also introduces thermoresponsiveness, self-assembly and semicrystallinity to poly(L-glutamate). An attempt is made to integrate phenyl amine end-functionalized PEO at the side-chain of polytyrosine (PTyr) through azo coupling to produce PTyr-N<sub>2</sub>-PEO conjugates with thermo-, photo-responsive and amphiphilic behaviors. An acrylic-based reactive polypeptide scaffold is also designed for easy functionalization to prepare zwitterionic polypeptide, amphiphilic polypeptide and polypeptide-based crosslinked gels with interesting properties.

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## Keynote Lecture-6

### Nano- generators from Macromolecules

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#### Abstract

The employment of materials with piezoelectric/triboelectric characteristics for micro- or nano-scale device fabrication, for power generation, is a potential area of research. Various polymeric systems or their derivatives have been identified as extremely interesting in this regard. However, the energy harvesting efficacy of many of them has been found to be inferior compared to most of the conventional inorganic substances in this domain. This aspect can be addressed, to a great extent, through various modification protocols.

The present work initially covers the investigations to modify the tribo-piezoelectric features of poly(vinylidene fluoride) [PVDF]. The embedding of suitable nanofillers within PVDF matrix is a viable strategy for modulating the  $\beta$  phase of PVDF with piezoelectric characteristics. Accordingly, hybrid nanocomposites have been developed with  $\text{TiO}_2$  and  $\text{SiO}_2$  as nucleating agents, through the first part of this work. The characterization has been done by employing X-ray diffractometry, FTIR, TGA and DSC. The hybrid filler incorporation approach has been found to cause considerable increase in peak voltage compared to the performance of PVDF alone.

The second part of the work presents the development of piezoelectric polymer mats, from ethylene vinyl acetate- millable polyurethane-nanohydroxy apatite (EVA-MPU/n-HA) composite systems, through an electrospinning technique. The evaluation of *in-vitro* biocompatibility features of the EVA-MPU/n-HA systems has been done for their possible utilization in the bio-medical field. The physiological motion of human body- parts has subsequently been used as the input for triggering tribo-piezoelectricity, and for developing LED sensors/ buzzers.

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## Keynote Lecture-7

### Hierarchically Architected Semicrystalline Polymer Aerogels

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#### Abstract

Since their discovery by Kistler, aerogels have developed huge interest among material scientists because of their unique characteristics, such as high porosity, low density, low dielectric constant, low thermal conductivity, large specific surface area, etc. The demand for polymer-based aerogels with superior comprehensive properties has escalated in various fields of application, such as packaging, thermal insulation, acoustic insulation, filtration, adsorption, electromagnetic interference (EMI) shielding, energy harvesting, and environmental remediation. In the first part of my talk, the preparation of hierarchically porous crystalline aerogels of syndiotactic polystyrene (sPS) and blends of poly(L-lactide) (PLLA) and poly(D-lactide) (PDLA) will be discussed along with their multifunctional applications in the fields of microelectronics, thermal management, acoustic insulation, and oil/solvent spill cleanup.<sup>1-3</sup> In the second part of my talk, fabrication of anisotropic polyvinylidene fluoride (PVDF)/MXene hybrid aerogels by unidirectional freezing of thermoreversible gels will be discussed.<sup>4</sup> These aerogels display distinct properties along the freezing and perpendicular to the freezing (transverse) directions. These anisotropic aerogels are flexible and flame-retardant, that possess anisotropic compression performance, heat transfer, electrical conductivity, and electromagnetic interference (EMI) shielding.<sup>4</sup> In the last part of my talk, I will discuss the facile fabrication of unprecedented isotropic and anisotropic nylon-11 aerogels. The energy harvesting performance of nylon-11 aerogels was studied by fabricating piezoelectric nanogenerators, and the anisotropic aerogel delivers a higher peak-to-peak open circuit voltage of ~ 30 V, with over 4-fold improvement as compared to that of isotropic aerogel.<sup>5</sup>

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## **Keynote Lecture-8**

### **Upcycling of post-consumer recycled ABS**

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#### **Abstract**

A sustainable closed-loop circular plastic economy would become a reality if post-consumer recycled (PCR) commodity plastics can be upcycled into higher-performance materials with facile processability.<sup>1,2</sup> Such circularity will be realized when the upcycled plastics can be (re)processed into custom-designed structures through energy/resource-efficient economically congenial and industrially viable approachable and scalable methods.<sup>3</sup> Here, we have introduced a novel method for the first time to upcycle one of the majorly used engineering plastic acrylonitrile butadiene styrene (ABS) into a recyclable, robust adaptive dynamic covalent network (ABS-vitrimer) in melt. In a first of its kind, a designer bio-based crosslinker having pre-installed imine bond as the covalent adaptable network (CAN) was synthesized (here imine containing castor oil, iCO) which is sterically and thermally stable and forms a robust adaptive dynamic covalent network in the melt state to form PCR-ABS Vitrimers. This designer crosslinker, besides offering a transient network helps bridge the fragmented ABS chains that are usually not so far exercised in melt state in ABS system. This study is thereby addressing a long-standing challenge of upcycling PCR ABS in the melt by producing stronger, tougher, solvent-resistant 3D objects obtained from PCR-ABS waste.

## Keynote Lecture-9

### Design and Development of Non-ionic Amphiphilic Architectures for Transdermal Drug Delivery

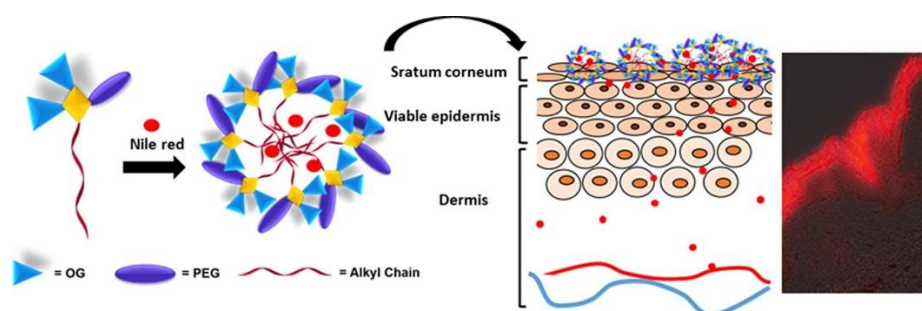
**Sunil K. Sharma**

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The delivery of many bioactive molecules to their target sites can be improved by utilizing different classes of nanocarriers. Amphiphilic nanocarrier systems are known to have enhanced permeability and retention effect and thus can circulate themselves in the blood for longer duration and are reported to be effective for drug delivery. In response to the increasing need for easy-to-prepare and versatile nano-transport systems for biomedical applications, the importance of polymers and dendrimers has been well recognized. A new class of non-ionic amphiphiles have been synthesised following chemo-enzymatic methodology and using glycerol, polyglycerol, polyethylene glycol (PEG), and alkyl/perfluoro-alkyl moieties as the building blocks. The amphiphiles synthesized were observed to aggregate in aqueous medium. Their aggregation behaviour was studied using Dynamic light scattering (DLS), fluorescence spectroscopy, and cryogenic electron microscopy (*cryo*-TEM). The inner hydrophobic core of these aggregates in aqueous medium is capable of encapsulating lipophilic guest. The biomedical application of synthesized amphiphiles was further investigated for trans-dermal drug delivery on excised human skin using Nile red encapsulated in the nanocarrier. The release profile of drug/dye encapsulated amphiphiles was studied under physiochemical conditions in the presence of immobilized lipase Novozym 435.

An overview of this research area will be given during the conference.



**Keywords:** Amphiphiles, nanoaggregate, drug/dye, encapsulation, transdermal delivery

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## **Keynote Lecture-10**

### **Engineered nanomaterials from waste resources and their polymer composite applications**

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#### **Abstract**

Nanoparticles are widely used because of their unique tunable properties and applications in automotive, electronic, textile, energy, aerospace and biomedical fields. The development and applications of nanoparticles derived from natural sources such as plant or animal are gaining more attention due to the high cost and environmental hazards of the petroleum and mineral derived products. This presentation covers the range of nanotechnology applications in polymer composite and biomedical fields. These include the synthesis and characterization of various types of bio-nanomaterials obtained from renewable waste resources such as used eggshell, seashells, used coffee grinds, packaging waste and rice husk etc. The application of nanoparticles includes the drug delivery systems to control the release of drug in the body to protect the drug from enzymatic or chemical degradation, scaffold for bone regeneration, wound healing, biodegradable antimicrobial food packaging, automotive parts, carbon capturing and electronic devices.



## Keynote Lecture-11

### Emulsion-templated Porous Polymers as Scaffolds for Tissue Engineering

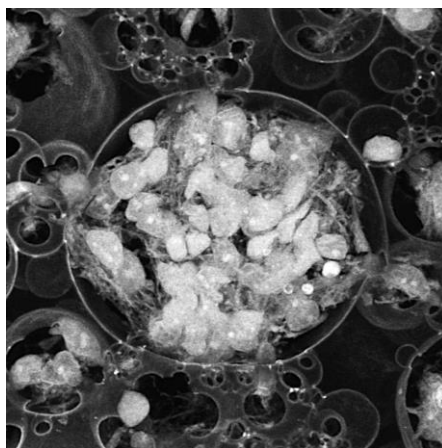
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#### Abstract

In the presentation, I will discuss some of our work on the development of highly porous polymeric materials as scaffolds for 3D cell culture, tissue engineering and regenerative medicine. The materials are produced by a technique known as emulsion templating, which generates porous polymers (polyHIPEs) with a very well-defined and fully interconnected network of pores in the size range 10-100 microns. Features such as the pore diameter, degree of interconnection, porosity, mechanical properties and surface chemistry can be varied to produce materials tailored for different applications. The main focus of the presentation will concern recent work on the development of degradable materials intended for tissue engineering and regenerative medicine applications. These are produced by light-activated thiol-ene network formation, which, due to the speed of cure, can be adapted to 3D printing (stereolithography) platforms. Recent results selected from current projects<sup>1-6</sup> focussing on a range of tissue engineering/regenerative medicine applications, including human neural precursor cells, human pluripotent stem cells, hematopoietic stem cells, osteoblastic cells and endometrial cells, will be presented.



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## Keynote Lecture-12

### Exploring eco-friendly synthetic strategies for Naphthalenediimide based Acceptor Polymers and their device applications

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#### Abstract

Naphthalene diimide bithiophene P(NDI2OD-T2) polymer, also known as N2200, is a commercially available donor-acceptor polymer, which is extensively investigated for its high electron mobility ( $> 0.85 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  in OFET), high power conversion efficiency (PCE)  $\sim 5\%$  in all-polymer solar cells (PSC)s, good solution processability, high crystallinity and light absorption capability near-visible and infrared region. Recently our group has demonstrated the energy storage applications of composites of N2200 with carbon nanotubes (CNTs).<sup>1, 2</sup> The traditional methods for synthesizing these conjugated polymers can be impractical for industrial-scale production due to the need for toxic pre-functionalized monomers and difficulties in purification. Our research group has been engaged in the development of the versatile acceptor polymers based on naphthalene diimide, by conventional and DHAP methods.<sup>3</sup> In my presentation I will discuss the research efforts from our group to develop cost-effective, scalable, and reproducible synthetic routes for P(NDI2OD-T2) polymer. Continuous flow polymerization, direct heteroarylation polymerization and recycling and reusing heterogeneous catalysts are some of the approaches that will be presented.<sup>2-4</sup>

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## Keynote Lecture-13

### Effect of Polymer Charge and Interface Concentration on Structure of Carboxylate Polymers at Oil-Water interface: Isotactic Poly(acrylic acid) PAA and Isotactic Poly(methacrylic acid) PMA

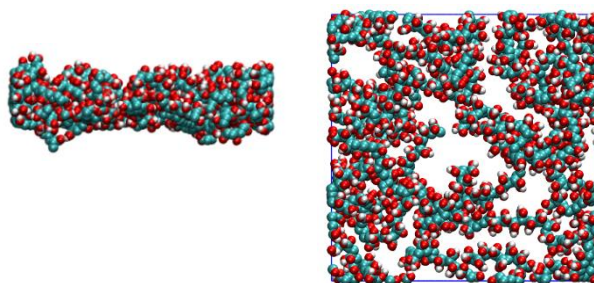
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#### Abstract

An understanding of the factors that govern adsorption of polyelectrolytes and the structure of adsorbed polyelectrolyte layers is important for control of the stability of emulsions and to regulate the properties of macromolecular monolayers. Adsorption behavior of *isotactic* Poly(acrylic acid) (*i*-PAA) and *isotactic* Poly(methacrylic acid) (*i*-PMA) at CCL<sub>4</sub>-H<sub>2</sub>O (oil-water) interface was studied by all-atom molecular dynamics simulations with varying charge density  $f$  and concentration of polyelectrolyte. *i*-PAA and *i*-PMA adopt planar extended conformation at interface in contrast to coiled in bulk water [1]. Adsorption occurs only for low values of degree of ionization ( $f < 0.2$ ) in agreement with experiment [2]. Uncharged *i*-PAA and *i*-PMA, and charged *i*-PMA chains undergo structural change from extended planar conformation to random coiled conformation with increase in interface concentration. The preferential orientation of backbone and side groups disappear with increase in interface concentration. The morphological properties of adsorbed film - film thickness and interface coverage, distribution of orientation of carbonyl, methyl, hydroxyl groups and the solvation behavior of COOH groups [3] of *i*-PAA in water as characterized by hydrogen bonding interactions will be presented. Although such conformational changes are expected from interpretation of pressure-area isotherms, MD simulations add strength along with provision of additional molecular level information. 90% of COOH groups are involved in the formation of a single H-bond between hydrogen of O-H group and water and 50-60% of these groups also form H-bond with oxygen of the C=O groups.



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## Keynote Lecture-14

### Characterization of isosorbide derived biobased polycarbonates and studies about their thermal and rheological properties for understanding of the mechanisms of their functionalities

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#### Abstract

With their high functionalities such as transparency, surface hardness, and others, biobased-polycarbonates (bio-PC) from isosorbides<sup>1-2)</sup> are the key bioplastics to realize engineering applications of biobased materials in automobile industry. However, controlled manipulation of the functionalities of bio-PC in a practical production is still challenging. A sufficient understanding of key behaviors of bio-PC is an important target for the controllable manipulation.

In this research project, the mechanisms of functionalities of bio-PC are studied with an approaching understanding of the macromolecular chain behaviors by rheological analyses and other analytical techniques. A commercialized petroleum-based polycarbonate (petro-PC) is also used for comparison with the bio-PC for more understanding of the mechanisms of functionalities. Figure 1 shows the dynamic mechanical analysis (DMA) result of 2 different bio-PCs having different melt flow index and thermal properties (bio-PC1 and bio-PC2). Figure 1 also shows the DMA result of the commercialized petro-PC. The dynamic modulus around room temperature supported by  $\beta$ -relaxation shows higher values from bio-PC1 and bio-PC2 than that of petro-PC. It indicates the higher physical performance of bio-PCs than that of petro-PC at room temperature, and it is also supported by  $\gamma$ -relaxation results from the low-temperature range. The peak top position (temperature) of  $\alpha$ -relaxation of bio-PCs and petro-PC are different, and this result corresponds to the result of  $\tan\delta$  and from DMA and thermal properties from Differential Scanning Calorimetry (DSC). The differences in other functionalities such as impact strength are also studied under discussion about the effect of rheological behaviors.

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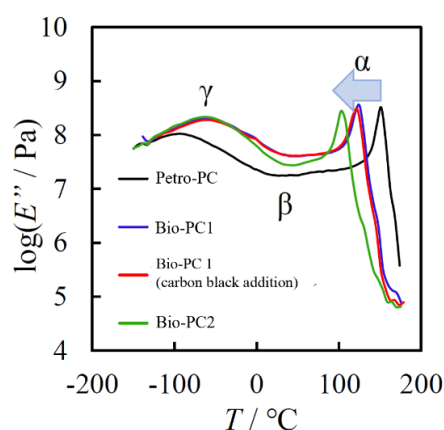


Figure 1. DMA result of bio-PC1, bio-PC2, and petro-PC

## Keynote Lecture-15

### Design of Drug Delivery Vehicles for Healthcare

**Pralay Maiti, Sudipta Senapati, Aparna Shukla, Arpan Biswas, Arun K. Mahanta**

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#### Abstract

Variety of molecules has been developed for long term drug release by controlling hydrophilic-hydrophobic balance for effective healthcare. Different generations of molecules are designed through urethane linkages using small spacer 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. Drug release becomes sustained from the intricate superstructure following the non-Fickian diffusion process resulting massive cancer cell killing as compared to meagre killing rate from the pure drug arising from its burst release. The superstructure is found to be a good biomaterial and its drug loaded conjugate as carrier 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 in subcutaneous, below the tumor site, which completely heal the melanoma. No side effect is observed, as opposed to conventional/control system, due to sustained drug release from the superstructure as evident from histopathological studies of sensitive body organs and biochemical parameters. Thus, new design of vehicle heals the melanoma tumor by enhancing the bioavailability of drug and specific interaction without having any side effects as opposed to conventional chemotherapeutic treatment. New design of vehicle will be discussed in details which heal the melanoma and breast tumors by enhancing the bioavailability of drug and specific interaction without having any side effects. Biomaterials for overall healthcare technology will be discussed including bone healing, stent and suture based on shape memory polymers.

## Keynote Lecture-16

### Tailormade Synthesis and Tunable Properties of Polythiophene graft Block Copolymers

U. Basak,<sup>1</sup> U. Halder,<sup>1</sup> S. Mondal,<sup>1</sup> D.P. Chatterjee<sup>2</sup> and A. K. Nandi\*<sup>1</sup>

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#### Abstract

We have synthesised a water-soluble polythiophene graft block copolymer, polythiophene-graft-poly(caprolactone-block-dimethylaminoethyl methacrylate)(PT-*g*-PCL-*b*-PDMAEMA, P) using combined polymerization techniques e.g. oxidative polymerization, ring-opening polymerization (ROP), atom-transfer radical polymerization (ATRP), and click chemistry.<sup>[1]</sup> The final polymer was characterized by <sup>1</sup>H NMR and FT-IR spectroscopy. Self-assembly behavior of the P1 polymer was investigated by HRTEM and DLS study. The results show variation of nanostructures from micelle to vesicle to multi-vesicular assembly with the variation of pH from 3 to 7 to 10. The dc-conductivity values at pH 3, 7, 10 are  $0.40 \pm 0.09$ ,  $0.11 \pm 0.04$ , and  $0.12 \pm 0.04$   $\mu\text{S/cm}$ , respectively and the highest value at pH 3 is for the uncoiled polythiophene chain arising from the ionic repulsion of protonated -N(CH<sub>3</sub>)<sub>2</sub> group of grafted PDMAEMA block. The I-V characteristic data shows semiconducting nature with signature of organic mixed electronic and ionic conductivity (OMEIC) at pH3. To simplify the difficulty of multistep process we recently reported an one pot synthesis of polythiophene(PT)-graft block copolymers with thermo-sensitive poly(diethyleneglycol methyl ether methacrylate)(PDEGMEM) and PDMAEMA using ATRP technique.<sup>[2]</sup> The polymers PT-*g*-PDEGMEM<sub>10</sub>-*b*-PDMAEMA<sub>3</sub>(P1), PT-*g*-PDMAEMA<sub>10</sub>-*b*-PDEGMEM<sub>3</sub>(P2) and PT-*g*-PDMAEMA<sub>6</sub>-*ran*-PDEGMEM<sub>8</sub>(P3) are characterized by <sup>1</sup>H-NMR and SEC techniques. P1 and P3 exhibit micellar morphology but P2 shows vesicular morphology, pH, temperature and sequence dependent absorbance peak, and dc-conductivity (P2>P3>P1) indicates semiconducting nature. I-V property shows pH dependent memory and OMEIC property. At pH3, on photoirradiation the photocurrent gain of P2, P3 and P1 are 7.9, 6.6 and 3.5, respectively. Thus PT-graft block copolymers exhibit tunable properties depending on *proximity and preponderance* of block sequence from PT backbone.

#### References

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## Keynote Lecture-17

### 3D printed scaffolds from plasticized Polyhydroxybutyrate (PHB)/Polylactic acid (PLA) blends reinforced with strontium doped hydroxyapatite (Sr-nHAp)

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## Abstract

The current research focusses on biocompatible polymeric blends from PLA/PHB reinforced with a bioactive filler employing a low cost and stable FDM technology to successfully prepare bone repair scaffolds. Strontium doped natural hydroxyapatite (Sr-nHAp), which was derived from caprine bones were preferred, as HAp has similar properties of human bone (Ca/P=1.67) and increases the bioactivity of the polymer matrix, thereby mitigating the negative aspect of the PLA and PHB. The composite filaments with a diameter of 1.75mm were developed by using twin screw extrusion at varioable loading of HaP and were subsequently 3D printed using FDM. To assess the Sr-nHAp and the biocomposite scaffold for use in bone tissue engineering, various in-depth characterizations such as scanning electron microscopy, x-ray diffraction, fourier transform infrared spectroscopy and particle size analysis were undertaken. The loaded Sr-nHAp-PLA/PHB 3D printed specimens exhibited improved compressive strength as compared with pure PLA scaffolds. The antimicrobial activity of the powder samples were done wherein 3%Sr-HAp showed significant antibacterial property, and thus this composition was optimized for further studies.

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## **Keynote Lecture-18**

### **Elucidating the Structural Insights of Rieske Oxygenases in Plasticizer Degradation**

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#### **Abstract**

Plastic/plasticizer pollution has emerged as a pressing global environmental challenge, driven by the widespread use of plastics. This issue is exacerbated by the release of toxic substances known as plasticizers into the environment, posing potential health risks. To address this concern, we identified *Comamonas testosteroni* KF1 as a highly efficient bacterium in plasticizer degradation. Subsequently, we characterized all the enzymes involved in the degradation pathways of plasticizers and polyethylene terephthalate (PET) within this microorganism.

Notably, we successfully determined the long-anticipated molecular structures of key plasticizer-degrading enzymes, specifically phthalate dioxygenase, terephthalate dioxygenase, and isophthalate dioxygenase, employing X-ray crystallography. These crystal structures revealed that these enzymes exhibit distinctive structural features characteristic of Rieske Oxygenases (ROs). Intriguingly, their catalytic domains displayed unique structural attributes when compared to related ROs, indicative of their specialized evolution to catalyze specific reactions.

Furthermore, our structural analyses unveiled that the binding of substrates to these enzymes is contingent upon the precise spatial arrangement of arginine residues within the active site. Through biochemical assays and mutational analysis, we confirmed that arginine residues play a pivotal role in mediating substrate specificity and regiospecificity of these enzymes. These findings provide a solid foundation for the future engineering of these enzymes, with potential applications in the biodegradation of PET and plasticizers.

## Keynote Lecture-19

### Design of self-folding shape-memory elastomer composites based on polyphosphoesters

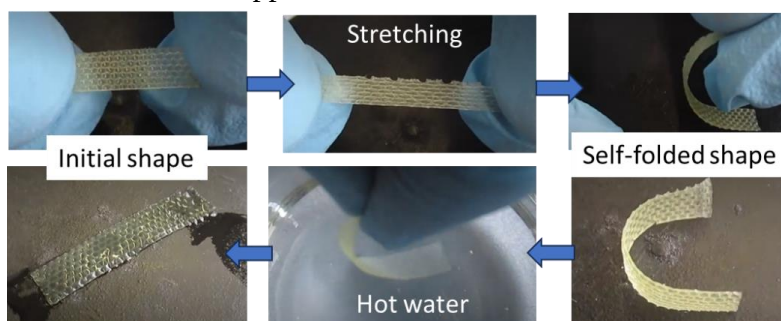
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#### Abstract

Today, the strong demand for advanced devices able to hold specific functions implies the continuous development of innovative materials. Imparting groundbreaking properties to existing materials, such as the ability to degrade after use, is one example of improvement which paves the way to unlock specific and advanced applications, especially in the biomedical field. In addition, the development of innovative strategies for fine-tuning the design of polymer composites makes it possible to synergistically combine advanced materials into functional devices. In this frame, we developed functional sheets presenting simultaneously degradability, mechanical self-folding, elastomer behavior and shape-memory properties. This was successfully achieved by developing sheets of shape-memory elastomer composites based on fully degradable materials and specifically designed to afford composition asymmetry of the sheet sides providing self-folding ability. Following a new concept to design a composite sheet able to self-fold in various shapes depending on the orientation of the uniaxial stretching,[1] a honeycomb-structured poly( $\epsilon$ -caprolactone) electrospun nanofiber mat was embedded in a photo-crosslinked polyphosphoester elastomer matrix. Remarkably, these self-folding sheets were obtained by a one-step process being an upfront alternative to conventional multi-layered laminates reported in the literature. They are also characterized by a different roughness on each side. The initial shape of these mecanomorph self-folding sheets can be retrieved thanks to the shape memory properties of the designed material. Based on preliminary *in vitro* biocompatibility tests, biomedical applications can be foreseen.



#### Reference

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## Keynote Lecture-20

### Nanostructured Polysaccharides Materials for Water Purification

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#### Abstract

The design and synthesis of nano-architected cellulose and chitin can act as efficient materials for water purification. The talk aims to study and compare the performance of a polyvinylidene fluoride (PVDF) electrospun membrane, unmodified cellulose nanofiber (CNF) based PVDF membrane, and Meldrum's acid (2,2-dimethyl-1,3-dioxane-4,6-dione) modified CNF-based PVDF membranes against the Fe<sub>2</sub>O<sub>3</sub> nanoparticle filtration and crystal violet (CV) dye adsorption. Herein, we introduced a facile method to produce a unique green adsorbent material from cellulose nanofibers (CNFs) via a nonsolvent assisted procedure using Meldrum's acid as an esterification agent to enhance the adsorption toward positively charged crystal violet dyes. Most of the surface modifications of cellulose nanofibers have been done using toxic organic solvents like pyridine, dimethyl acetate, (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO), etc. So far, this is the first report on the surface modification of cellulose nanofibers via a nonsolvent assisted procedure. Both CNF-based PVDF membranes were prepared by successive coating of modified and unmodified CNFs on to the surface of a PVDF electrospun membrane. All the demonstrated membranes showed high filtration capacity against the Fe<sub>2</sub>O<sub>3</sub> nanoparticles. With the 10 mg/L of crystal violet (CV) aqueous solution, CV adsorption of PVDF electrospun membrane, and unmodified CNF-based PVDF membrane was around 1.368 and 2.948 mg/g of the membrane respectively, whereas it was 3.984 mg/g of the membrane by Meldrum's acid CNF-based PVDF membrane. The demonstrated Meldrum's acid modified CNF-based PVDF membrane was proven to be the efficient media that can concurrently eliminate the Fe<sub>2</sub>O<sub>3</sub> nanoparticles and CV dyes from the water. The investigation into the surface chemistries of cellulose nanofibers beyond the adoption of toxic solvents can enhance the economic usefulness of the process and also yield a new eco-friendly adsorbent material that is agreeable to adsorbing various toxic pollutants.

## Keynote Lecture-21

### **Continuous Flow Process: A New Paradigm in Process Intensification for the Production of Functional Polymers for Optoelectronic Devices**

**Anil Kumar**

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### **Abstract**

Continuous flow process provides a potential alternative to batch synthesis 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 telescoping 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 an “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 and polymers with precise control over critical molecular design parameters. It also enables one to carry out material synthesis at higher temperatures that were outside the domain of an organic synthetic lab. We have been exploring continuous flow processes for the synthesis of conjugated polymers, nanoparticles and nanofibers, fine chemicals, miniemulsion polymerization etc. In this presentation, I will review some of the recent advances in these directions and some results from our laboratory.

## Keynote Lecture-22

### Surface-anchored *clickable* coatings

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#### Abstract

Reactive coatings are those that permit installation of desired segments in a post-coating step; several approaches have been developed to design polymers that can covalently anchor to the substrate while at the same time provide a handle for further functionalization. Here, we present a simple approach to prepare surface-anchored coatings that can be functionalized with desired segments in a post-coating step; to achieve this, we prepared a hetero-diester of itaconic acid (IA), namely 2-hydroxyethyl, propargyl itaconate (HEPI), which upon free-radical initiated polymerization yielded a polymer, PHEPI. This polymer is endowed with three important features: i) the pendant hydroxyl groups can react with Si-OH groups on suitably treated glass/silicon surfaces; ii) the pendant propargyl groups can help install chosen segments onto the coating, via azide-alkyne reaction, to render the desired properties to the surface, and iii) thermally induced crosslinking of the coating that occurs at  $\sim 140^{\circ}\text{C}$ , which helps create robust surface-anchored coatings of desired thickness. Derivatization of PHEPI coatings was easily done by treatment with a variety of organic azides, such as PEG-azide, cetyl azide, fluoroalkyl azide, etc., to yield surfaces with distinct characteristics; the derivatized surfaces were characterized by contact angle measurements, IR and XPS. Further, we demonstrate that this polymer can also be spray-coated onto paper, and thus it serves as a reactive primer for covalently modifying their surface properties at a late stage, in a process termed *spray-click-bake*. In addition, we also show that the propargyl groups in Si-coated PHEPI can be clicked using photoinitiated thiol-yne reaction, which in turn permitted the photo-patterning of coated substrates. In summary, this simple approach, starting from readily available and bio-sourced itaconic acid, provides ample scope for further elaboration to generate designer surfaces that could form the basis for a range of potential applications.



## Keynote Lecture-23

### Controlling Molecular Self-assembly for Task-specific Porous Organic Polymers

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#### Abstract

The intriguing self-assembled architectures in nature fascinate researchers to tune the morphology of the synthetic materials.<sup>1</sup> Morphology and textural features of materials are essential parameters to influence their physicochemical properties, such as porosity, adsorption, diffusion kinetics, and optoelectronic properties.<sup>2</sup> Morphological tunability of any supramolecular/ macromolecular architectures demand detailed elucidation of the molecular self-assembly processes. In the present talk, I will discuss the self-assembly processes leading to the morphological evolution of hypercrosslinked porous organic polymers from nanospheres to nanosheets obtained through the solvent knitting process and the impact of morphology on polar molecule separation from water.<sup>3</sup> In addition, I shall explain the molecular-level picture of an intriguing phenomenon of the dynamic covalent chemistry-directed room-temperature transformation of discrete organic imine cage-to-covalent organic framework (COF) film at the liquid-liquid interface. The unfolding of the cage leading to the generation of imine intermediates, followed by their interface-assisted preorganization and subsequent growth of the COF film, are elucidated through detailed spectroscopic and microscopic investigations.<sup>4</sup> The interfacial cage-to-COF transformation provides a facile route for the faster fabrication of free-standing COF films with high porosity and crystallinity, demonstrating excellent performance towards molecular sieving and high solvent permeance.

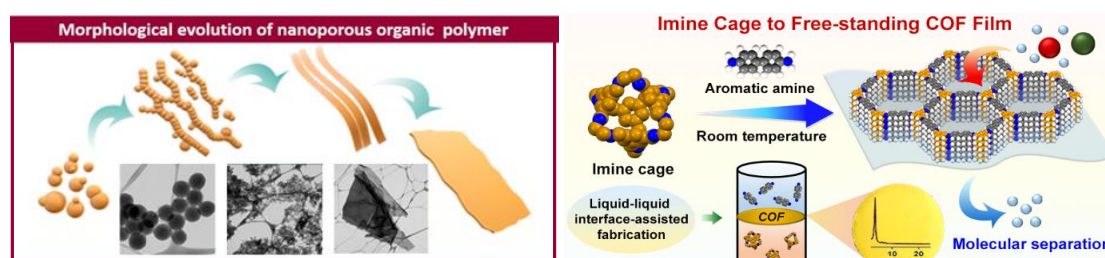


**Figure 1:** Schematic illustration of deciphering the self-assembled nanoporous structures leading to hypercrosslinked polymers and crystalline nanoporous film at the liquid-liquid interface.

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## **Keynote Lecture-24**

### **Polysaccharide-based copolymers and their biomedical applications**

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#### **Abstract**

Recently in authors' laboratory, various polysaccharide-based hydrogels have been developed that found potential application as superabsorbent material<sup>1</sup>, as cargo carrier<sup>2-4</sup>, and also as rapid hemostatic agent. Moreover, different copolymeric micelles have also been synthesized and found to be suitable towards the delivery of hydrophobic drug *in-vitro*<sup>5-6</sup>. The synthesized hydrogel as well as the micellar systems have demonstrated enhanced biocompatibility, UV resistance as well as thermoresponsive shape memory behaviors.

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## Keynote Lecture-25

### Heterogeneous Catalysis in Prebiotic Chemistry and the Transition from Geochemistry to Biochemistry

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A long-standing question in the Origins of Life field is which biopolymer emerged first--RNA, enzymes (proteins) or lipid membranes because in extant biology each requires the other? Enzymes catalyze biopolymerization of DNA, RNA, proteins, and all other biomolecules but are themselves polymers of amino acids and require DNA and RNA, and membranes are needed for many function, including importantly, ATP synthesis, to drive all bioreactions. Previous work has thus focused on non-enzymatic synthesis of either one biopolymer or other. However, we note that a fundamental property of all living systems is that they are mutually-codependent in their ecology. Therefore, rather than a sequential development of biopolymers, we **postulate** that prior to the emergence of cellular ecosystems, a “protobiogeochemical ecology” (prebiotic broth) existed, that was predicated on the principles of molecular **Mutualism, Selection and Catalysis by minerals and dissolved ions** in the **Origins of Life (MuSeCoL)**. We take a Systems Level approach to demonstrate mutual, nonenzymatic **coevolution** of RNA, peptides and unique amphiphiles with **simultaneous isomer selection** (e.g.,  $\alpha$ -amino acid over  $\beta$ -,  $\gamma$ -,  $\delta$ -amino acids configurational isomer selection) as catalyzed by minerals and dissolved metals in a **complex, multicomponent prebiotic broth**.

## Keynote Lecture-26

### Structural Change and its Mechanism of OBDD Triggered by Temperature Change

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#### Abstract

Block copolymers exhibit a variety of morphologies as a function of a volume fraction, temperature, a molecular architecture, and so on. One- or two-dimensional structures, i.e., lamellae or cylinders show a continuous change in a structural period. For example, the period continuously increases with the decrease of the interfacial area between the constituent blocks by the temperature drop for a UCST system. This is easily realized by the stretch of the block chains and the squeeze of the lateral molecular distance. However, this procedure is not possible for spheres, a three-dimensional structure, because the interface is not continuous. When the molecules forming the spheres stretch with the same lateral distance, it causes the formation of voids between them. In order to prevent it, it is necessary to increase the number of the constituent molecules per domain by the evaporation and condensation mechanism, which requires a lot of time to reach the equilibrium. In this paper, we investigated the temperature change of the period in a OBDD structure. This structure consists of three-dimensionally continuous interfaces throughout the system. The continuous change as one- or two-dimensional structures show, or the evaporation and condensation mechanism in spheres is obviously impossible.

We employed two systems; a blend of a polystyrene-*b*-polyisoprene diblock copolymer (SI1,  $M_n = 4.5 \times 10^4$ ,  $M_w/M_n = 1.06$ , PS:PI = 70.2:29.8 vol.%), polyisoprene homopolymer ( $M_n = 5.5 \times 10^3$ ,  $M_w/M_n = 1.05$ ) and dioctyl phthalate (DOP), and a polystyrene-*b*-polyisoprene diblock copolymer (SI2,  $M_n = 15.1 \times 10^4$ ,  $M_w/M_n = 1.03$ , PS:PI = 62:38 vol.%).

The OBDD structure formed in the blend showed a drastic change in the period and the SAXS intensity on the temperature drop (Fig. 1). This result implies the discontinuous change, which is further studied by TEM using the SI2 specimen.

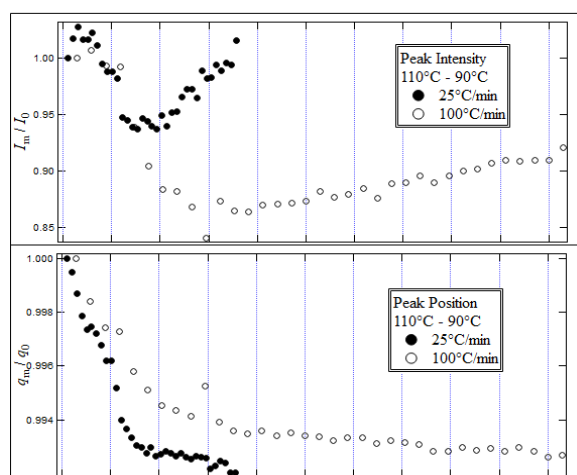


**Fig.1** Change in the intensity and the peak position of the 1<sup>st</sup> peak from the gyroid phase.

## Keynote Lecture-27

**Random copolymers of *N*-alkyl-*N*-(3-(isopropylamino)-3-oxopropyl)acrylamide [alkyl = *n*-propyl and isopropyl] and poly(ethylene glycol) methyl ether acrylate as efficient nano-carrier for drug delivery**

Sourov Mondal,<sup>1</sup> Archana Kumari,<sup>1</sup> Kheyanath Mitra,<sup>1</sup> Payal Gupta,<sup>1</sup> Ranjeet Singh,<sup>2</sup> Bikram Roy Laskar,<sup>2</sup> Partha Pratim Manna,<sup>2</sup> Biswajit Ray<sup>\*1</sup>

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**Abstract**

Here we report the synthesis of two new *N*-alkyl-*N*-(3-(isopropylamino)-3-oxopropyl)acrylamide [alkyl = *n*-propyl and isopropyl] monomers and their control polymerization via RAFT polymerization using two RAFT agents 1-phenylethyl phenyl dithioacetate and 2-(Dodecylthiocarbonothioylthio)-2-methylpropionic acid as RAFT agents. Their random copolymerization with poly(ethylene glycol) methyl ether acrylate (PEGA: CH<sub>2</sub>=CHCO<sub>2</sub>(CH<sub>2</sub>CH<sub>2</sub>O)<sub>*n*</sub>Me, Mn = 480, *n* = 9 on average) macromonomer at different composition have also been carried out. Thermoresponsiveness, self-assembly property in aqueous medium and thermal properties of these polymers have been studied. Lower critical solution temperature of these copolymers increases with increase in PEGA content. Glass transition temperature of these copolymers decreases with increase in PEGA content. Apparent hydrodynamic diameter increases with increase in PEGA content to about 20% PEGA content. To explore the possibility to use of their copolymers, having LCST value close to the body temperature, as nano-carriers for anticancer Doxorubicin drug delivery, *in vitro* drug loading and release study and antitumor studies against Dalton's lymphoma (DL) tumor cells have also been performed. Drug loaded polymer reduced the cell viability, induce cytotoxicity and inhibit long term growth of the cells in concentration dependent manner. *In vivo* study also revealed that the drug loaded copolymer considerably protects the animals bearing such cells via the enhancement of life span, reduction of tumor volume and prevention of metastasis. Thus, these copolymers have been shown as efficient drug delivery nano-carrier.

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## **Invited Lectures**



## **Invited Lecture-1**

### **Multi-stimuli Responsive Molecular Materials: Design, Synthesis and Applications**

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#### **Abstract**

Natural responsiveness of living beings have inspired researchers to develop stimuli-responsive (bio)polymers for construction emerging materials for application in healthcare, sustainability, and energy applications. Such polymers exhibit physical/chemical/conformational transformations upon changes in external pH, temperature, electric/magnetic field, etc. Compared to single/dual-stimuli responsive polymers, multi-stimuli responsive polymers offers more versatility, functionality and control and thus are more preferred for the construction of sensors and actuators for engineering and biomedical applications. However, precision synthesis of such materials is essential for their subsequent application. This is hindered by (a) challenging and multi-step synthesis protocols requiring stringent reaction conditions and (b) the difficulty in tuning various material parameters.

We have developed a facile green and cost-effective synthesis protocol to prepare well-defined multi-stimuli responsive polymers and (bio)polymers for the construction of materials with tunable wettability, self-healing materials, antifouling materials and nanocarrier for anti-cancer drug delivery.

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## Invited Lecture-2

### Control over Nano- and Secondary Structures in Peptide Self-Assembly

G. Ghosh,<sup>\*1,2</sup> R. Barman, A. Mukherjee, U. Ghosh, S. Ghosh, G. Fernández

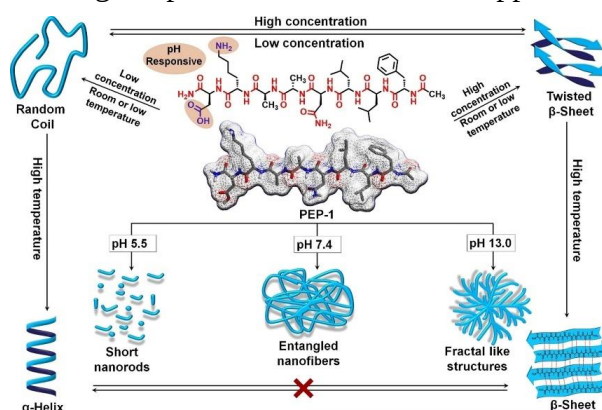
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#### Abstract

Control over nano- and secondary structures of self-assembled peptides has gained great attention because of their numerous biological applications. In this study, we demonstrated the extensive morphological and conformational versatility exhibited by a biologically active peptide, PEP-1. PEP-1 can be self-assembled into six distinct nanostructures and four different secondary structures through the subtle interplay between noncovalent interactions in which pH, concentration, and temperature play a crucial role. PEP-1 exhibited pH-responsive behavior because of the presence of basic and acidic amino acids. PEP-1 formed nanofibers and twisted  $\beta$ -sheet as secondary structures at pH 7.4, whereas fractal-like structures with almost unaltered conformational structures were observed at pH 13.0. Interestingly, secondary structures were completely demolished and very nanorod-like structures were found at pH 5.5. The twisted  $\beta$ -sheet with nanofibers exhibited by PEP-1 at pH 7.4 (high concentration and at RT) was the kinetically stable state which could be transformed into another kinetically stable state (random coil formation with irregular nanoparticles) at RT upon dilution. Both the kinetically controlled states (at high and low conc.) at RT further transformed into thermodynamically stable states upon thermal annealing. At high temperatures, PEP-1 revealed well-organized strong  $\beta$ -sheet secondary structures with 2D sheet-like nanostructures and  $\alpha$ -helical conformations with short nanofibers at high and low concentrations respectively. It is worth mentioning that PEP-1 also exhibited significant biocompatibility and notable antibacterial properties. These findings suggested that our system has great potential for biomedical applications.



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### Invited Lecture-3

## Piezo-mediated Polymerization for Fiber Reinforced Polymer Composites with Adaptive Mechanical Properties

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### Abstract

Common engineering materials fail under repeated mechanical loading. Materials that adapt to external mechanical loading environments by changing their structure and mechanical properties can prevent material failure. One such example is bone, which remodels itself to adapt and strengthen according to the experienced local mechanical stimuli. Inspired by this, our efforts are directed towards developing synthetic analogous material using mechanical responsive piezoelectric particles. The fiber-reinforced polymer composites are prepared by in-situ piezoelectric particle-assisted polymerization. Piezoelectric particles act as an initiator when activated using mechanical vibrations and help to improve the polymer composite's strength [1]. In the presence of mechanical stimuli, piezoelectric particles can drive the rearrangement of polymer networks in polymer composites. This rearrangement leads to the tuning of local mechanical properties that result in the mechanical adaptation in polymer composites according to the experienced mechanical stimuli. A robust fiber-reinforced polymer composite system like this can offer an added potential for real-world applications. Here, the selection of chemistry plays a vital role in achieving the adaptive properties, and further studies are focused on making the chemistry reversible for repurposing or recycling the polymer composites [2].

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## Invited Lecture-4

### Electrospun Polymer Nanofibers for Controlled & Sustained Drug Release

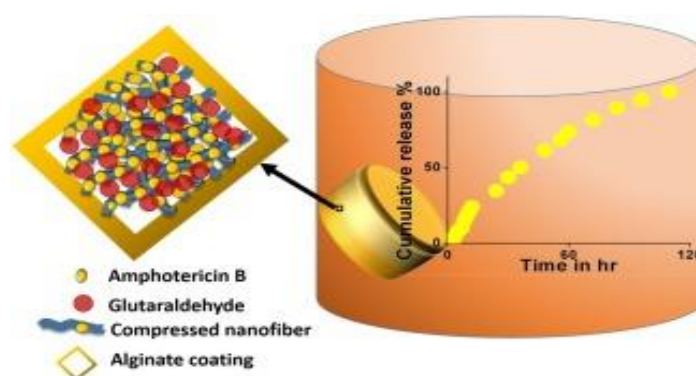
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#### Abstract

Electrospinning is a technique to fabricate nanofibers by applying high voltage to a polymer solution. We work with different polymers (PES, PAN, PMMA, Cellulose etc.) and Block co-polymers (PS-b-PMMA) to obtain the electrospun nanofibers. These electrospun nanofibers are then functionalized to provide the additional features such as porosity, core and shell morphology, hollow fibers, alignment, pyrolysis to yield carbon nanofibers etc. for specific applications. Some of these applications being pursued in our group include using them as electrode material for energy storage devices, biosensors, environmental pollution control and health related issues. One such application was the use of the nanofibers to develop an oral drug delivery vehicle for Amphotericin-B. In the work, we engineered the electrospun gelatin nanofibers to enable their use for controlled release of AmB in the form of oral tablets while focusing on loading realistic drug doses of AmB as per the clinical guidelines for the treatment of Visceral Leishmaniasis <sup>2</sup>.



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## Invited Lecture-5

### Cationic Copolymerization of Vinyl Ethers with 2,3-Dihydrofuran

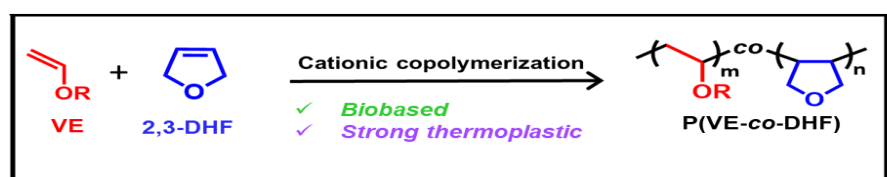
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<sup>1</sup>Polymer Research Centre and Centre for Advanced Functional Materials, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur - 741246, Nadia, West Bengal, India.

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#### Abstract

The thermomechanical and optical properties are significantly influenced by stereochemistry of the polymers. Thus, controlling the tacticity is a key consideration in polymer synthesis. Isotactic poly(vinyl ether)s (PVEs) have recently been identified as a new class of semicrystalline thermoplastics with valuable mechanical properties.<sup>1</sup> Thermoplastics represent a 5 million metric ton per year market of such petroleum-based materials. However, to reduce the carbon footprint these highly used commercial polymers should be derived from sustainable resources. The synthesis of new materials from petroleum feedstock is quite challenging as it requires the development of new renewably sourced polymers that match the physical performance as well.<sup>2</sup> Recently, the use of 2,3-dihydrofuran (2,3-DHF)<sup>3</sup> has gained adequate attention as this cyclic vinyl ether can be prepared by one-step cyclization of biorenewable alcohols such as 1,4-butanediol.<sup>4</sup> Notably, PVEs can only be prepared through cationic polymerization.<sup>5</sup> In the synthetic area of macromolecular science, copolymerisation is an advantageous method for synthesizing materials with desired functions that cannot be achieved in homopolymers. Herein, we envisioned that cationic copolymerisation of other VEs with 2,3-DHF can address the aforementioned aims purposefully. We perform the copolymerisation of 2,3-DHF with various alkyl VEs such as ethyl, propyl, isobutyl VEs. However, the copolymerization of different types of monomers is inherently challenging due to difference in reactivity ratio of comonomers; hence copolymerisation kinetics is also investigated. We anticipate that this type of materials will show satisfactory performance like the engineering thermoplastics such as commercial acrylonitrile butadiene styrene (ABS) terpolymer, polycarbonate (PC), etc.



**Scheme 1.** Schematic representation of synthesis of P(VE-co-DHF) by cationic polymerization.

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## Invited Lecture-6

### Di-Fmoc based minimalistic dipeptide building blocks as functional hydrogelators

**Priyadarshi Chakraborty**

Department of Chemistry

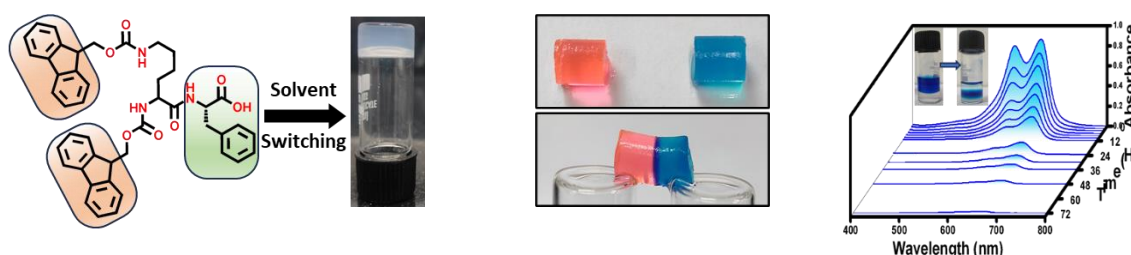
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#### Abstract

Short peptides are excellent hydrogelators due to their high aggregation propensity resulting from the unidirectional H-bonding and  $\pi$ -stacking. Explicitly, peptides modified with the 9-fluorenylmethoxycarbonyl (Fmoc) group have shown remarkable self-assembly/hydrogelation ability due to the intrinsic hydrophobicity,  $\pi$ -stacking ability, and aromaticity of the Fmoc group. Intriguingly, peptides modified with two Fmoc moieties have recently emerged as better building blocks for hydrogelation than their mono Fmoc counterparts.<sup>1,2</sup> Here, we present a de novo building block, Fmoc-Lys(Fmoc)-Phe (Lys = lysine, Phe = phenylalanine) with an additional Fmoc group protecting the Lys side chain, and a Phe residue at the C-terminus. We anticipated that the building block containing two Fmoc groups and the aromatic Phe residue would bestow higher hydrophobicity and  $\pi$ -stacking interactions. The Fmoc-Lys(Fmoc)-Phe building block produced hydrogels at a very low concentration, accompanied by self-sustaining and self-healing behavior. The network structure of the peptide hydrogel was modified by integrating edge-functionalized graphene oxide nanosheets, bestowing conductive properties. The hydrogels showed remarkable dye absorption capacities, indicating their potential use as supramolecular materials.



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### Invited Lecture-7

## Effect of dispersion on the gas barrier property of hybrid 3D nanofillers incorporated segmented polyurethane nanocomposites

Subhash Mandal<sup>1,2</sup>, Debmalya Roy<sup>\*2</sup>, Kingsuk Mukhopadhyay<sup>2</sup>, Mayank Dwivedi<sup>3</sup> and Mangala Joshi<sup>\*1</sup>

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### Abstract

The hybrid 3D carbonaceous nanofillers i.e. functionalized carbon nanotube (f-MWCNT) immobilized into edge functionalized few layer graphene (f-FLG) were incorporated into segmented thermoplastic polyurethane (STPU) by twin screw extrusion (TSE) technique. The nanofillers was loaded in different weight percentages (0.25, 0.5, 1.0, 2.0 and 5 wt%). The supramolecular self-assembly route (SSAR) was espoused to enhance the level of dispersion of nanofillers at higher percentages into STPU followed by TSE. The phase morphology of prepared nanocomposites was studied and analysed by scanning electron microscope (SEM). The phase morphology unveiled uniform dispersion at higher nanofillers loading of 2 wt% through SSAR followed by TSE. The permeability of the film prepared using 2 wt% hybrid 3D nanofillers strengthened STPU nanocomposite exhibited significant improvement of gas barrier property with reduction of He (helium) gas permeability from 1287 (for neat polyurethane film) to 472 cm<sup>3</sup>/m<sup>2</sup>/day. The developed nanocomposites were also evaluated by X-ray Diffraction (XRD), Attenuated Total Reflection Fourier Transform IR (ATR-FTIR) spectra and Thermogravimetric Analysis (TGA).

**Key words:** Polyurethane; 3D nanofillers; extrusion; supramolecular self-assembly route; gas barrier property, permeability.



## **Invited Lecture-8**

### **Designing Functional Polymers for the Biomedical Applications**

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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 treatment and diagnosis in a single system. A new class of metal-ligand-based nanocarrier in a polymer backbone has been designed as a theranostic system. An NMR experiment is performed at room temperature to prove the MRI capabilities of copolymer nano-aggregates. Cell viability studies suggest the biocompatibility nature of the copolymer. Flow cytometry and epi-fluorescence microscope experiments demonstrate the dual-imaging ability of the newly designed copolymer. The much higher relaxivity ratio ( $r_2/r_1$ ) of the present method establishes the superiority of our system as one of the best contrast agents known to magnetic resonance imaging practitioners.

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## Invited Lecture-9

### Low entangled UHMW-polymers

**D. Romano<sup>\*1</sup>, S. Raman<sup>1</sup>, J. Zhao<sup>1</sup>, N. Sharahili<sup>1</sup>, A. Alsubhi<sup>1</sup>, M. Puthiyaveetil<sup>1</sup>, R. Gote<sup>1</sup>, F. Li<sup>1</sup>, J. Mayet<sup>1</sup>, J. van der Eem<sup>1</sup> and S. Rastogi<sup>1</sup>**

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#### Abstract

High Performance polymers are a subject of considerable interest due to their enhanced properties (mechanical, optical, electrical, thermal, etc...) especially when used in lightweight composites. Higher mechanical properties (especially impact strength, tensile strength and modulus) are often achieved by increasing the molecular weight of the polymer produced. In this perspective, considerable attention is posed in achieving high or ultra-high molecular weights (UHMW). However, the major drawback of UHMW is a significant increase of the melt viscosity caused by the high number of entanglements formed, leading to major challenges in the melt processing. Recently, a major development in the processing of the UHMW-polyethylene is achieved by direct synthesis of the polymer having a reduced amount of entanglements. By tailoring the reaction conditions during the polymer synthesis and making a meticulous choice of the catalytic system, it is possible to synthesize low-entangled-UHMWPE. The resulting polymer can be uniaxial as well as biaxial solid-state processed without using any solvent. The resulting solid-state processed tapes have unprecedented breaking tenacity (>4.0 GPa) and tensile modulus (>200 GPa) [1]. The fundamental concept of producing low-entangled UHMW polymers is of generic nature and can be applied for all polymeric materials. The current research activities focuses on polymer synthesis, characterization and processing of polyolefins (polyethylene, polypropylene, poly-*trans*-1,4-butadiene) [2,3], polylactones (polylactides, poly- $\epsilon$ -caprolactone) [4] and alternating polyketone [5]. Correlations between the entangled state (as determined by a combination of characterization techniques) with the catalytic system used (homogeneous and heterogeneous), molecular characteristics and properties of the uniaxial oriented tapes is discussed.

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## Invited Lecture-10

### Donor–Acceptor–Donor type Triphenylamine based Electroactive Monomers : Electropolymerization and Electrochromic Applications

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#### Abstract

Electrochromic materials (ECMs) which reversibly modulate optical transmittance by applying potentials are the key components for energy saving and colour-tuning applications, especially in smart window technology which switch between dark state and a colourless state to control solar heat and increasing the energy efficiency of buildings sectors. Organic ECMs include conducting polymers and small organic molecules that have a large degree of conjugation, have the advantages of good optical switching, fast response time, flexible device fabrication, large coloration efficiency, low driving voltage, and easy molecular design. The present talk deals with the design and synthesis of electroactive triphenylamine (TPA) based different donor-acceptor-donor (DAD) moieties. These are subsequently electropolymerized on conductive surface to have polymers which are subsequently explored by extensive cyclic voltammetry studies. These TPA based DAD type EC polymers are exhibiting strong colour change at low working potential. The effect of core or the effect of substituent on the central acceptor on the electrochromic parameters and the subsequent application of these EC polymers in form of electrochromic device will be elaborated in the talk.

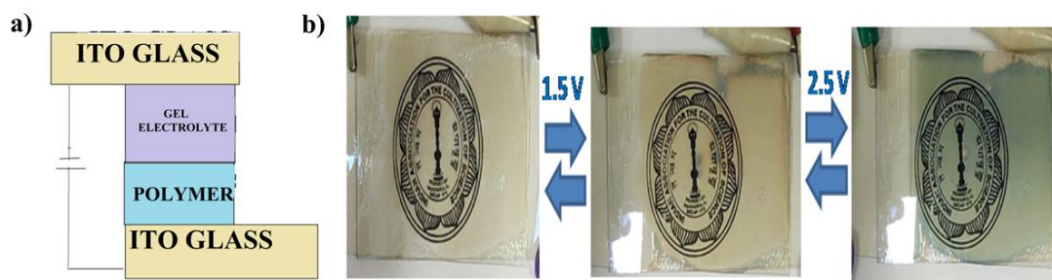


**Figure1:** a) Schematic diagram of the electrochromic device and b) the device (5 x 5 cm<sup>2</sup>) showing the colour change upon applying potential.

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## **Invited Lecture-11**

### **Agar based Materials for Packaging and other Applications**

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### **Abstract**

Environmental and ecological concerns from conventional non-degradable packaging materials are at alarming level and need attention. Biodegradable materials are environmentally friendly and are considered for packaging applications. However, their moderate strength, processability, and susceptibility to environmental exposure – like moisture and microbes – restrict their usage. Agar, a seaweed derived polymer, is demonstrated as a potential packaging material. Plasticizers and reinforcement were employed to modulate strength and elongation at break properties. Chemical crosslinking and surface modification helped in improving water resistance. Synergy between reinforcement and crosslinking further enhanced the properties due to covalent bond formation between reinforcement and agar. Antifungal and antibacterial properties were introduced for prolonging shelf life of the packaged goods. The developed material was transparent and demonstrated heat sealing ability. The processes developed will not only help develop materials for packaging applications, but also for wound healing dressings and as substrate for flexible electronics. The talk will discuss the journey of our group while working with agar and the learnings during the progress.

## **Invited Lecture-12**

### **A Glimpse of Polymer Materials and Technologies for Defence Applications**

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#### **Abstract**

Polymer technologies are very interesting and fascinating materials technologies. It is a wonder that a gaseous molecule by virtue of polymer chemistry and technology can be transformed to a so high impact resistance materials that could stop a Bullet! On the other hand, the resilient rubber component requirement may be small but essential, because without a simple rubber gasket or seal, a big gear and machine may be non-functional!

High performance polymeric materials including composites have their certain advantages over the classical metal/alloys and ceramic materials being lightweight materials having high specific strength, processing flexibility and corrosion resistant properties. Hence the polymeric materials have attracted special attention for their engineering and structural applications in defence such as in aero-structures, spacecrafts, missile & naval systems as well as in armour applications, in addition to their other civilian applications.

Polymer composites are fabricated with the reinforcing fillers such as glass, carbon and kevler fibers/fabrics embedded into polymer matrices such as thermoplastic and thermosetting resins. Thermosetting composite technologies are well established and dominating the composite world in which more than 95% of such composites are based on epoxy and polyester resins. The processing technology for thermosetting resin composites are relatively easy compared to the thermoplastic technology. However, over two decades, high-performance thermoplastic composites are demanded and its technologies are up-coming because of their certain advantages over the thermosetting counterpart especially impact resistant property and recyclable possibility.

Based on the finding at author's Laboratory, some of the polymer materials and their technologies will be presented along with their defence applications, such as (i) high performance resins (phthalonitrile resin and PEEK) and their components and composites, (ii) rubber and thermoplastic seals and gaskets, (iv) high-performance fibers and their composite structures and (iv) functional futuristics technologies.

## Invited Lecture-13

### Click Reactions: Small Molecules to Macromolecules

Debasis Samanta <sup>a, b</sup>

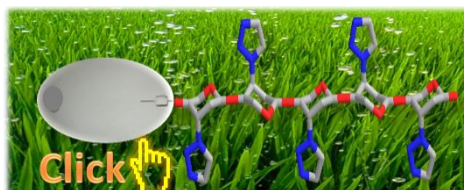
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#### Abstract

Around two decades back the term “Click Chemistry” was coined by Nobel Laureate K. Barry Sharpless and others to classify very efficient chemical reactions based on widest scopes, formation of a single product, eco-benign conditions etc. Although reactions like Diels Alder reaction, nucleophilic ring opening reaction, thiol-ene reaction etc falls under this category, most of recent research for applications of click chemistry concept have been focussed on copper (I)-catalyzed azide-alkyne cycloaddition reactions (CuAAC) or simply click reaction. This is particularly because of efficiency, orthogonality, availability of starting materials, catalysts etc. Last year's Nobel Prize shared by Sharpless and others is also testimony to the importance of click reactions in various fields ranging from materials science to biotechnology. Recently we have shown the click reactions can be used conveniently to functionalize various surfaces ranging from glass, silica or leather-like materials. Applications range from controlling hydrophobicity to dye degradation and development of new-age materials. In the presentation we will mainly focus on our recent results for the immobilization of polytriazoles to various surfaces by click reactions. We will also discuss on the challenges we faced while performing AABB-type<sup>1</sup> or AB-type<sup>2</sup> click polymerizations particularly on cellulose surfaces for the development of leather-like materials. Along the same line, improvement of hydrophobicity of leather surfaces after immobilization of click polymers will also be discussed.<sup>3</sup> Finally, a brief discussion about our effort on the development of the suitable catalyst for performing reactions on biological macromolecules will also be discussed.



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## Invited Lecture-14

### Polyvalent Interaction Facilitated Improvisation of Li-S Battery Performance

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#### Abstract

In Li-S batteries, the Sulfur undergoes various changes during the charging-discharging experiments, hence they dissolve in battery electrolytes. The sulfur redox is also sluggish. To address these issues, we designed and prepared carbon materials with positive charges on their surface. In the first set of experiments, graphite was ball-milled with Nickel Phthalocyanine, which was subsequently carbonized.<sup>1</sup> The Nickel cations attract the negative charge-bearing polysulfides and suppress polysulfide dissolution. In the next set of experiments, graphite was ballmilled with Nickel sulfate and Cobalt chloride.<sup>2</sup> The nickel cations intercalate into the layers of graphenes due to cation -  $\pi$  interaction. We found that the nickel cations suppress polysulphide dissolution better than cobalt cations. Therefore, we have synthesized an organogel of polypyrrole with Nickel Phthalocyanine to host sulfur and polysulfides. Batteries fabricated using these materials showed impressive performance while using high sulfur loading.

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## Invited Lecture-15

### Value-added Biocomposites from Agro-biomass residues

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#### Abstract

Biodegradable polymers and renewable materials are promising alternatives for sustainable replacement of single-use plastics & green technologies for microplastics mitigation. The utilization of single plastic has progressed rapidly worldwide in recent decades due to its lightweight, mechanical properties, and low cost. High plastic consumption with increased micro-plastic contamination causes severe detrimental impacts on human health, soil and aquatic ecosystems. With the Government of India (GoI) decision to ban single-use plastic from the year 2021, it is important to develop commercially-viable and scalable biodegradable and renewable polymer based processing technologies to meet the huge demands of the country. This brings in an opportunity for the indigenous synthesis, fabrication, and processing of biomass-derived bio-plastics and biodegradable polymers such as cellulose derivatives, poly(lactic acid) (PLA), poly(hydroxybutyrate) (PHB), and polyvinyl alcohol (PVA) due to their renewability, sustainability, low energy consumption during production, non-toxicity to living entities, and low-cost. Moreover, development of composite formulations using renewable derivatives such as bamboo or agro-waste residues such as rice, sugarcane and wheat will induce bio-plastics with high thermal, barrier and mechanical stability, which can aid in the production of a variety of daily-use plastic products. Scalable extrusion based processing technologies for biomass-based plastics production finds potential application in plethora of sectors involving electronics, food packaging, and biomedical applications. Life cycle assessment (LCA) provides a platform for evaluation of sustainability in developing novel innovations that can be scaled to pilot and further at the industrial level to substitute or replace the conventional technologies. It aids the stakeholders in deciding the industrial scale production feasibility, ecological hotspots in production processes, and potentially harmful effects of the proposed technologies on the ecosystem. Recently, several eco-friendly novel technologies such as electric vehicles, fuel cells, batteries, biofuels, and green hydrogen energy are being proposed for replacement of non-sustainable petroleum-based materials and fuel sources like hard coal, petrol, and plastics. The development of life cycle-based studies for these emerging novel technologies will allow to evaluate and screen different processes based on sustainability and environmental impact parameters. The environmental impacts in a quantified manner for carbon footprints or global warming potential and its comparison with the sustainable systems will aid the consumer, government, and manufacturers in selecting the appropriate sustainable systems. The life cycle analysis covers the ecological impacts generated during production, utilization as well as after shelf life of a product. The end-of-life LCA can suggest and compare the ecological impacts of conventional and sustainable technologies for assessing the potential harmful effects of a disposed product on the environment.

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## Invited Lecture-16

### Acetabular liner made of UHMWPE and its composites with inborn plateau finish and their testing

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#### Abstract

Ultra-high molecular weight polyethylene (UHMWPE) has been considered as the gold standard of acetabular liner in the metal-on-polymer total hip joint replacements (THR) since 1960. However, the life of a metal-on-polymer total hip arthroplasty (THA) is still limited to 15-20 years, mainly due to excessive wear debris generation during its operation, leading to osteolysis and aseptic loosening. Researchers attempted to improve the tribological characteristics of UHMWPE liners with better processing techniques, bio-compatible reinforcements and superior bearing surface finish. The objective of the present work is to design and develop medical-grade UHMWPE and UHMWPE-MWCNT composite based acetabular liners for THR by an ingenious manufacturing technique for their *in vitro* evaluation using a novel 'Ball-on-Cup' tribometer with a synthesized synovial fluid analogue as the lubricant, following the international guidelines. To achieve the same, processing parameters are optimized to obtain UHMWPE products having the relative density of  $\sim 98\%$  and Vickers hardness of  $\sim 5.0$ , where the latter is further improved by 77% with the reinforcement of 0.25 wt.% MWCNT. After achieving the desired mechanical properties of UHMWPE and UHMWPE-MWCNT samples, rubber moulds of novel design are employed to manufacture the machining-free acetabular liners having plateau finished bearing surface with  $R_a < 100$  nm. *In vitro* wear test of newly developed acetabular liners is performed against stainless steel femoral head using a 'Ball-On-Cup' tribometer, designed and fabricated as per the ISO-14242-3, under a synthesized solution of 2% w/v high molecular weight sodium alginate and 0.75% w/v Gellan gum to create a rheological environment similar to synovial joint. The wear debris obtained from the test rig has a significant morphological resemblance with those retrieved from human bodies while using THA and it is confirmed that adhesive wear and fatigue wear are the leading causes of material loss under *in vitro*. Total volume of wear debris generated from the UHMWPE-MWCNT liner is found to be 52% less compared to that of pure polymer liner with a 33% reduction in linear wear depth. After achieving a significant resemblance in recreating *in vivo* conditions under *in vitro*, it is concluded that UHMWPE-MWCNT may be considered as a potential aspirant for the bearing material in a next generation metal-on-polymer THR in order to increase its longevity.

## Invited Lecture-17

### Designing Thin Film Nanocomposite Membranes by Interfacial Polymerization for Separation of Biomolecules

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#### Abstract

The versatility of membrane technology in biomolecule separation has captured significant attention due to its effective separation efficiency. Thin film composite (TFC) membrane, a prevalent type among composite membranes, consists of a thin selective layer and a support layer. The ultrathin selective layer ensures effective separation efficiency, while the support layer provides mechanical properties and mass transfer [1]. A noteworthy development within this domain is the integration of nanoparticles into thin film composite membranes, commonly known as thin film nanocomposite (TFN) membranes. TFN membranes are considered by their composite structure integrating nanomaterials into a thin film, exhibit enhanced properties that make them promising candidates for membrane applications with excellent selectivity. This lecture focuses on the development of TFN membranes by incorporation of nanomaterials such as clay, graphene oxide (GO), cellulose nanocrystals (CNC) etc. as nanofiller and emphasizing their enhanced separation efficiency [2-4]. In our work, emphasis has been given to develop customized thin film nanocomposite membrane based on incorporation of functionalized nanomaterials through interfacial polymerization method. Thermally and mechanically stable, antifouling, solvent resistant membranes have been developed to enhance the separation performance. Nanomaterial incorporated membranes showed excellent separation efficiency for the individual components. In this lecture, all the aspects of thin film nanocomposite membranes from chemistry to engineering for molecular separation will be discussed.

The effectiveness of TFN membranes in biomolecular separations highlights the advancements in selectivity, permeability, and resistance to fouling. My research group has conducted specific applications of polyamide TFN membranes, showcasing their impact in technological contexts. TFN membranes have been prepared using the interfacial polymerization (IP) process and applied for separation of resveratrol, oxyresveratrol, tea polyphenols and antibiotics, achieving the rejection efficiencies in the range of 90%-95% [2]. Our ongoing research efforts have focussed the use of TFN membranes for future technologies considering environmental aspects, which offer a comprehensive perspective on the promising role of the membrane technology in advancing separation processes.

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## Invited Lecture-18

### Polymer Membrane : Heart of the Hydrogen Value Chain

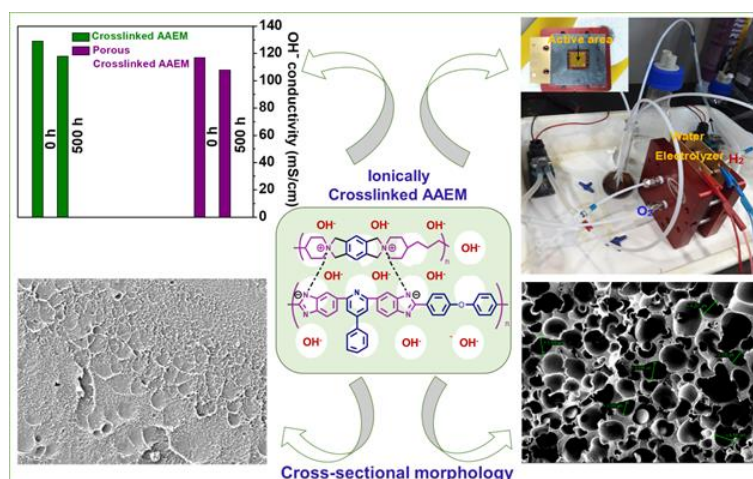
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#### Abstract

The development of polymer-based ion exchange membranes (IEMs) with higher ionic conductivity, desirable mechanical strength, low acid leaching and high alkaline stability are the prime challenges to be achieved for the successful use of these membranes in various types of electrochemical devices such as fuel cell, water electrolyzer etc. Our group has developed several strategies to make IEMs from various polymers with a special focus on a class of polymers namely polybenzimidazoles (PBIs). Synthesis of tailor made PBI structures, development of a novel IEM fabrication process, blending of PBI with suitable polymers, and formation of PBI hybrid nanostructures are the few novel strategies so far, we have pursued to address the key challenges. I wish to discuss few examples arising from these approaches towards the development of PBI based IEMs and their application in proton exchange membrane fuel cell, water electrolyzer etc. and especially focusing on on the development of PBI based alkaline anion exchange membranes (AAEMs).



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## **Invited Lecture-19**

### **Multi-compartmental biodegradable polymeric particles for programmable drug release**

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#### **Abstract**

In this particular talk, I would like to discuss about our work related to the synthesis of multi-compartmental polymeric particles for delivering multiple drugs at a desired fashion to treat complex diseases. One of the aim of this fascinating study was to engineer tri-compartmental polymeric microcarriers by electrohydrodynamic co-jetting technique to encapsulate three PD (Parkinson's disease) drugs incorporated at a desired drug ratio with high encapsulation efficiency (~100%) for an efficient management of PD. This essentially required a combination of LD (Levodopa), CD (Carbidopa), and ENT (Entacapone) at a fixed drug ratio of 4:1:8. Ideally, the drug ratios need to be maintained even after being released from the particles. This was quite challenging as LD and CD were hydrophilic, whereas ENT was hydrophobic. An appropriate combination of FDA-approved biodegradable and biocompatible polymers such as PLA, PLGA, PCL, and PEG was used to make disc shaped tricompartamental microcarriers, so that a desirable drug release profiles for all 3 PD drugs entrapped in their respective compartment (having no or minimal drug-drug interactions) can be attained. Furthermore, *in vitro* release study demonstrated the simultaneous release of all three therapeutics in a sustained and controlled fashion. Additionally, a pharmacodynamics and pharmacokinetics study in Parkinson's-infected rats induced by rotenone showed a remarkable improvement in PD condition for the microparticles-fed rats as compared to the ones having market formulations (oral), thereby showing a great promise towards efficient management of PD. In addition to PD, I will also discuss about related systems for treating other complex diseases, showing the enormous potential of these multi-compartmental particles.

## **Invited Lecture-20**

### **Multifunctional Application of Fluorescent Carbon Nanomaterials**

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#### **Abstract**

Fluorescent carbon nanomaterials (CNMs) are potential candidates for numerous modern nanotechnologies and biomedical research. Owing to their simple, one-pot synthesis, unique excitation-dependent emission, excellent photochemical stability, and high biocompatibility, these water-dispersible CNMs have shown great potential as an alternative source to conventional organic fluorescent dyes and inorganic semiconductor quantum dots<sup>1</sup>. Considering these advantages of CNMs, we have synthesized fluorescent CNMs from various fruits, vegetables and agriculture waste in straightforward, green and cost-effective ways for white light emitting material,<sup>2</sup> chemical sensing<sup>3-4</sup>, biomedical applications (bio-imaging and theranostics)<sup>5-6</sup> and invisible ink<sup>7</sup>.

The details of synthesis, characterization, photophysical properties and their multifunctional applications of synthesized fluorescent nanomaterials will be discussed during my presentation.

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## **Invited Lecture-21**

### **Morphology change and controlled release from nanoassemblies of stimuli-responsive polymer architectures**

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## **Abstract**

Stimuli-responsive polymer architectures have been explored for wide ranging applications for the past two decades. Their self-assembly in aqueous solution into nanocarriers is of particular interest. We have synthesized amphiphilic block copolymers, dendronized polymers, and linear-dendritic copolymers using a combination of various synthetic methods such as atom transfer radical polymerization (ATRP), ring-opening polymerization (ROP) and azide-alkyne click reaction (CuAAC). Different stimuli-responsive groups such as pH-responsive (acetal), redox-responsive (disulfide) and light responsive (UV and visible light) groups were installed in the polymers using functional monomer approach. Alternatively, polymers that are inherently stimuli-responsive by virtue of their molecular structure were employed. Self-assembly of the synthesized polymers in aqueous solution showed micelles, vesicles and rod-like morphologies. Stimuli-responsive morphology change or disassembly was studied using TEM and DLS techniques. To explore the potential of these polymer assemblies as nanocarriers for controlled drug release, hydrophobic as well as hydrophilic drugs were encapsulated and their stimuli-responsive release was shown in cellular uptake studies.

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## Invited Lecture-22

### "Side-Chain Substituted Poly(lactic acid)s: Synthesis, Structure, and Properties"

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#### Abstract

Recently, the side-chain-substituted poly(lactic acid)s (SPLAs, Figure) have attracted much attention as novel bio-based plastics that overcome the weakness of poly(L-lactic acid) (PLLA). However, their structure–property relationship is still not available. In this study, we synthesized crystalline SPLAs with isopropyl and *sec*-butyl side chains [P(L-iPr) & P(L-sBu), Figure]. Crystallization, microstructure, and thermal properties of the SPLAs were systematically investigated and compared with PLLA [1–2].

P(L-iPr) and P(L-sBu) ( $M_n = 60\text{--}70$  kg/mol) were synthesized by ring-opening polymerization of the cyclic dimers of the L- $\alpha$ -hydroxy acids obtained by diazotization of the L- $\alpha$ -amino acids [1–3]. It was found that WAXD crystallinity of P(L-iPr) (60%) was higher than that of P(L-sBu) (30%). Solvent and thermal annealing gave crystal polymorphs of P(L-iPr) ( $\alpha$ - &  $\beta$ -forms). On the contrary, no polymorphism was seen in P(L-sBu) irrespective of annealing conditions. The maximum spherulite growth rates of SPLAs were in the order of P(L-iPr) ( $>4.2 \mu\text{m s}^{-1}$ )  $>$  PLLA ( $0.17 \mu\text{m s}^{-1}$ )  $\approx$  P(L-sBu) ( $0.16 \mu\text{m s}^{-1}$ ). The observed maximum and equilibrium melting points ( $T_{m,\text{max}}$  &  $T_m^\circ$ ) of SPLAs were in the order of P(L-iPr) ( $222/240^\circ\text{C}$ )  $>$  P(L-sBu) ( $193/\text{n.d.}^\circ\text{C}$ )  $>$  PLLA ( $177/200^\circ\text{C}$ ). Thus, we demonstrate that side-chain substituents have a great effect on the structure and properties of SPLAs. P(L-iPr) rather than P(L-sBu) would be a better candidate as excellent bio-based crystalline plastics.

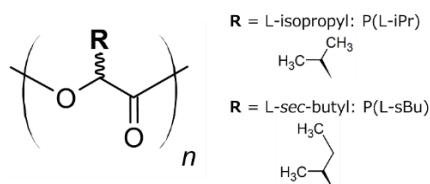


**Figure.** Chemical structure of side-chain-substituted poly(lactic acid)s.

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## Invited Lecture-23

### Engineered Polymeric Micro-Nano Structures for Tissue Repair and Regeneration

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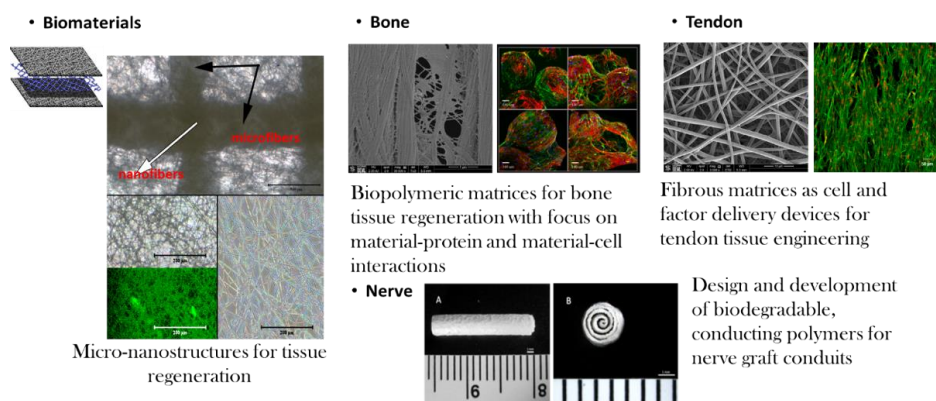
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#### Abstract

Polymeric biomaterials and their structures are used as an alternative to biological grafts in tissue repair and regeneration. Our research efforts are focused on using semi-synthetic polymers to create micro-nanostructured grafts to improve tissue engineering and drug delivery. The micro-structures of the engineered grafts provide mechanical strength to enable tissue repair while nanostructures direct stem cell growth under varying stimuli to promote tissue-specific healing<sup>1-3</sup>. Semi-synthetic polymers combine the advantageous mechanical/degradation properties of synthetic materials with the inherent biological functions of natural materials. These novel materials and structures address several unmet needs of the current clinically used products and structures in terms of biocompatibility, mechanical strength, and bio-erosion. The primary focus of our research is the application of 1) a cellulose biomaterial platform for load-bearing bone healing, 2) small drug molecules and nanocarriers for soft-tissue repair and regeneration, and 3) electrical stimulation for neural tissue repair and regeneration. This presentation will summarize our significant findings, continued innovation, and teaching and mentoring activities in biomaterials science and engineering.



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## Invited Lecture-24

## Conjugated polymer Framework and their Applications

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## Abstract

Conjugated polymer framework (CPF) have recently attained tremendous research attention due to their multifaceted applications including energy storage<sup>[1]</sup>, catalysis<sup>[2]</sup> and separation<sup>[3]</sup> that originates from their unique combinations of properties like extended  $\pi$  conjugation, microporosity and high surface area. These materials, without sidechains or functional groups on their back bone, are generally insoluble in common organic solvents. Whereas, CPF with sidechain are solution processable for electronic device applications. Herein, we have recently developed a series of triazine based CPF by conjugating different moieties like thiophene, carbazole, fluorene unit with triazine ring through a phenyl ring linker. The effect of side chain polarity on self-assembly, photophysical, electrochemical, band gap and electronic property of these CPF were also systematically studied. When these CPFs were reacted with Lewis acids and bases, significant optical switching and conductivity changes were observed indicating efficient nonoxidative doping/dedoping. These materials show a wide range of potential applications ranging from catalysis, electrocatalysis, lithium battery, electrochromism, electroluminescence. Synthesis scheme of such thiophene and triazine based CPF is shown in Figure 1.

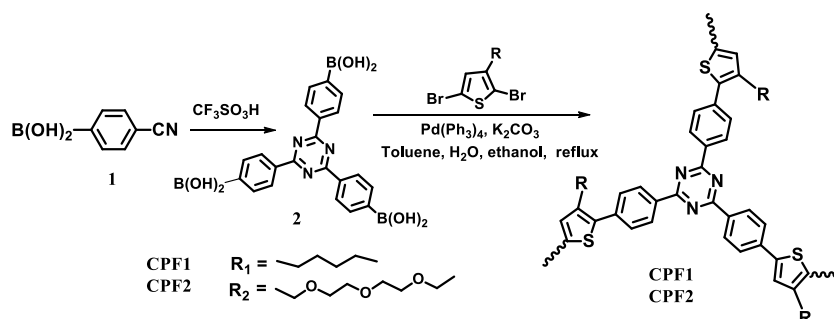


Figure 1 Synthesis scheme for preparation of polymer CPF1 and CPF2.

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## Invited Lecture-26

### Nano-hydroxyapatite Enfused Traditional Nepali Paper-Based Composite Scaffold Films for Bone Tissue Engineering

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#### Abstract

The composite scaffold was prepared via sequential mineralization technique to deposit the hydroxyapatite nanoparticles (nano-HAp) onto the traditional Nepali paper, called *Lokta* Paper. The experiments were conducted with four groups of scaffolds with variations in incubation times and concentrations of mineralizing solutions. The deposition of the nano-HAp onto the paper was attested by Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), and Scanning Electron Microscopy (SEM). It was found that with an increase in the number of mineralization cycles, the HAp content increased and that the deposition of the HAp was found to be independent of the mineralizing solution's concentration. *Lokta* paper/nano-HAp composite film was prepared using the solvent casting method. For this, the HAp was synthesized using the *sol-gel* technique for its incorporation into the composite film. The FTIR and XRD verified the formation of the nano-HAp on the surface of the paper film. Further, the SEM analyses demonstrated the deposition of the HAp crystals on the *Lokta* paper/HAp nanocomposite film. Furthermore, human osteosarcoma epithelial cell culture and the MTT assays were performed to investigate the biocompatibility of the samples. Increasing the HAp content in the scaffolds resulted in enhanced cell viability. Comparing the cell viability of the paper scaffold and the nanocomposite film, even the cell viability of 1<sup>st</sup> cycle mineralized scaffold was found to be better than that of the film. *Lokta* paper, itself in its pristine form, had similar cell viability as *Lokta* paper/nano-HAp film demonstrating the paper as an excellent biomaterial for bone tissue engineering.

*Lokta* paper; mineralization; hydroxyapatite; scaffold; composite film

**Keywords:** *Lokta* paper; mineralization; hydroxyapatite; scaffold; composite film

## Invited Lecture-27

### Biostable Collagen Crosslinked by Dialdehyde Chitosan-Gallic acid for Biomedical Applications

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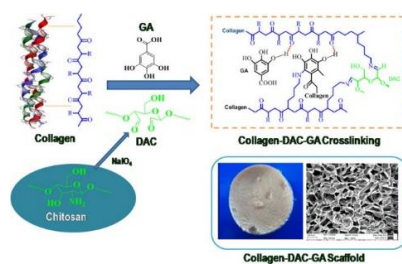
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#### Abstract

In this study, we have prepared the biostable collagen scaffold which is crosslinked by dialdehyde chitosan (DAC) with presence of Gallic acid (GA) and characterized its physico-chemical, biostable and biocompatible properties. The digital photographic and SEM images of the prepared collagen scaffold are exposed well with properly oriented interconnected porous natured structure. The appearance of diffraction peaks showed slightly crystalline characteristic when compared to others. The thermogram measurements indicate significantly increased denaturation temperature ( $T_D$ ) and decreased decomposition rate. FT-IR result suggests the structural integrity of collagen which favours molecular stability. The dialdehyde groups from DAC crosslinked with collagen functional groups that increase the molecular crosslinking owing to the large number of amino groups in its molecular chain. This scaffold exhibited 87% resistance against collagenolytic degradation by collagenase activity.



The results showed that the improved biostability which prevents the free access of the collagenase to binds with the collagen triple helical chains. This scaffold confirms high biocompatibilities, enhanced cell proliferation and adhesions properties. This result gains new insight into the collagen scaffold to improve the biostability. This could be a suitable method to prepare collagenous biomaterials for tissue engineering, regenerative medicine and drug delivery applications.

**Keywords:** Collagen; Collagenase; Dialdehyde chitosan; Gallic acid; Scaffold; Biostable.

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## Invited Lecture-28

**Organic Polymer-based Thermoelectric Materials: Insights into Structure, Doping Mechanisms, and Nanocomposite Formation****N. Raveendran,<sup>1,2</sup> I. Vijitha,<sup>2,3</sup> N. Jacob,<sup>1,2</sup> B. Deb<sup>2,3</sup> and Vijayakumar Chakkooth<sup>\*1,2</sup>**<sup>1</sup> Chemical Sciences and Technology Division (CSTD), CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram 695019, India.<sup>2</sup> Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India<sup>3</sup> Centre for Sustainable Energy Technologies (CSET), CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram 695019, India.*\*Corresponding author's E-mail: cvijayakumar@niist.res.in***Abstract**

Thermoelectric polymer nanocomposites have garnered increasing attention owing to their potential in energy conversion applications, particularly in converting waste heat into electricity. Our studies explored the intricate roles of doping and charge transfer in optimizing the thermoelectric properties of organic polymers. Through the strategic preparation of polymer nanocomposites and the use of molecular dopants, significant improvements in electrical conductivity and Seebeck coefficient were achieved. A range of polymer composites with different doping agents were synthesized and characterized, revealing that the degree of polymer aggregation and nature of the dopant are critical factors affecting the thermoelectric performance. Advanced analytical methods were used to confirm the formation of charge-transfer complexes and to identify shifts in the electronic structure of the materials, thereby elucidating the underlying physics responsible for the enhanced thermoelectric output. A prototype device is fabricated to demonstrate the practical applicability of these findings. Our study offers critical insights for designing high-performance thermoelectric materials with implications for sustainable energy-conversion technologies.

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## Invited Lecture-29

### Mutiscale Modeling and Simulations of Particle-Polymer Hybrid Materials

Haritha Pindi, Deepak Singh, Monmee Phukan, Talem Rebeda Roy and Balaji Iyer\*<sup>1</sup>

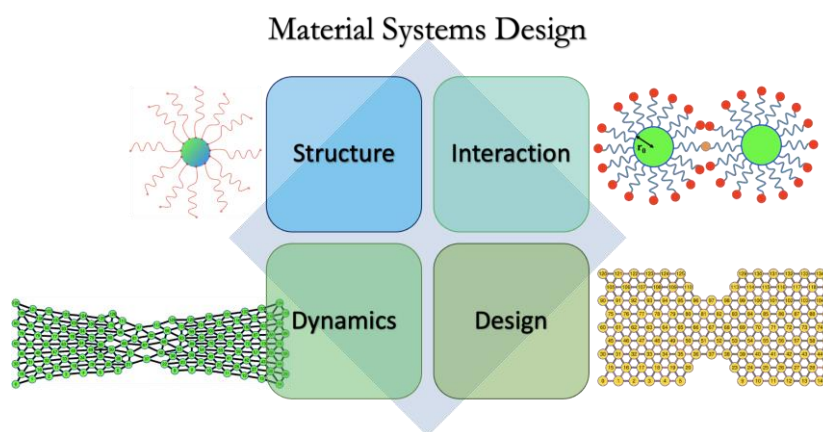
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#### Abstract

Interacting functionalized polymer grafted nanoparticles (PGNs) form extended networks with hexagonal close pack structure[1]. The resulting hybrid material network has an hierarchy of interactions over length scales of few Å to several  $\mu\text{m}$ . Using a multicomponent, multiscale model combined with stochastic simulations we track the dynamic response of such particle-polymer hybrid networks composed of PGNs. We show that both the local and the collective dynamics of such networks depend on features associated with PGN building blocks. In particular, we elucidate the effect of grafting density, length of the grafted polymers, and energy of the functional groups. The effect of the features on rheology and mechanical response are analysed using appropriate frameworks[2]. The analysis is used to establish design criteria for development of novel polymer composites with tunable rheological, mechanical and optical properties.



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### **Invited Lecture-30**

## **Polymers for fish packaging applications**

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### **Abstract**

Packaging is an important part of any food commodity for extending its shelf life, facilitating storage, distribution and sales. Fish is a highly perishable commodity and has to be handled and packed quickly in order to retain its nutritive quality and inherent characteristics. Packaging for fishery products is vital in enhancing its value and uniqueness in the international and domestic trade. Synthetic polymers in the form of trays, films, cups etc. are currently being used for fish packaging based on the type of end product and the properties of the packaging material. These polymers are highly capable and durable in ensuring a safe and quality product with the intended shelf life. However, the synthetic polymers are not biodegradable and end up in landfills or in oceans, causing harm to the environmental and marine living organisms. Currently a lot of alternatives are being looked into and biopolymers from natural sources is researched widely. Biopolymers degrade in the soil and reduces the carbon levels in the atmosphere and can be advocated. Several biopolymers like polylactic acid finds end use application in food industry in a limited way. The physical properties or strength of biopolymers are yet to fully match with that of synthetic polymers. Along with PLA, other films from PBAT, PHT, and their combinations in addition to starch, cellulose, protein, chitosan and seaweed-based films are being researched widely for enhancing their physical properties and end use applications. Different packaging systems like, vacuum, modified atmosphere, retorting, active and intelligent, sous-vide, aseptic, shrink and skin packaging etc. are also practiced worldwide for enhancing its keeping quality. A brief of different polymer and biopolymer-based packaging materials and packaging systems for enhancing the shelf life of fish and fishery products has been explained.



## Invited Lecture-31

### Sustainable Advanced Materials – A Case Study

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#### Abstract

A complex ecosystem of polymerization, resource utilization, and sustainability studies highlight the dynamics shaping our polymer-dependent world. The current focus on sustainable development is evolving new approaches for advanced materials based on renewable feedstocks. Understanding the influence of structural variation and nanocomposite formation on the polymerizability of the monomer as well as the product properties is considered important. In this presentation, the development of polymerizable monomers, the effect of monomer structural variation and polymer properties of cardanol derived materials using recently developed polymerization process and sustainable approaches will be presented. The effect of structural variation like the presence of unsaturation or alkyl substituents and the formation of nanocomposites on the crystallization, melting and polymer properties will be presented. The application of controlled polymerization processes for the design of new materials and multifunctional additives like polymeric surfactants, functionalized fillers, and adhesives with tunable properties will be presented.

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## Invited Lecture-32

### Molecular Engineering of Cross-linkable, Organic Electrochromic Materials: Effect of Hyper-Crosslinking in Carbazole-Diphenylamine Derivatives

S. Balakrishnan,<sup>1,2</sup> R. Venugopal,<sup>2,3</sup> A. Harikumar,<sup>1</sup> B. Deb<sup>2,3</sup> and Joshy Joseph\*<sup>1,2</sup>

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#### Abstract

Electrochromic (EC) devices respond to applied voltage through changes in their optical properties such as transmittance, reflectance and absorbance. Triphenylamine derivatives are promising organic EC materials due to their easy synthesis, low oxidation potentials, high charge carrier mobilities, electrochemical stability, coloration efficiency and tunability of electrochromic properties via substitution.<sup>1</sup> Further, the cross-linking strategy provides added advantage to the small molecule-based EC devices in terms of better-quality EC films with enhanced electrochromic properties. In our earlier work, we have adopted a donor- $\pi$ -donor design strategy for the design of cross-linkable electrochromic molecules, with two diphenylamine donor groups bridged by a  $\pi$ -core, such as fluorene, and tetraphenylethylene and two styrene moieties that can be cross-linked are attached to the diphenylamine groups.<sup>2,3</sup> The  $\pi$ -core in these derivatives influence the electrochromic properties via differential electronic coupling of the donor units in the neutral and oxidized states. In this work, we explore the EC properties of two carbazole-diphenylamine derivatives, **C-Sty2** and **C-Sty3**, with two and three thermally cross-linkable styryl units, respectively, following a donor- $\pi$ -donor design, where both the carbazole moiety and cross-linking styrene groups modulate the photophysical and EC properties.<sup>3</sup> Both styryl derivatives formed rigid, uniform, and transparent films with high solvent resistance and exhibited excellent thermal and electrochemical stability upon cross-linking. **C-Sty3**, with three cross-linkable styryl units, could form more extended cross-links, leading to hyper-cross-linked films with distinct, regular, and porous morphology compared to **C-Sty2**. A comparison of the EC properties of two polymers with the same electroactive groups reveals the significance of hyper-cross-linking in the EC properties of these cross-linked polymers.

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### Invited Lecture-33

## Molecular simulation-inspired development of hierarchical carbon fibres-reinforced high-strength light-weight hybrid polymer composites

Gaurav Manik<sup>1,\*</sup>, Rupam Gogoi<sup>2</sup> and Sachin Kumar<sup>1</sup>

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### Abstract

The demand for high performance light-weight fibre-reinforced polymer composites, which are current state-of-the-art need for structures of varied types, is rising exponentially for a wide range of applications spanning across automotive, aerospace, sporting and other industrial sectors. There is a need for development of hierarchical carbon fibres (CF) through utilizing the universally acceptable and remarkable tool of molecular simulations to screen the right strategy of functionalization and coating of CF in a polymer matrix. CF may be molecularly modeled as multiple stacked graphitic layers placed in a PP matrix. In order to enable a strong and effective load transfer from matrix to CF, it is important to reinforce the fibre-matrix interface through increasing fibre-matrix chemical interactions and enhancing physical inter-locking at the interface. For ensuring the former, various type of functionalization strategies have been adopted in past with different functional groups. Molecular simulations have helped screen and propose the superior functionalization route. To enable useful mechanical interlocking of fibre with matrix, functionalized carbon nanotubes (CNT) and similar materials have been appropriately coated onto the CF. The interfacial strength (IFSS) of fibre-matrix interface are estimated by performing a fibre pull-out molecular simulation protocol which expresses significantly improved mechanical properties. The experimental findings estimated using single fibre fragmentation test and mechanical properties compare well with the molecular simulation results. This work reviews similar investigative efforts that pave interesting ways for molecular simulation-assisted development of hierarchical CFs through functionalization and subsequent coating with suitable nano-fillers.

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## Invited Lecture-34

### Sustainable and green polymers for coating, adhesive and other applications

**P.Aruna**

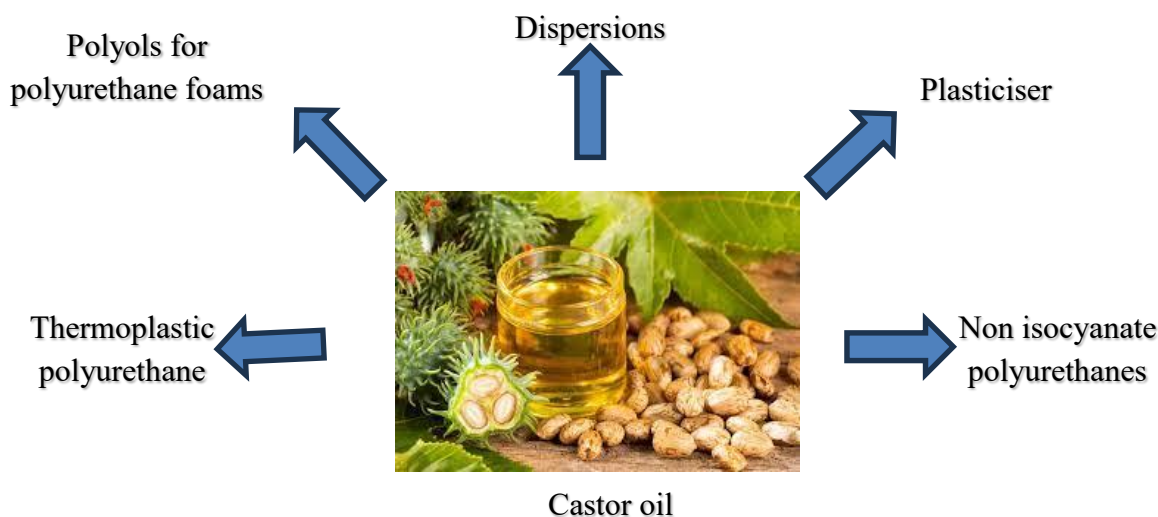
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#### Abstract

Due to the strict environmental legislations in the recent past, academia and industry, both are looking into eco-friendly and solvent free polymer coatings with very low to zero VOC emission. In addition, depleting fossil fuel sources have also contributed to increasing interest in renewable/biobased resources especially biomass and vegetable oils. Since there is a huge demand for edible oil, there is a thrust on utilisation of non edible oils like linseed oil, cardanol, castor oil etc for industrial applications. Castor oil is a non edible oil and India ranks first in the export of castor oil to other countries. However, very less value addition is being done in our country presently.

We have been working on the development of biobased products for coating and adhesive applications with special emphasis on the utilization of castor oil as raw material in the place of petroleum based resources. Another approach is the utilization of CO<sub>2</sub> for developing polymeric materials such as polyurethanes (through isocyanate free routes) which are a type of polymers having unique properties are widely used in almost all the fields in the form of elastomers, fibres, sealant, coatings, adhesives, foams etc. Keeping the environmental issues in view, castor oil and to some extent cotton seed oil have been employed in our group to develop waterbased polyurethane coatings, adhesives and other additives.

The various modifications of castor oil have been carried out for applications as dispersions, raw materials for foam formulations, plasticizer for PVC and epoxies. Currently, we are exploring the possibility of utilizing castor oil for developing bioplastics (thermoplastic polyurethanes) which may be industrially viable. This presentation will summarise all the above research findings and the way forward to develop novel, ecofriendly products.



## Invited Lecture-35

## Sustainable Approaches Towards Polymer Nanoparticles and Their Applications in Drug Delivery and Catalysis

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### Abstract

Cross-linked polymers are very useful because of their applications in drug delivery, tissue engineering, chemical sensing, cosmetics, etc. Instead of the conventional copper-based reagents for the development of star-branched polymers, we have established novel and environmentally benign methods, whereby a 1,3-dipolar cyclo-addition reaction using less toxic reagents like iodosobenzenediacetate [ $\text{PhI}(\text{OAc})_2$ ],  $\text{NaOCl}$ . In aqueous medium, these core crosslinked polymers produce polymeric nanoparticles (CCNP), which could potentially serve as a carrier of hydrophobic drug molecules. The polymeric NPs were also shown to successfully encapsulate a hydrophobic drug, doxorubicin. This new green synthetic strategy for CCNP formation may thus be employed effectively for the development of new polymeric architectures with potential applications in the field of advanced material science and smart drug delivery.

It is important to replace the conventional toluene chlorination process to produce industrially important benzaldehyde with eco-friendly processes. In that direction, we have developed a couple of polymer-conjugated magnetic nanoparticles as non-chlorinated, acid-free, noble metal-free 'green catalysts' that are effective in water at room temperature that can be quickly recovered by simple method and reused without loss in catalytic activity

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## Invited Lecture-36

### Micro/Nanoencapsulation of Phase Change Materials for Energy Storage Applications

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#### Abstract

A considerable portion of moderate energy (household) needs can be met using materials with large latent heat storage ability called PCM (phase change materials), provided energy exchanges take place with the surrounding environment. Phase transformation of PCMs during energy exchange causes unconventional challenges problems in application development using these materials. Micron/nano sized enclosures (higher heat transfer area) are preferred geometries for accommodating PCMs, provided the shell wall should be chemically, mechanically, and thermally stable with reasonably good thermal conductivity.

PCM molecules could be: (i) organic PCM (long chain paraffin, fatty acids, fatty alcohols, etc.), (ii) Inorganic PCM (salts, salt hydrates, etc.), and (iii) Eutectic PCM (mixture of two PCMs either organic/inorganic nature). Major research revolves around selection of right PCM, the corresponding shell material, and the technique(s) to be adopted for enclosing PCM as core targeting a specific application. Polymer is the most preferred shell material for enclosing PCMs following conventional emulsion/suspension, etc. polymerization technique. Paraffin being non-reactive are easier to encapsulate compared to PCMs being functional groups (fatty acids/alcohols). Similar challenges are also observed while encapsulating salts/salt-hydrates due to their non-reproducible physical properties during thermal cycles. Out of several methodologies developed for encapsulating different PCMs only a few are highlighted in this discussion: e.g. (i) understanding core-shell interactions while enclosing organic PCMs (paraffin, ester, and fatty acid) inside barium crosslinked pectin (polysaccharide) shell following ionic gelation, (ii) complex polymeric microstructure with programmable architecture during hexadecane encapsulation using Emulsion-templated *in situ* polymerization, (iii) hexadecane encapsulation using CaCO<sub>3</sub>, through self-assembly and developed materials were characterized and applied in various applications.

**Invited Lecture-37****Thermo-mechanically processed Chitosan with cyclic carbonate based plasticizers: Preparation and Physicochemical properties****Sukanya Satapathy\* and Aruna Palanisamy\****Polymers and Functional Materials Department, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, Telangana, India**Corresponding author's E-mail: [sukanya@csiriict.in](mailto:sukanya@csiriict.in)***Abstract**

Chitosan films with cyclic carbonate based plasticizers (ethylene carbonate, propylene carbonate, their mixture and carbonated diglycidyl ether of bisphenol A) were prepared by thermo-mechanical mixing and compression molding techniques. Cyclic carbonates are widely used as green and sustainable solvents in the academic as well as industrial level. To understand the applicability of these plasticizers in chitosan, their properties were compared to one of the most commonly used plasticizer, i.e. sorbitol. The plasticized chitosan films were characterized for their mechanical and thermal properties. It was observed that cyclic carbonates(5 wt.%) were sufficient for processing/plasticizing the chitosan matrix resulting in desirable mechanical properties as compared to sorbitol(30 wt.%) plasticizer. An increase in tensile and tear strength was observed for the carbonate based plasticizers. The cross section analysis of all the films by scanning electron microscopy showed a compact and homogenous surface. Such thermo-mechanically processed chitosan films would be economically viable and have applicability in packaging sector.

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## **Invited Lecture-38**

### **Embedded-enzymes for faster degradation rate and chemical recyclability**

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### **Abstract**

Scheming biocomposites with embedded enzymes can help to eradicate problems related to the slow degradability of common biobased and/or biodegradable materials. Efficaciously interfacing an enzyme in the polymer matrix and attaining programmable degradation is challenging. However, properly designed, this approach can accelerate the degradation process when the polymer material comes in contact with degradation medium, such as body fluids, soil or marine environment or offer a green chemical recycling route. We have developed strategies for production of enzyme-embedded (IL) cellulose acetate (CA) and polycaprolactone (PCL) materials, that exhibit significantly accelerated and still tunable degradation rates during simulated composting and in aqueous solutions. CA/IL 5% and PCL/IL 5% showed accelerated degradation under simulated thermophilic composting condition compared to their plain counterparts which is equivalent to more than 40% and 30% biodegradation rate respectively. Furthermore, the chemical recyclability of PCL was facilitated by the embedded enzymes. As an example enzyme-embedded PCL/IL5% films were chemically recycled in a 3:1 methanol/tetrahydrofuran mixture at 60°C without additional external catalyst and the results were compared with plain PCL. The embedded enzymes clearly served as biocatalysts resulting in significantly faster degradation, leading to a mixture of 6-hydroxyhexanoic acid methyl ester and oligomeric products with  $M_n=340$  and  $M_w=6370$ . The product mixture could also be repolymerized to new PCL. These embedded-enzyme materials have large future potential in multitude of applications where biodegradation or chemical recycling are the preferred end-of-life options, from biomedicine to consumer products and agriculture.

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## Invited Lecture-39

### Self-assembly of similarly charged polyelectrolyte chains in dilute aqueous solution

Shivalika Sharma, Mehak Jain, Raju K. Singh, Jyoti R. Seth, and Kamendra P. Sharma

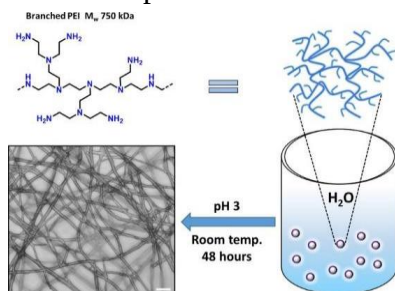
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#### Abstract

Similarly charged species are seldom attractive. For e.g., colloids with similar charges on their surface can be assembled into colloidal crystals by optimizing the ionic strength, i.e., the concentration of counter-ions in the solution. Charged polymers are trickier to assemble in the sense that the conformational degrees of freedom are multi-fold.

In my talk, I would speak about pH assisted and light-responsive self-assembled



microstructures of a cationic polymer, Polyethyleneimine (PEI), a well-known gold-standard non-viral vector for gene transfection. Generally, PEI is complexed with oppositely charged molecules to derive self-assembled polyplexes which are used for various drug delivery applications. However, our recent experimental observations suggest that at pH values between 2.5 to 4, neat PEI chains in explicit water undergo a completely unprecedented and never observed before kind of self-assembly process.<sup>1</sup> The self-assembly is extremely slow, irreversible, and occurs under quiescent conditions to form a 3-D fibrillar network comprising hollow fibrils (Figure 1). The transition of PEI { $\approx 0$  (nm)} chains into micron-sized fibrillar network follows coalescence of smaller PEI chains to form  $\approx 100$ -200 nm spheroidal aggregates accompanied with conformational/ morphological transitions into anisotropic rod-like aggregates which assemble end-to-end to form a network structure. Further, it will be shown how these self-assembled structures show light responsiveness under similar pH conditions.<sup>2</sup> My lecture will mainly focus on our experimental results; however, some PMF calculations based on MD simulations will also be shown to support the experimental findings. We believe that our work will initiate to seek more understanding in the gene delivery through hyperbranched PEI-based polyplexes which encounter several levels of low pH conditions once transfected into cells.<sup>3</sup>

**FIGURE 1.** Branched PEI chains ( $\sim$  nm in size) self assemble at pH 2.5-4 to form micron sized structures which resemble tubular morphology.

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**Invited Lecture-40****Ag nanoparticles/Poly (vinyl alcohol) composite films: The tuning of morphology and conductivity****S.Sirohi\*<sup>1</sup>, Mittal<sup>1</sup>, R. Nain<sup>1</sup>, N. Jain<sup>1</sup>, R. Singh<sup>1</sup>, S.Dobhal<sup>1</sup>, B.Pani<sup>1</sup> and D. Parida<sup>2</sup>**<sup>1</sup>*Bhaskaracharya College of Applied Sciences, University of Delhi, Delhi 110075, India*<sup>2</sup>*Swiss Federal Laboratories for Materials Science and Technology (Empa),  
St Gallen, Switzerland**\*Corresponding author's E-mail: siddharth.sirohi@bcas.du.ac.in***Abstract**

In this work, the influence of shape of silver nanoparticles (AgNPs) on photocatalysis and electrical conductivity was investigated. AgNPs of different shapes of AgNPs were prepared using various concentrations of NaBH<sub>4</sub>. The obtained AgNPs were characterized using particle size analysis, UV–visible spectroscopy and high-resolution transmission electron microscopy. The colours of colloidal solutions were observed to be influenced by the shape of the nanoparticles. Yellow and blue AgNPs were spherical and triangular in shape, respectively, whereas distorted spherical particles showed a red colour and the presence of both particles in one solution resulted in a green colloidal solution. AgNPs of different morphologies were used to prepare Ag/poly(vinyl alcohol) (PVA) composite films.

The Ag/poly(vinyl alcohol) (PVA) composite films were investigated for their electrical conductivity. Owing to the better charge carrier generation and uniform distribution in the PVA matrix and enhanced surface plasmon resonance, blue AgNPs (triangular shaped) exhibited superior conductivity performance compared to the other Ag nanoparticles. The values for maximum conductivity for the blue and yellow AgNPs were  $3.45 \times 10^{-4} \Omega^{-1} \text{cm}^{-1}$  and  $2.67 \times 10^{-4} \Omega^{-1} \text{cm}^{-1}$  respectively.

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## Invited Lecture-41

### Polyethylene surface modification: Surface free energy of sulfonated films

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#### Abstract

The modification of organic surfaces is a subject of theoretical and practical importance. The interfacial chemistry of polymer is relevant to many applications such as wetting, adhesion, compatibility and gas/liquid permeability. Polyolefins is a relatively inert hydrocarbon, stable leads to materials with low surface energies, wherein their considerable incentive for introducing polar functional groups on the polymer surface used for a wide range of applications. Gas phase sulfonation of polyethylene is industrially practiced to impart superior hydrocarbon barrier properties of polyethylene. A more controlled method is surface sulfonation involves gaseous  $\text{SO}_3$  suitably diluted with nitrogen to moderate the reactivity of sulfonating agent. The surface polarity and wetting properties of the sulfonated polyethylene were evaluated by contact angle measurement.

The contact angle is sensitive to chemical composition of the top molecular layer and it is relatively simple, inexpensive and popular technique for characterizing the polymer surfaces. In the present work, we have measured surface free energy of sulfonated HDPE films with different solvents namely water, formamide, diiodomethane using contact angle goniometry at ambient temperature. Dispersion forces and polar attractive forces combine by using Geometrical mean method. The surface free energy of HDPE films increases with the extent of sulfonation. The sulfonated films were characterized by UV-VIS absorption and reflection spectrometry, SEM, FT-ATR, contact angle goniometry and XPS. The degradation was observed as extensive carbonization on the surface with the time of sulfonation and increased  $\text{SO}_3$  gas concentration. The sulfonation at low concentration and shorter time period improves these two properties of HDPE surfaces

**Invited Lecture-42****Multi-material Additive Manufacturing with Lightweight Closed-Cell for enhanced Mechanical and Functional Properties****Ajeet Kumar\****Department of Design, Indian Institute of Technology Guwahati**\*Corresponding author's Email: ajeetkumar@iitg.ac.in***Abstract**

This work studies the novel concept of multi-material additive manufacturing by filling closed-cell lattice structures with secondary material. Filling closed cells incorporate new functional properties that unfilled or open-cell lattice structures cannot otherwise achieve. Filled closed cells also prevent materials from escaping the cellular cavity that can prove advantageous while combining dissimilar materials. For this, a hybrid 3D printing and foaming process is developed, which involves simultaneous 3D printing and foam-filling of closed-cell lattice structures on an open-source fused filament fabrication (FFF) 3D printer. This hybrid system targets direct digital manufacturing (DDM) by combining two separate processes into a single process, eliminating post-process operations. Here, the global closed-cell sea-urchin (SU) lattice structure is 3D printed with thermoplastic polyurethane (TPU), and the secondary functional material filled in the lattice structures is polyurethane (PU) foam. The load vs. deformation responses of the composite of PU foam and TPU lattice structures has shown higher stiffness, energy dissipation, and damping characteristics which otherwise could not have been achieved by the lattice structure alone. Possible applications for these could be protective equipment, shoe midsoles, and other energy absorbing and damping devices.

**Invited Lecture-43****Liquid Metal Embedded Soft and Multifunctional Elastomeric Architectures for Soft Matter Engineering****Shib Shankar Banerjee***Department of Materials Science and Engineering, Indian Institute of Technology Delhi, New Delhi-110016, India**Corresponding author's E-mail: ssbanerjee@mse.iitd.ac.in*

Functional elastomers with incredible toughness and stretchability are indispensable for applications in soft robotics and wearable electronics. Furthermore, coupled with excellent electrical and thermal properties, these materials are at the forefront of recent efforts toward widespread use in cutting-edge electronics and devices. Herein, we introduce novel soft, multifunctional elastomeric architectures with integrated eutectic gallium-indium liquid metal (LM) alloy inclusions. Viable strategies of incorporating LM into the elastomer matrix via both solid and liquid state polymer processing benefices a homogeneous droplet-matrix morphology mitigating the modulus mismatch issues existing in rigid filler filled elastomer composites. The resulting material exhibits outstanding mechanical features like, ultra-stretchability, enhanced tearing energy, crack-growth resistance, and reduced hysteresis loss over an unfilled elastomer. Moreover, the multifunctionality of the resulting composite material substantiated via the remarkable enhancement of dielectric permittivity, and thermal conductivity ratifies the immense potential of LM-filled elastomeric systems for multifarious high-end engineering applications. The experimentally determined results have been also rigorously analysed and validated using theoretical models like Eshelby's and modified Eshelby's approach, modified Cole-Cole model, and Bruggeman formulation. Henceforth, this work provides a facile and scalable pathway to develop liquid metal-embedded soft elastomeric composites accentuating their instrumentality toward potential applications in soft-matter engineering.

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## Invited Lecture-44

### Printable Elastomer Composite Sensor based “Smart Mask” for Point of Care Diagnostics

**Titash Mondal**

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#### Abstract

Flexible strain sensors are becoming more and more used in the field of human healthcare. However, the precision is frequently limited by issues like noise and crosstalk in the sensor's output signal. Therefore, it is imperative to design a strain sensor through inexpensive engineering, thereby justifying its mass utility. This work reports on the development of a crosstalk-free strain sensor for unobtrusive respiratory monitoring using stencil printable graphene/liquid elastomeric. Printing eliminates complicated fabrication and encourages the process's thrift. A wearable mask had the sensor attached to it, and a homemade sensor console was created. With an SNR of -12.85 dB, the console showed that it could identify the respiratory profile at both room temperature and at a low temperature of -26°C. Newly developed sensors could produce breathing signals as a result of strain-induced temperature and humidity nullification. A model experiment was carried out to verify the strain mechanism's fidelity. The console showed outstanding stability (during 500 cycles) with sensitivity values of 117.49 (0.17-0.34% strain) and -196.56 (0-0.17%). The console might use Bluetooth to wirelessly transfer the data and precisely identify conditions like tachypnea, eupnea, etc. These results address important limitations in the development of flexible sensors by emphasizing selectivity, sensitivity, and stability.

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**Invited Lecture-45****Effect of Polycarbonate on Flammability and Mechanical Properties of Macro Crosslinked Wood Plastic Composite Manufactured from (HDPE/LDPE/UHMWPE)-g-MA/(rPET/LDPE)-g-MA Reinforced with Rice Husk****U. Meekum\****Institute of Engineering, Suranaree University of Technology, Maung, Nakorn Ratchasima, Thailand;**\*Corresponding author's Email: umsut@g.sut.ac.th***Abstract**

Decreasing processing temperature of poly(ethylene terephthalate) waste (rPET) and ultra-high molecular weight polyethylene (UHMWPE) to prevent rice husk fiber (RHF) decomposition during the manufacturing of wood plastic composite (WPC) was accomplished by blending technology. The peroxide/silane macro crosslinked (XWPC) was also successfully performed for properties enhancement. This publication, polycarbonate (PC) was explored as the blended flame retardant in XWPC. The commercial retardant was employed for bench marking. The results showed that the retardant had solution effect on XWPC. The increasing in flowability but decreasing in mechanical properties upon increasing the retardant loading were observed. The optimal retardant dosing was 1 phr. Adding PC as flame retardant on the XWPC was revealed that flammability was decreased, mechanical properties were generally decreased, HDT was increased, and water absorption was merely increased when the PC loading was gradually increased. The noticeable superior flammability was explained by gas dilution mechanism derived from the PC decomposed carbon dioxide. The SEM analysis revealed that compatibility in the blended matrix and at fiber/matrix interfacial were the main cause of the obtained mechanical properties. It was found that obvious phase separation and inferior fiber/matrix bonding were found when the PC loading was increased. PC blending not exceed 10 phr was suggested.

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## Invited Lecture-46

### Advanced technologies for controlling pests

**GVN Rathna<sup>1\*</sup>, Ashwini Dhobale<sup>1</sup>, Amarnath Singam<sup>1</sup>, Dhiraj Mishra<sup>1</sup>, Kirthi Lakhan<sup>1</sup>,  
 Sravanya Konchada<sup>1</sup>, Naresh Killi<sup>1</sup>, and B. Shantha Kumari<sup>1</sup>**

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#### Abstract

Conventional chemical pesticides like pyrethroids, organophosphates, organochlorines, carbamates, etc. have been in practice for decades. The extensive application of these pesticides is toxic to the ecosystem and more importantly, poses a threat to the farmers who are continuously being exposed to these chemicals. Hence the regulations are being directed to reduce their use and are encouraging the development of novel technologies and products that contribute to Integrated pest management. Consequently, pheromones (secreted by insects or animals) are being used for auto-confusion/mating disruption of pests to control feeding the crops. Though these methods are in practice, they tend to be expensive and not affordable to low-income farmers. Hence, they are compromised by using the pheromones.

To reach out to farmers an affordable integrating pest management needs to be designed and developed, accordingly in our lab, we have developed eco-friendly and biodegradable polymeric material immobilized with pheromone that can sustain pheromone release for about 60 to 90 days (i.e. complete crop season). The first part of my talk is about the design and development of novel gels for the controlled release of methyl eugenol to control fruit-fly. The second part is a demonstration of indigenous biodegradable nanomaterial for the controlled release of pheromone to control Bollworm. A bottom-up approach was followed to develop these two indigenous technologies, which enabled us to attract an Agri company for the transfer of technology. The insights of these technologies will be presented.

Bulk material



Nanomaterial



Gel



Fruit fly

Pest Control

Nanofiber mat



Dispenser



Dispenser

## Invited Lecture-47

### An insight into the role of polyproline's secondary structures during thermal phase transition and bulk phase separations

Arjun Singh Bisht, Prabir Kumar Maiti, Sneha C and Raj Kumar Roy\*

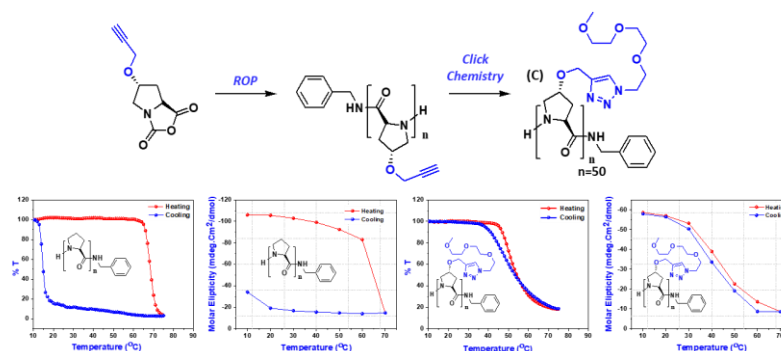
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#### Abstract

Proteins are composed of amino acids, which play an essential role in their structure and functions. One of the 20 naturally occurring amino acids, proline, is the only one with a five-membered pyrrolidine ring attached to its side chain. Polyproline is unique among other polypeptides due to its cyclic side-chain and lack of an amide backbone that donates H-bonds. It is common for polypeptide backbones to assume -trans conformation, while polyproline can assume both -cis and -trans conformations. The conformation around the tertiary amide bonds in polyproline is crucial to the formation of their secondary structures. When the backbone amides are exclusively cis or trans, polyproline assumes a PPI (right-handed helix) or PPII (left-handed helix) secondary structure.<sup>1</sup> Different factors, such as temperature, solvent, substitution at C4-position, etc., can stabilize a particular secondary structure (PPI and PPII).<sup>2</sup>

In my presentation, I will describe a rational design of polyproline to stabilize PPI and PPII structures independently either via functionalization or copolymerization approach. Subsequently, I will explain how thermal phase transitions of polyprolines are related to their secondary structure.<sup>3</sup> Finally, I will discuss the role of polyproline's secondary structure during bulk phase separation of polyproline-based block copolymers.



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## **Invited Lecture-48**

### **Development of Reprocessable, Self-Adherable High-Performance Carbon Fiber Reinforced Vitrimer Composites**

**Sravendra Rana\*, Harsh Sharma, Gun Jin Yun\***

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#### **Abstract**

In the present study, carbon fiber reinforced (CFR) vitrimeric composites are developed through vacuum assisted resin infusion molding (VARIM) process. The system allows the repeated reversal of fatigue damage *via* reversible covalent adaptable networks (vitrimers) where heating the material to a temperature beyond its glass transition temperature is helpful to achieve self-healing in the materials and thus enhancing the reliability and safety of the components. In addition, the vitrimeric system and its composite show excellent mechanical, reprocessing, shape-memory, and self-adhering properties. The developed CFRP vitrimer composites can be rapidly dissolved in thiol solvent (2-mercaptoethanol), due to the thiol-disulfide exchange reaction, resulting in the efficient recycling of carbon fibers (CFs). Scanning electron microscopy, X-ray diffraction, and Raman spectroscopy show that the recycled CFs have almost the same chemical structure and composition as the virgin CFs. The recycled CFs can be used to prepare “2nd generation” composite materials with excellent mechanical properties for non-structural applications (e.g., sports, automotive etc.).

#### **Acknowledgment**

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## Invited Lecture-49

### Rise of Benzoxazines: Conventional to Innovative Applications

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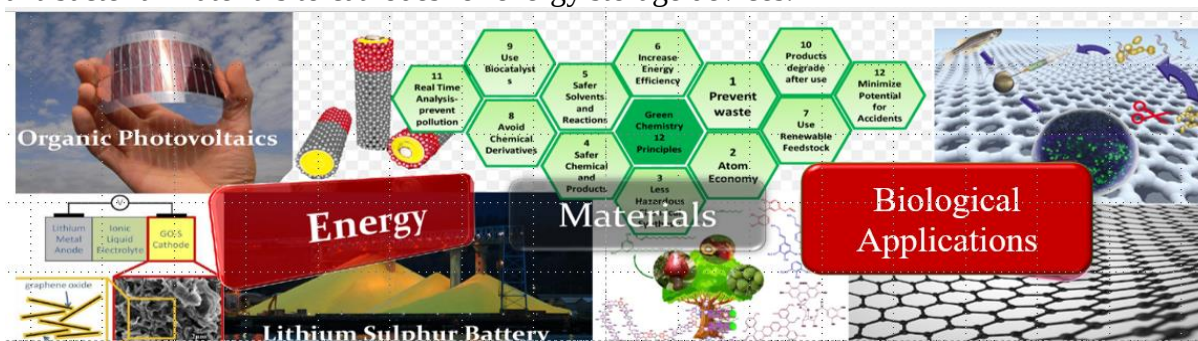
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#### Abstract

Depleting fossil fuel reserves and increasing waste reservoirs are among the world's most pressing problems. This calls for exploring naturally occurring building blocks for developing bio-based polymers. Polybenzoxazines is a new class of thermally curable thermosets being pitched as superior alternates of phenolics. In this work, we intend to exploit the options of synthesizing partially bio-based polybenzoxazines following green chemical principles of atom economy, bio-renewable feedstock, solventless synthesis, and nontoxic waste generation. In addition, the molecular flexibility of benzoxazine moiety has been utilized by studying the relation between higher functionality and properties. These polymers have shown improved thermal stability compared to their non-green counterparts and the ability to copolymerize with other industrial wastes/resources, thus finding wide applicability from adhesive and antibacterial materials to cathodes for energy storage devices.



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## Invited Lecture-50

### Pathway Complexity in Supramolecular Polymerization and Heterostructures by Seeding Effect

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#### Abstract

Herein, we unravel supramolecular copolymerization between two amide-functionalized chiral dipolar naphthalene monoimide (NMI) monomers (**O-NMI** and **S-NMI**) through manipulated kinetic and thermodynamic pathways and showcase sequence-controlled supramolecular polymerization for programmed synthesis of complex blocky "star" topology.<sup>1</sup> **O-NMI** and **S-NMI** differ by a single heteroatom (oxygen vs. sulfur) and show distinct supramolecular polymerization (SP) features in an organic solvent, decane. **O-NMI** initially forms kinetically-controlled metastable nanotapes that transform into thermodynamically-controlled helical 1D fibres over 24 hours. In contrast, **S-NMI** only forms stable spherical aggregates under similar conditions. The presence of multiple competing intermolecular interactions (dipole-dipole interactions and different H-bonding modes) dictates the energy landscape of the two distinct self-assembly pathways in **O-NMI**, while the absence of competing self-assembly pathways in **S-NMI** is ascribed to the predominance of amide-amide H-bonding that supercedes other interactions. Furthermore, we generated unprecedented blocky supramolecular star topologies with segregated domains of self-assembled **S-NMI** "core" and multiple **O-NMI** "arms" in a kinetically controlled route via surface-catalyzed hetero-seeded SP by sequential addition of the two monomers. Contrastingly, under thermodynamic conditions, statistical copolymerization with random distribution of the two monomers led to the formation of temporally controlled chiral nanofibres via achiral metastable spherical hetero-aggregates. The sequence of microstructural organization (statistical vs. block) between the two monomers determines the chiroptical properties of the two distinct resultant supramolecular copolymers generated through different thermodynamic and kinetic routes. Successfully extending this strategy to water produced temporally controlled 2D polymers with monolayered thickness that showed a promising response towards protein adsorption and time-dependent regulation of enzyme activity.<sup>2</sup>

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## Invited Lecture-51

### Dynamics and Rheology of Nanoparticle Grafted Ring Polymers

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#### Abstract

Abstract: The dynamics of ring copolymers or nanoparticle grafted ring polymers are investigated in the framework of optimized Rouse Zimm theory in dilute solutions. The multiscale nature of the system may be modelled in terms of monomers of varying size connected to each other through harmonic springs with different spring constants. The intrinsic viscosity and the mechanical moduli directly measure the viscoelastic properties of such ring polymers. The intrinsic viscosity and the size of the ring copolymer increases with an increase in the size and the number fraction of the nanoparticles. The mechanical moduli exhibit a size independent universal scaling behaviour both in the low and high frequency region. In the low frequency regime, the mechanical moduli are dominated by the collective relaxation mode corresponding to the slower relaxation rates. In the high frequency regime, mechanical moduli are primarily characterized by the local modes of motion corresponding to the higher relaxation rates. The intermediate power-law regime is typically representative of the topology of the grafted ring copolymers, which are due to the contribution of the non-trivial eigenvalues representing the multimode relaxation. Increase in the number fraction of the nanoparticles increases both the width of the intermediate frequency regime and the magnitude of the viscoelastic relaxation moduli. The loss moduli exhibit a characteristic bimodal peak in presence of hydrodynamic interactions with an increase in the number fraction of the nanoparticles. The intramolecular relaxation dynamics of ring polymers in dilute solutions may be modulated by manipulating molecular architecture and interactions.

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## Invited Lecture-53

**Synthesis, Characterization, and Anticancer Activity of Phenolic Carbaldehyde Based Chitosan Functionalized Thiosemicarbazones****Hari Sharan Adhikari<sup>1\*</sup>, Rameshwar Adhikari<sup>2,3</sup>, Paras Nath Yadav<sup>2</sup>**<sup>1</sup>*Institute of Engineering, Pashchimanchal Campus, Department of Applied Sciences, Tribhuvan University, Pokhara 33700, Nepal*<sup>2</sup>*Central Department of Chemistry, Tribhuvan University, Kathmandu 44600, Nepal*<sup>3</sup>*Research Center for Applied Science and Technology, Kirtipur, Kathmandu 44600, Nepal**\*Corresponding author's Email: adhikaripkr687@gmail.com***Abstract**

Functionalization of chitosan as salicylaldehyde and 2-acetylphenol-based chitosan thiosemicarbazone involving amino group at C2 position of pyranose ring was confirmed by comprehensive characterization by spectroscopic and analytical ways. Both the low molecular weight ( $M_w$ ) chitosan oligosaccharide (CS) ( $M_w < 3000$  Da, degree of deacetylation (DDA) = 87%) and the crab shell chitosan (CCS) ( $M_w = 350$  k Da, DDA = 67%) functionalized thiosemicarbazones were found thermally stable till the commencement of chitosan backbone disruption at 200 °C. The MTT assay profiles showed a conspicuous enhancement in the *in vitro* antitumorigenic and anticancer activity of native chitosan upon its functionalization as phenolic carbaldehyde chitosan thiosemicarbazones. Further, the assays more often revealed a further lowering of cell viability with chitosan oligosaccharide derivatives in comparison to high molecular weight chitosan derivatives, and a lower viability of the MCF-7 cancer cells than the tumorigenic MDCK cells. Both the low  $M_w$  chitosan with high DDA and high  $M_w$  chitosan with low DDA, the chitosan-functionalized salicylaldehyde based thiosemicarbazones, were found to have minimal toxicity with  $IC_{50} > 600 \mu\text{g mL}^{-1}$  against the mouse embryonic normal fibroblast NIH3T3 cells. These results were indicative of more protonation and enhanced anticancer activity of chitosan oligosaccharide derivatives, and preferential cytotoxicity of chitosan biomaterials against the tumorigenic and cancer cells with more negatively charged cell surfaces.

**Keywords:** 2-Acetyl phenol, Anticancer activity, Chitosan, Chitosan thiosemicarbazones, Functionalization, Salicylaldehyde

## Invited Lecture-54

### Surface Functionalisation of Poly (amidoamine) and Poly (propylene imine) Dendrimers for Drug Delivery Applications

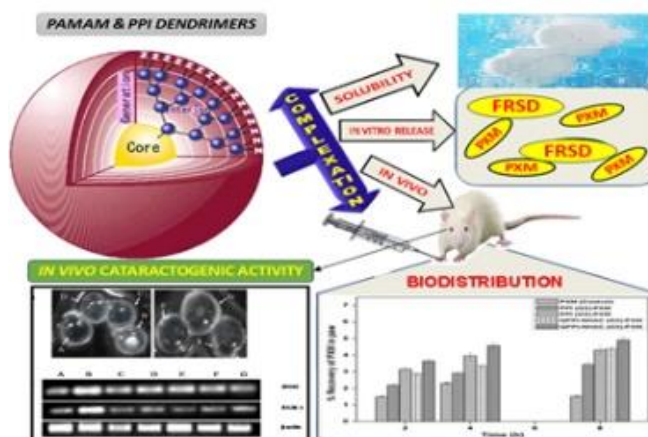
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#### Abstract

Dendrimers are highly branched polymers with tailor making surface functional groups with spherical core-shell nanoarchitecture. They can be synthesised with different generation numbers and based on their size they can be used as diverse nanocarriers for biomedical applications. Currently, surface modification of poly(amidoamine) (PAMAM), poly(propylene imine) (PPI) and poly(ethylene imine) (PEI) has been widely applied for gene and drug delivery. Drugs can be loaded in multiple ways including complexation and/or conjugation to surface functional groups and/or encapsulation inside the core of the dendrimers. We have developed various potential dendrimers through simple surface modifications using poly(amidoamine) and poly(propylene imine) dendrimers and demonstrated them as drug carriers using Piroxicam (PXM) and Furosemide (FRSD) as model drugs and proved an excellent improvement in delivery as compared to the drug molecule alone (without modified dendrimer). The drug carrying potential of functionalised dendrimer has significantly solubilized the PXM drug to the tune of 50 folds and FRSD to the tune of 109 folds compared to its intrinsic solubility and ensured promising loading of drugs. The drug release noticed under *in vitro* conditions from PXM prolonged up to 570 min and from FRSD up to 510 min and hence it becomes suitable for sustained/delayed release. Further, the modified dendrimers in both the cases showed increased cell viabilities on Vero cell lines which are correlated to its reduced cytotoxicity with increased biocompatibility. The potential of drug delivery was established based on the solubility, *in vitro* release and toxicity results. It is noticed that the efficiency of the modified dendrimers in drug delivery application depends on the number of modified functional groups and the degree of complexation of respective drug molecules. Similarly, the efficacy of the developed dendrimer encapsulated curcumin nanoparticles was demonstrated to prevent the selenite induced cataract in wistar rat pups as a model through the expression of pro-inflammatory genes using *in vivo* and human infant lens epithelial (HLE-B3) cells *in vitro* systems. Compared to native curcumin, the solubility increased nearly 345-fold and also the *in vitro* release of curcumin prolonged 17 times. Furthermore, nanocurcumin alleviated cataracts in orally dosed rat pups at 2.5 mg/kg body weight (b.w.) in both pre- and post- selenite treatment comparatively much higher doses (75 mg/kg b.w.) in earlier studies. Thus, the developed non-toxic dendrimer formulations can offset major limitations to their native counterpart with increased solubility, sustained release and increased bioavailability. They prevented oxidant mediated cataract development and hence they are found promising.



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## Invited Lecture-55

### Exploring the Impact of Orientation and Nature of Filler Material on Water Droplet Bouncing: Insights from Molecular Dynamics Simulations

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#### Abstract

This study investigates water droplet bouncing and its underlying mechanisms, focusing on filler nature and orientations (as shown in Fig. 1). Employing molecular dynamics (MD) simulations, we explore three distinct filler shapes (square, rectangle, and cylinder) with varying angles and hydrophobic or hydrophilic properties. We systematically varied water droplet velocity to examine its impact on detachment from the surface.

Furthermore, the nature of the underlying surface itself also warrants attention. The hydrophobic nature of the filler, rather than the surface, exerts a significant influence on this process. Fillers characterized by their hydrophobicity and surface roughness demonstrate a remarkable ability to repel water droplets, preventing excessive spreading and facilitating efficient detachment. This unique trait of hydrophobic fillers leads to a rapid departure of the water droplet from the surface, in contrast to hydrophilic fillers that encourage droplet adhesion and hinder rebound. The interplay between filler properties and water droplet behavior reveals a nuanced relationship, shedding light on the intricate physics involved in droplet-surface interactions.

Surprisingly, filler properties have a more substantial influence on bouncing behavior than surface characteristics in conjunction with velocity. Overall, this research provides valuable insights into the complex relationships among filler orientations, material properties, and droplet velocity in water droplet bouncing. These insights have broad implications for optimizing processes involving water droplets and surfaces, paving the way for further exploration and advancements in related fields.

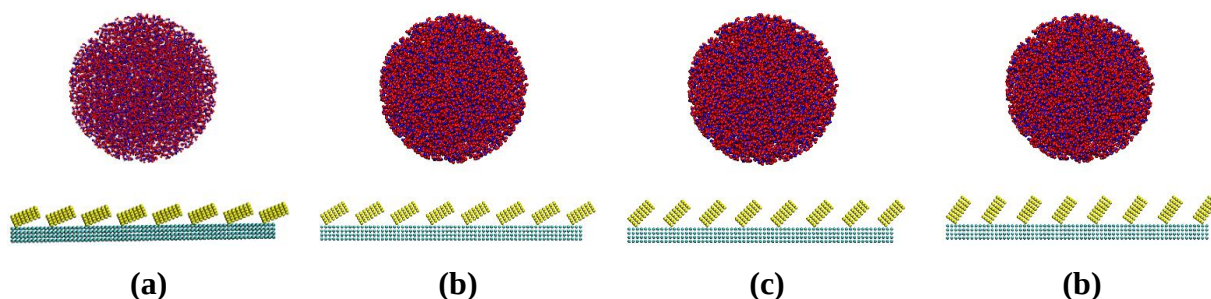


**Fig. 1:** Simulated models of water droplet with surfaces having varying filler orientations of  $\theta$  = (a) 20°, (b) 30°, (c) 45°, and (d) 60°.

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## Invited Lecture-56

### Strained Bronsted Pair Catalysis for Glycoside Bond Formation

Pavan K. Kancharla\*

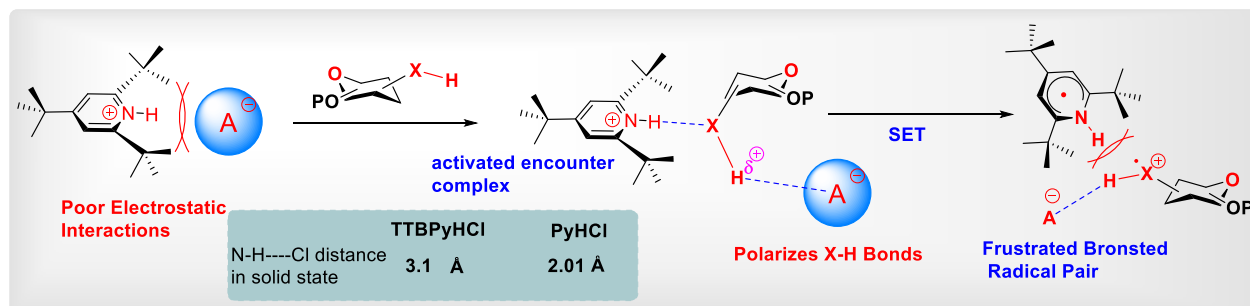
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#### Abstract

Organocatalysis has emerged as a significant tool for organic synthesis over the past two decades. Enormous progress has been made in utilizing the small molecule organocatalysis to control organic reactions' enantioselectivity and diastereoselectivity. Glycosylation is arguably the most significant reaction in carbohydrate chemistry and controlling the anomeric selectivity in glycosylation reactions is of prime importance. Our laboratory is focused on developing new organocatalytic methods for the construction of various glycosidic linkages and controlling the anomeric selectivities. The focus of the talk will be mainly on one of the unique concepts developed in our laboratory, "Frustrated Bronsted-Pair Catalysis" and including some of the other aspects of glycoside bond formation.



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**Invited Lecture-57****Development of Sustainable Ceramic-Based Flexible Composites for  
Advanced Multi-Functional Applications****Debabrata Ganguly and Santanu Chattopadhyay***Rubber Technology Centre, IIT Kharagpur, Kharagpur-721302**Corresponding author's Email: santanu@rtc.iitkgp.ac.in***Abstract**

In the current context of sensitive environmental concerns, including pollution and waste disposal, there has been a growing focus on greener technologies, lower carbon footprints, sustainability, and the principle of exploitation of 3R (Reduce-Reuse-Recycle) s. Additionally, there has been a demand for multi-functional smart materials to address such burning issues. In this presentation, we developed smart multi-functional composites using various ceramic wastes. In one such systems, a smart stimuli-responsive composite was made using white cement and slag in a Hydrogenated Nitrile Rubber (HNBR) matrix. This composite demonstrated notable changes in modulus and volume during wet-dry cycles and also displayed enhanced electrical conductivity and improved radiation shielding characteristics upon adding a meagre amount of carbon black to the system. In other systems, the addition of Silicon Carbide filler significantly enhanced mechanical properties and thermal conductivity, making it suitable for applications that demand lower electrical conductivity combined with higher thermal conductivity, e.g., in applications like in EVs. Magneto-rheological composite systems were also developed featuring ceramic fillers with magnetic properties, which enhanced and helped customize various technical properties in-field depending on the end usage. Liquid silicone rubber displayed advantages over HNBR solution in terms of magnetorheological aspects.

Furthermore, the utilization of various energy harvesting methods like piezoelectric, pyroelectric, thermoelectric, and triboelectric has gained importance. Elastomer composites being flexible and primarily used in places of friction, wear, and tear makes them the most promising candidate in the field of electricity generation through friction. Ceramic waste, including white cement, slag, and MXene, proved effective in the triboelectric cohort, generating considerable units of voltage and current.

These ceramic-based materials have potential applications in lightweight shielding materials, microfluidic valves, printed circuit boards, e-automotive components, magnetorheological devices, magnetostrictive applications, and as triboelectric generators.

**Keywords:** Sustainability, Carbon Footprint, Ceramic Waste, EMI shielding, Electrical & Thermal Conductivity, MR Fluid, Triboelectricity.



## Invited Lecture-58

### Triphenylamine-Anthracene Derivatives based Conjugated Microporous Polymers for Visible Light Driven Photocatalytic Reactions

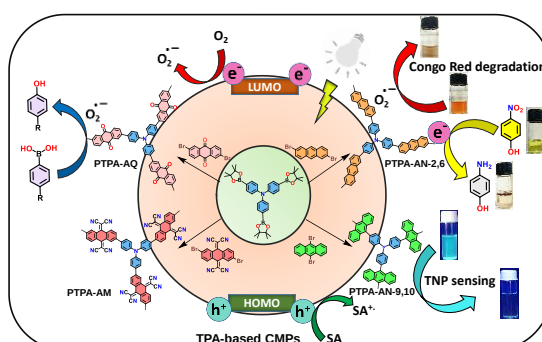
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#### Abstract

Triphenylamine (TPA)-based donor–acceptor conjugated microporous polymers (CMPs) with various anthracene derivatives as acceptors namely 9,10-dibromoanthracene (**AN-9,10**), 2,6-dibromoanthracene (**AN-2,6**), 2,6-dibromoanthracene-9,10-dione (**AQ**) and 2,2'-(2,6-dibromoanthracene-9,10-diylidene)dimalononitrile (**AM**) were synthesized via Suzuki–Miyaura cross-coupling reactions. By changing the acceptor moiety in these CMPs, their Brunauer–Emmett–Teller (BET) surface area and the photophysical properties can be tuned. Thus, higher BET surface areas were obtained for **AQ** (400 m<sup>2</sup>/g) and **AN-2,6** (362 m<sup>2</sup>/g) derivatives as compared to the **AM** (43 m<sup>2</sup>/g) and **AN-9,10** (210 m<sup>2</sup>/g) derivatives due to the effective blocking of the pores. Therefore, the **TPA-AQ** based CMP having higher BET surface area, suitable HOMO–LUMO positions and an optimal band gap (1.94 eV) showed a better visible-light driven oxidative hydroxylation of various phenylboronic acids to phenols with yields up to 96%.<sup>[1]</sup> Interestingly, the **TPA-AN-9,10** based CMP showed bright cyan fluorescence in THF dispersion and exhibited fluorescence-based sensing of various nitroaromatics, with low detection limit of 34 μM and high Stern–Volmer constant of 5.8×10<sup>3</sup> L.mol<sup>−1</sup> for 2,4,6-trinitrophenol.<sup>[2]</sup> On the other hand, **TPA-AN-2,6** based CMP showed efficient photocatalytic reduction of various nitroaromatic micropollutants such as *p*-nitrophenol ( $k = 0.164 \text{ min}^{-1}$ ) and degradation of Congo red from water with ultrafast kinetics ( $k = 0.047 \text{ min}^{-1}$ ) which are much better than most of the previously reported CMPs. These photocatalysts showed high thermal stability and recyclability for at least five cycles without losing their photocatalytic activity significantly.



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## Invited Lecture-59

### Design of multifunctional polymeric carriers 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. 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. However, some non-degradable polymers accumulate in the body resulting in the cytotoxicity and thus the reduction in their gene transfer ability. Even though, low molecular weight polymers, which can be eliminated via kidney is an alternative, exhibits lower colloidal stability and DNA condensation due to their reduced number of electrostatic interactions thus reduced transfection efficiency. As biodegradable polymers are designed to contain a combination of various functional components, it is likely that engineered systems for non-viral gene delivery, especially with the application of biodegradable ester linkage will eventually be constructed. This biodegradable linkage approach to vector development is giving way to a safety profile where low molecular weight polyethylenimines are coupled with diacrylates and sugar alcohol linkers to yield high molecular weight poly (ester amine) (PEAs) with reduced cytotoxicity and high transfection efficiency. 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.

**Invited Lecture-60****Development of fish scales based biocompatible piezoelectric sensor for biomedical applications****Nikhil Dilip Kulkarni, Abir Saha and Poonam Kumari\*<sup>1</sup>**<sup>1</sup>*Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Assam  
781039, India.**\*Corresponding author's E-mail: kpmech@iitg.ac.in***Abstract**

Developing self-powered piezoelectric nanogenerators for biomedical applications is challenging because of toxicity, biocompatibility, and complicated fabrication approaches. Bio-resources are increasingly used to fabricate devices that are ecologically sustainable. Leftover fish scales (FS) in varying quantities were reinforced with Polyvinylidene fluoride (PVDF) matrix to develop highly flexible piezoelectric nanogenerators (PENGs) to gauge their energy harvesting capability. Morphology and structure confirm uniform dispersion of FS particles inside PVDF matrix. Role of FS loading on mechanical and dielectric behavior of PVDF is also investigated. A 56% and 67% enhancement in ultimate tensile strength and Young's modulus values for composite sample over pure PVDF matrix is recorded. PENGs were checked for its piezo response under various loading conditions using human hand (finger tapping, twisting, and bending). A maximum voltage of around 8 V is observed for finger tapping condition. Compressive stress by the human finger is sufficient to drive the biowaste hybrid to generate energy which could be used in biomedical application domains.

## Invited Lecture-61

### Simultaneous bioremediation and bioelectricity generation by an integrated process of PVB-TiO<sub>2</sub> photocatalysis and magnetic-field microbial fuel cell from diesel pollution

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## Abstract

Oil such as diesel can be introduced into the ocean by natural, accidental, and intentional spills. It causes huge damage to the biodiversity. To reduce the environmental impact, an efficient remediation technology should be established. Adding Neodymium-Iron-Boron magnets can enhance the bioelectricity generation for a double-chamber cubic microbial fuel cell (MFC)[1]. An integrated process combining photocatalytic and magnetic-field MFC (MF-MFC) technologies was developed for diesel pollutant bioremediation in our previous study [2]. The synthetic diesel pollutant (500 mg/L) was treated by the photocatalytic system which used the Polyvinyl Butyral Resin (PVB)-TiO<sub>2</sub> sponge cube (2 cm × 2 cm × 2 cm, TiO<sub>2</sub> 1.25 g/L) and illuminated for 3.5 h in the first stage. In the second stage, the chicken manure digester effluent as seed inoculum and photocatalyzed diesel solution as carbon source were fed in the anode, and K<sub>3</sub>[Fe(CN)<sub>6</sub>] 0.05M was used as the cathode in the double-chamber MFC. The MFC was incubated at a temperature of 35°C and fed the diesel solution every 3 days with the sequencing batch model. The results show this photocatalytic and MF-MFC intergradation process can effectively remove the diesel pollutants based on the high COD removal value (85.46±7.96%) and simultaneously generate bioelectricity with an average voltage of 87.10±14.76 mV, average current density of 219.94±37.27 mA/m<sup>2</sup> and average power density of 19.71±6.73 mW/m<sup>2</sup>.

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## Invited Lecture-62

### Interplay of monomer geometries in designing the functionalized microporous thin films for separation

Ketan Patel\*<sup>1,2</sup>

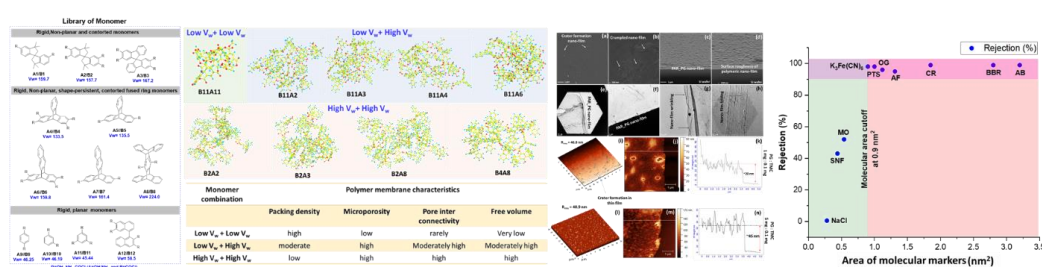
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#### Abstract

Polymeric membranes with enhance mass-transport and solute selectivity are highly anticipated for liquid separation.<sup>1,2</sup> To enable membrane-based separation of a large-scale unit operation, membranes with high mass transport and solute selectivity (permeability-selectivity trade off) becomes essential to process large volume of liquids over realistic membrane area.<sup>3</sup> The present work focuses on increasing mass transfer by enhancing microporosity, reducing the thickness and solute selectivity by increasing crosslinking density of the polymeric membranes. Rigid, non-planner, contorted and shape-persistent monomers that occupy high van der Waals volume ( $V_w$ ) are preferred. As a function of selecting monomers with shape persistent and high van der Waals volume, we intent to restrict conformational mobility in the chain packing, allowed a structure to occupy more steric space. This enables in enhancing microporosity and interconnecting porosity. The correct choice of monomers and polymerization with a reaction kinetics assisted in producing polymeric membrane with the ultra-low thickness ( $\sim 10$ -20 nm) and enhance microporosity. As a result, we observed enhance water mass transport as compared to the state-of-the-art the membrane without compromising solute selectivity.<sup>4-6</sup> Concomitant separation of energy minerals and controlled MWCO also achieved.<sup>7</sup>



**Scheme 1.** Choice of monomer selection based on their van der Waals volume and Computation study of various proposed monomers combination; Thickness; MWCO

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**Invited Lecture-63****Polymer Complexation Theory and Application to IDPs**

**Aritra Chowdhury (2), Souradeep Ghosh (1), Soumik Mitra (1), Arindam Kundagrami (\*1), Benjamin Schuler (\*2)**

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**Abstract**

Polymer complexation, an association of oppositely charged polyelectrolytes, is a fascinating aspect of charge polymers. The thermodynamics of such processes includes an interplay of enthalpy and entropy contributed from several components of the complex system, and it is a challenge to identify the dominant ones which govern the equilibrium of the complexed structures. We describe a general minimal theory of the phenomenon originating from basic polymer physics. In addition, we describe how the theory can be applied to quantitatively explain the experiments on thermodynamics of complexation of intrinsically disordered proteins (IDP).

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## **Invited Lecture-64**

### **Polyhydroxy Alkonates: Sustainable Biopolymers for Future**

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#### **Abstract**

The emergence of global demand for biopolymers is increasing due to the landfill problem and less capability of recycling single-use plastic. Polyhydroxy Alkonate (PHA) is a sustainable biopolymer synthesised from the greener biological route through microbial fermentation. PHA has more environmental impact in terms of biodegradability as compared to polylactic acid (PLA). The inherent properties of PHA, such as Flexibility, Strength, and Thermal stability, make it difficult to use as a potential polymer for different segments of application. Polyhydroxy alkonate is modified through Biological, Chemical, and Physical routes to improve such properties by considering its crucial area of application. Different co-polymers of PHA, like polyhydroxy valerate and polyhydroxy butyrate-co-3-hydroxy hexanoate, are synthesised through biological routes to produce flexible PHA. These kinds of biopolymers have similar properties as compared to flexible commodity biopolymers. It opens up its application in medical devices and packaging material. Similar properties can be achieved through chemical and physical modification routes with the addition of different plasticizer, co-agents, and chain extension additives.



## Invited Lecture-65

### Predicting polymer properties using graph-based multi headed attention transformers with hierarchical aggregation

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#### Abstract

The development of new materials, especially polymers, is crucial to meet the demands of evolving technological applications. Traditionally, material discovery has heavily relied on time-consuming and costly experimental approaches rooted in the structure-property relationship. In contrast, computational methods such as Density Functional Theory (DFT) and Molecular Dynamics (MD) have limitations, particularly in handling the intricate multi-scale nature of polymers. In recent years, deep learning (DL) has emerged as a promising avenue for efficient and accurate material property prediction. In this work, we introduce graph-based techniques to predict the glass transition temperature (T<sub>g</sub>) demonstrated over a comprehensive dataset comprising of 7174 monomer SMILES (simplified molecular input line entry system) strings spanning the entire polymer space. Our approach is based on a graph-based transformer model with a trainable multi-headed attention block that transforms the graph representation using hierarchical aggregation and top-K pooling. The monomer depicted by SMILES strings, a popular Molecular representation scheme, is initially converted into a graph data structure, with node and edge embeddings representing atom and bond properties, respectively. After multiple training iterations, the node features of the final layers capture aggregated information from neighboring nodes and connected edges, weighted by trained attention weights. Consequently, the new representation space of the graph transformer effectively captures the relationships between the structure and the property, extracting crucial features such as backbone rigidity/flexibility important for T<sub>g</sub> prediction. Through rigorous evaluation, our model demonstrates a commendable R<sup>2</sup> value of 0.83 in the regression task for T<sub>g</sub> prediction, underscoring its efficacy in capturing essential information from the SMILES representations with a reduced inference time. The study further reveals that graph-based transformer representations for polymers yield predictive performance comparable to the widely adopted extended-connectivity circular fingerprint (ECFP) representation, such as Morgan fingerprints, for T<sub>g</sub> prediction.

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## Invited Lecture-66

### Wheat Stalk and Rice Husk Based Fibers for Reinforcement in Mechanical Strength, Surface Modification and Degradability

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Agricultural waste based microcrystalline cellulose (MCC) and nanocrystalline cellulose (NCC) can be used as fabricating fibers for polymer composites. In this work, MCC and NCC were extracted from the wheat stalk and rice husk by thermochemical and mechanical processes and compounded with a biodegradable polymer, the poly(butylene adipate-co-terephthalate) (PBAT) by melt extrusion process with variation in wt. fraction of the filler. The composites were characterized by fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), tensile strength, thermogravimetric analysis (TGA), contact angle measurements and gel permeation chromatography (GPC). These composites were found to increase in tensile modulus. The composites were found to be hydrophilic which induced high degradability of the materials on soil composting. The results were coherent with the wetting behaviour of PBAT on MCC (see Fig. 1). The lignocellulosic waste used in this project is one of the solutions to reduce plastic consumption, reinforce mechanical strength and induce biodegradability in the PBAT composites for smart applications.

**Keywords:** biodegradable polymer, scanning electron microscopy (SEM), gel-permission chromatography (GPC), tensile modulus, microcrystalline cellulose (MCC)

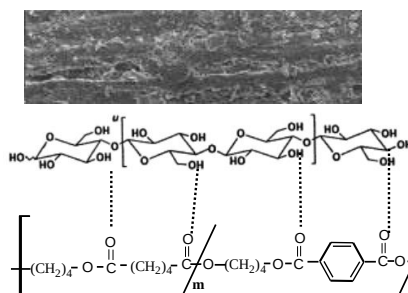


Fig.1 H-bonding involved during wetting of fibers with PBAT

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## Invited Lecture-67

## Dynamics of Nano Particle containing Polymer Thin films

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## Abstract

We show the influence of nano particles on the stability of thin homo-polymer films as well as their influence on modulating the phase separated morphology of thin polymer blends. First we show how addition different nano particles suppress the spontaneous instability in ultra thin polymer films engendered due to Disjoining pressure. While the instability gets completely suppressed above a critical Nano particle concentration ( $C_{NPC}$ ), the films do evolve and dewet at lower particle concentrations. We show that the length scale of dewetted features vary non monotonically with  $C_{NP}$  arguably due to complex interplay between polymer – particle interaction as well as alteration in viscosity of the polymer. We also show how different routes to engender dewetting, that is thermal annealing above glass transition temperature or solvent vapor exposure, the dewetting length scales might change. We also show how addition of nano particles alter the dynamics and stability of a polymer bilayer. We subsequently discuss how the as cast morphology of spin coated immiscible polystyrene/poly(methyl methacrylate) (PS/PMMA) thin films of different thickness ( $h_E$ ) and composition ( $R_B$ , volume ratio of PS to PMMA) changes due to addition of nano particles. We observe that addition of AuNP barely alters the generic morphology of the films with  $R_B = 3:1$ . In contrast, the presence of the particles significantly influences the morphology of the films with  $R_B = 1:1$  and  $1:3$ , particularly at higher  $C_{NP}$  ( $\approx 10.0\%$ ). X-Ray Photoelectron Spectroscopy (XPS) and X-Ray Reflectivity (XRR) of some samples reveal that the AuNPs tend to migrate to free surface through PS phase, thereby stabilizing this layer partially or fully (depending on  $C_{NP}$ ) against dewetting over a surface of adsorbed PMMA layer and influencing the as cast morphology as a function of  $C_{NP}$ .

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**Invited Lecture-68****Synthesis, characterization and properties of high-performance copoly(ether-imide)s via polycondensation reaction****Murugesan A\* and Loganathan***Polymer Science Engineering Lab, Department of Chemistry, Sri Sivasubramaniya Nadar**College of Engineering (Autonomous), Chennai, India- 603 110**\*Corresponding author E-mail: murugesana@ssn.edu.in***Abstract**

High-performance poly(ether-imide)s were synthesised with different derivatives of bisfluoro-diimide and bisphenol-A monomers via polycondensation reaction. Different rigid (imide) and flexible ( $-\text{C}(\text{CF}_3)_2-$ ,  $-\text{C}(\text{CH}_3)_2-$  and  $-\text{O}-$ ) functional moieties were incorporated in the bisfluoro-diimide monomers. Incorporation of bisfluoro-diimide and flexible linkages enhance the thermal and mechanical properties of the polymers, which could be improve the properties of high-performance polymers in the field of material science. Synthesis high-performance polymers were characterized using FT-IR, NMR, DSC and TG analysis. The structure of polymers and monomer were confirmed by NMR and FT-IR analysis. Thermal behaviours ( $T_g$  and degradation temperature) of the polymers were examined using DSC and TG analysis. The results suggested that the thermal properties have been enhance by the incorporation of effective functional moieties in the structure of polymer back-bone. Based on the result suggested that poly(imide-ether)s is an effective polymers for the preparation of material applications.

**Keywords:** Bisfluoro-diimide; Poly(imide-ether)s; Polycondensation; Incorporation; Flexible:**References**

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## Invited Lecture-69

### Polymeric additives applied to petroleum refineries

Dr. T. Senthilkumar\*<sup>1</sup>

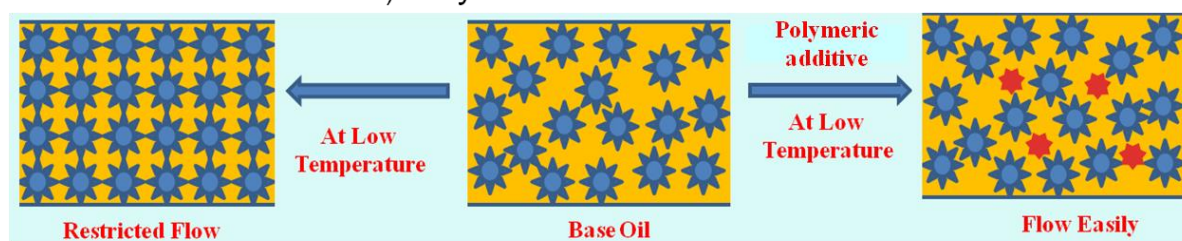
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#### Abstract

Polymeric additives, especially design, synthesis, and physicochemical characteristics, have enormous potential in addressing the challenges faced by petroleum refineries. In all the phases of petroleum refining, polymers are used as additives or fluids to enhance production efficiency, transporting in pipelines, and product upgradation.<sup>[1]</sup> I discuss the design and synthesis of various polymeric additives used as pour point depressants (PPDs), wax inhibitors, and bitumen modifiers. The performance evaluation of the polymeric additive formulations helps establish new correlations between the physicochemical properties and performances in a specific application. The knowledge of synthetic polymeric additives is applied to petroleum refineries to address the following key issues: (i) lowering the pour point of crude oil to improve the pipeline flow at low-temperature zones,<sup>[2]</sup> (ii) inhibiting the wax crystal growth by preventing the deposition of paraffin waxes on surfaces in contact with crude oils (iii) upgradation of viscosity grade base bitumen (VG10) to higher bitumen grades bitumens (VG20, VG30 and VG40).

#### a) Polymeric additives as PPD



#### (b) Polymeric additives as bitumen modifier



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## Invited Lecture-70

### Development of Discotic Liquid Crystals for the Application in Organic Electronic Devices

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#### Abstract

Liquid crystalline semiconductors seem to be a bright option for the application in organic electronics considering their good solubility, processability and excellent reproducibility along with the ease of purification.<sup>1</sup> Additionally, the addressability of their molecular alignment and self-healing of defects in the thin films by thermal annealing provides a major advantage over amorphous polymers and organic single crystals. This presentation reports several shape anisotropic molecules that stabilize columnar (Col) phases. Col phases are formed by the one-dimensional stacking of the disk/star/polycatenar shaped molecules, leading to an intimate overlap of the central aromatic units. The molecular design of these molecules is such that, they are able to form spontaneous columnar organization in response to stimuli like solvent and/or temperature. The Col phase provides a one-dimensional (1D) pathway for the migration of charge carriers akin to 'molecular wires'. Our present focus is on the application of such Col LCs in enhancing the efficiency in organic electronic devices such as organic solar cells (OSCs), organic light emitting diodes (OLEDs)<sup>2-3</sup> and organic field effect transistors (OFETs).<sup>4-5</sup> As expected, the gaps between the expectation and the performance of the molecules in such devices are to be addressed, which we are working on through the experience. In this presentation, I will be discussing our recent research on naphthalene and perylene based molecules.<sup>6-7</sup>

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## Invited Lecture-71

### **Challenges and Opportunities for Thermoplastic Elastomers (TPEs) as Potential Alternative to Conventional Rubbers in terms of EV, Renewable energy and other Technologies**

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#### **Abstract**

Thermoplastic elastomers (TPEs) are one of the fastest growing polymeric materials which combine the elastic and mechanical properties of cross-linked rubbers with the melt processability of thermoplastics. Styrenic thermoplastic elastomers like S-B-S block copolymers are most important class of soft TPEs. On the other hand, thermoplastic polyurethane (TPU) is the most important class of hard TPEs. The primary advantage of a TPE is its ability to reuse and recycle the production scrap and waste. Thermoplastic vulcanizates (TPVs) or dynamic vulcanizates are a special class of TPEs, produced by simultaneous mixing and crosslinking of a rubber with a thermoplastic. TPVs represent the second largest group of soft thermoplastic elastomers, after styrenic based block copolymers. The unique characteristics of TPEs make them very useful and attractive alternatives for conventional elastomers in a variety of markets, such as automotives, footwear, buildings and constructions, wires and cables etc. Automotive accounts for about 45 % of global polymer consumption. Within the automotive sector, ownership patterns are shifting toward electric vehicles (EVs), autonomous vehicles (AVs), semi-autonomous vehicles (semi-AVs), and various forms of ride sharing have entered the market. These shifts have created new functional roles for automotive polymers. The new opportunities will result from broader performance requirements, the need to bring smart functionality (smart polymers), more versatile fabrication process technology and shortened/shifting supply chains. Thermoplastic elastomers (TPEs) have attracted significant interest in the last few years, owing to their enormous specialized properties and wide range of applications.



## Invited Lecture-72

### Design and Development of $\pi$ -Conjugated Polymers as Efficient Probes for Detection of Environmentally and Biologically Concerned Analytes

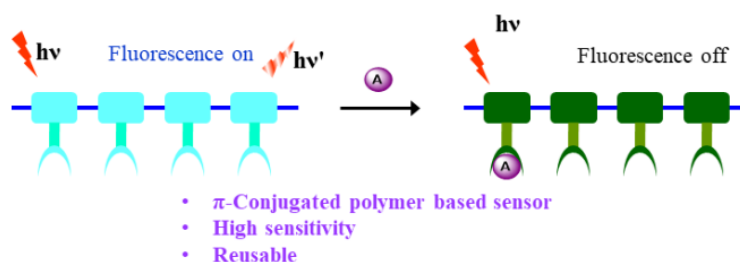
Chinmoy Behera,<sup>1</sup> Dipanjan Giri<sup>1</sup> and Sanjib K. Patra\*<sup>1</sup>

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#### Abstract

The  $\pi$ -conjugated polymers have been realized as emerging multifunctional materials for their technological promising future. Taking the advantage of 'molecular wire' effect, the emissive and electron rich *p*-type  $\pi$ -conjugated polymers with suitably desinged receptor units can act as effective, highly sensitive and excellent chemosensor for trace detection of environmentally and biologically concerned analytes. In this regard, we have developed a new class of  $\pi$ -conjugated luminescent polymers employing the 1,2,3-triazole group as appendage and in main chain in the polymer backbone as cheap and efficient chemical sensors for detecting explosives such as nitroaromatics (NACs).<sup>1,2</sup> Furthermore, we have also successfully designed and synthesized efficient fluorescent  $\pi$ -conjugated copolymers following the A-*alt*-B architecture having pendant coordinating sites such as diketopyrrolopyrrole segments. The resulting Fe(III) and Cu(II)-metallopolymers can efficiently and selectively detect biologically relevant molecules such as ATP and glycine.<sup>3,4</sup> In the presentation, our effort in judiciously designing the  $\pi$ -conjugated polymeric probes and its systematic studies for detection of environmentally and biologically concerned analytes will be discussed.



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## Invited Lecture-73

### Comparison of Cyclic Deformation Behavior between $\kappa$ -Carrageenan and Agarose Hydrogels

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#### Abstract

Polysaccharides form hydrogels via networking with intermolecular aggregation of helical fractions. It is known that two polysaccharides from seaweeds  $\kappa$ -carrageenan and agarose have different gelation mechanisms regarding interaction between the helices. Since  $\kappa$ -carrageenan is an anionic polysaccharide, the aggregation of the helical fractions becomes stable by the shielding effect of counter-cation species on the electrostatic repulsions between the helices. On the other hand, agarose is a neutral polysaccharide and the aggregation takes place by means of hydrogen bonding. This study have compared the cyclic deformation behavior of  $\kappa$ -carrageenan and agarose hydrogels to elucidate the relationship between the network structures of polysaccharide hydrogels and their mechanical properties. Both hydrogels have been prepared at different initial concentrations on cooling, and then the stress-strain curves during cyclic deformations have been measured at the same polysaccharide concentrations. It has been found that Young's modulus decreases with the initial concentration of  $\kappa$ -carrageenan hydrogels<sup>[1]</sup>, while the relation between Young's modulus and the initial concentration is opposite for agarose hydrogels<sup>[2]</sup>. Samples other than high- $\kappa$ -carrageenan hydrogels tend to show residual strains in each cyclic deformation, as shown in Fig.1. Optical rotation and IR measurements have been also performed to examine the effects of the initial concentration on the mechanical properties specific to each polysaccharide.

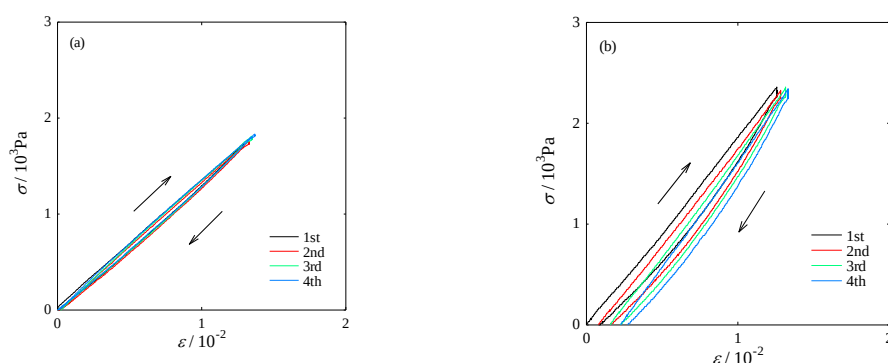


**Figure 1:** Stress-strain curves of four cyclic deformations for (a) high- and (b) low- $\kappa$ -carrageenan hydrogels.

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## Invited Lecture-74

### Nanoparticle-incorporated carbon foam derived from flexible polyurethane foam as a multifunctional material

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#### Abstract

Carbon foam (CF), a porous, lightweight, 3D interconnected, electrical conducting, open-cell, glassy foam, is mainly derived from carbonization of polymeric precursors. CF is mainly used in battery electrodes, cathode emission, metal slag filters, etc. The extraordinary properties of these foams can further be harnessed in modern technological applications such as electromagnetic interference (EMI) shielding, supercapacitor electrodes, and oil-water separation through nanofiller incorporation. In the present study, various nanofillers such as fumed silica (FS) and graphene oxide (GO) were incorporated into open-cell polyurethane (PU) foam followed by carbonization to prepare CF. The resulting foams exhibited improved electromagnetic interference (EMI) and microwave absorption properties. The CF was also *in-situ* coated with (i) NiCo<sub>2</sub>O<sub>4</sub> by hydrothermal method and (ii) poly(dimethyl siloxane) (PDMS) oil by vapor deposition. The NiCo<sub>2</sub>O<sub>4</sub> coating resulted in the deposition of nanoneedle-like structures, leading to the increased surface area of the porous foam. The NiCo<sub>2</sub>O<sub>4</sub>-coated foam showed improved EMI shielding and microwave absorption properties. The NiCo<sub>2</sub>O<sub>4</sub>-coated foam showed excellent charge storage capacity, with capacitance retention of ~97% after 10,000 galvanostatic charge/discharge cycles. On the other hand, PDMS oil coating, vapor-deposited at 320 °C for 14h resulted in a superhydrophobic CF with a water contact angle of 168°. The superhydrophobic foam displayed excellent oil-water separation properties.

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## Invited Lecture-75

### Designs of Bio-inspired Polymeric Functional Coatings

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#### Abstract

The nature-inspired wettabilities that either extremely repelled or allowed effortless sliding of different liquids (oil/water) in air or underwater are with immense potential for various prospective applications. In common practice, essential chemistry and appropriate topography that conferred the special liquid wettabilities were mostly and generally achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issues. In the literature, very few designs are capable of providing durable bio-inspired wettability—but fabrication processes remain generally complex. Moreover, the integration of various other relevant physical properties with such durable liquid wettability is highly challenging to achieve. Hence, design of robust bio-inspired liquid wettability following a simple fabrication process that would allow to integrate different and relevant physical properties is utmost important for various fundamental and applied contexts. Related to this, recently, our research group has extended 1,4 conjugate addition reactions between amine and acrylates at ambient conditions to develop tolerant and functional liquid wettability.<sup>1-10</sup> The controlled tailoring of different bio-inspired liquid wettability from the porous and chemically reactive interfaces—following strategic post modulation of the chemically reactive interfaces will be discussed in this invited lecture. A strategic association of adequate crosslinkers can provide a highly tolerant and hard superhydrophobic coating on geometrically complex and soft materials. Such a simple chemical approach also allowed to reveal important fundamental aspects related to different bio-inspired wettability. Taking advantage of the durable bio-inspired wettability, the synthesized nature inspired interfaces were successfully applied to demonstrate some practically relevant applications—including controlled release of small molecules, oil/water separation, water harvesting, sensing, anticounterfeiting etc.<sup>1-10</sup>

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## **Invited Lecture-76**

### **High Performance Adsorbent Materials**

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#### **Abstract**

The application of high-performance Adsorbents materials in solving environmental problems has recently sparked a lot of attention due to their unique physical and chemical properties, which make them advanced to traditional adsorbents. The ability to functionalize materials by attaching specified functional groups to their surfaces enables the formation of a variety of designed High Performance Adsorbents materials for the removal of organic and inorganic pollutants. This work contains a thorough investigation and analysis of the application of sophisticated adsorbent materials in the treatment of contaminated wastewaters containing various oils. It will also concentrate on recovery methods and possible solutions for nanomaterial regeneration and reuse.

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## **Invited Lecture-77**

### **Ion exchange membranes: a potential battery separators**

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#### **Abstract**

Ion-exchange membranes are inherited with a fixed positive or negative charge on the polymer matrix and an exchangeable cation or anion. Their utility in battery applications lies in the tuning of charge density as well as porosity. We have developed different types of membranes from thermoplastic engineering polymers by solvent as well as melt extrusion methods and demonstrated their best applicability in battery and alkaline hydrogen generation applications.

In a vanadium redox flow battery, oxidative stability and mitigation of vanadium crossover are serious concerns. The issues were addressed by a charge-tuned polypropylene-based membrane where Donnan exclusion was dominant. The best membrane showed 70% capacity retention at a 200 mA/cm<sup>2</sup> current density in 100 charge-discharge cycles. The membrane developed by melt extrusion showed over 85% capacity retention in 200 charge/discharge cycles at 100 mA/cm<sup>2</sup> current density with an average capacity decay of 0.03% per cycle, 99% columbic efficiency, and 76% energy efficiency. In an identical experimental condition, Nafion-117 showed merely 24% capacity retention. The calculated diffusion coefficients for V<sup>3+</sup> and VO<sub>2</sub><sup>+</sup> were  $1.41 \times 10^{-8}$  and  $7.62 \times 10^{-8}$  cm<sup>2</sup>/s, respectively, about one order lower than Nafion-117, suggesting the formation of dense membranes without the formation of microvoids, the inherent issue of solvent-cast membranes.

**Invited Lecture-78****Biopolymer-based Films and Coating as Sustainable Alternative to Non-biodegradable Plastic Packaging for Shelf-life Extension of Fruits and Vegetables****Santosh Kumar***Department of Food Engineering & Technology**Central Institute of Technology Kokrajhar**Corresponding author's Email: [s.kumar@cit.ac.in](mailto:s.kumar@cit.ac.in)***Abstract**

Fruits and vegetables are highly perishable and they have short postharvest shelf-life because of their continuous respiration and transpiration even after harvesting. In addition, ripening and reactive oxygen species (ROS) that produced during electron transport can directly damage cells and reduce the quality of fruits and vegetables. About one-third of the fruits and vegetables are wasted every year due to mechanical damage, microbial spoilage, and physiological processes after harvesting, particularly during handling, storage, packaging, or transportation. Edible coating of fruits and vegetables is an inexpensive, simple, and effective method, which provide barrier on food surface resulting in decreasing respiration rate, moisture loss, and microbial spoilage, and therefore maintaining quality and extending the shelf-life of coated fruits and vegetables. In this context, biopolymer-based edible coatings are gaining importance in prolonging postharvest shelf-life of fruits and vegetables due to their edible, biodegradability, compatibility with food and environment-friendly nature. Biopolymers are obtained from renewable resources such as plants (starch, cellulose, other polysaccharides, proteins), animals (proteins, polysaccharides, lipids), microbes (xanthan, dextran, pullulan) and polymers synthesized chemically from naturally derived monomers (polylactic acid). Incorporation of natural fillers or nanomaterials improves functional properties such as antimicrobial and/or antioxidant activities of the biopolymer-based composite. Plant-extracts and compounds derived from plant (e.g., essential oil) are effective in imparting antimicrobial and antioxidant properties to biopolymer-based composites. Therefore, the biopolymer based edible coating incorporated with natural active compounds is the sustainable way that can prevent the weight loss, retain firmness, and reduce the load of food-borne pathogens, and thus can extend the shelf-life of the coated fruits and vegetables from a few weeks to a month.



**Invited Lecture-79****Recent developments in polyurethanes for biomedical stress sensor applications****S. N. Jaisankar**

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**Abstract**

Thermoplastic polyurethane (TPU) is a class of versatile elastomeric materials that offers both flexibility and high-performance mechanical properties in coating, film, sheet, footwear and adhesives. Recently, polyurethanes (PU) are playing a significant role in power generation, sensor and battery applications. The piezoelectric sensors can capture the tiny amount of energy generated by human movements like shoulder, hand, foot and arm. We have assembled these sensors with TPU as one component along with PLA, polyamide and other materials and studied piezoelectric measurements. A series of polyurethane elastomers were synthesized using aliphatic isocyanates and sustainable polyols in combination with PLA. The molecular weight in the range of 1600-1700 PLA diol was used. The morphology, melting, glass transition and crystallinity were studied using various characterization techniques. These materials meet specific criteria: favourable biocompatibility, non-toxicity and overall harmless to the human body and in applications such as wearable sensor devices.

## **Invited Lecture-80**

### **Molecular Modeling and Simulation of Biodegradable Polymeric Materials**

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#### **Abstract**

The molecular modeling and simulation studies of some biodegradable polymers and their nanocomposites are reported here. In particular, studies on the nanocomposite of poly (vinyl alcohol) (PVA) and keratin-derived peptides for application in direct methanol fuel cell (DMFC) and studies on biodegradable polymer nanocomposites containing cellulose nanocrystals (CNC) are discussed. Low methanol permeation through the polyelectrolyte membrane and good ionic conductivity of the membrane are two essential properties for the selection of membranes for DMFCs. We have investigated the effect of the presence of peptide chains derived from keratin on the methanol permeation and ionic conductivity of PVA-based matrix in alkaline medium through molecular dynamics (MD) simulations. In order to conduct the simulations, a molecular model of the nanocomposite was developed by packing several chains of PVA in a cubic simulation box with keratin-derived peptide (5 wt %) and water. The geometry optimized and equilibrated polymer nanocomposite model is used for longer MD simulations to investigate the methanol diffusion and hydroxyl-ion (OH<sup>-</sup>) mobility in the system. We have also employed molecular simulations on simplified representations of biodegradable polymer-CNC systems to study the effect of CNC on the mechanical and gas barrier properties of the polymer. The dimensions of actual CNCs (length ~ several 100 nanometers and diameter ~ several tens of nanometers) make them computationally intractable through atomistic simulations. In this work, we have considered crystalline cellulose nanorods of significantly smaller dimensions dispersed in amorphous polymer matrix. The effect of crystalline cellulose on the mechanical and gas barrier properties of the polymer has been studied.

## Guest Lecture

# Advancing Additive Manufacturing Through Innovations in Large Area Liquid Crystal Display (LCD) Vat Photopolymerization

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**Keywords:** 50-inch LCD VPP, Quasi collimated backlight, Local dimming, Mass customization

## Abstract

Large-area LCD vat photopolymerization (VPP) presents a novel additive manufacturing approach, enabling high-speed printing of large, high-quality polymer parts. Our researchers have engineered customized 32-inch and 50-inch LCD-based VPP systems leveraging advanced backlight design and controls. Key innovations we have implemented include a quasi-collimated UV LED backlight module we refined to achieve 86% uniformity across the LCD screen area and a regional light control circuit utilizing local dimming to control the unwanted curing and reduce material waste. Together, these optimize print resolution while preventing unwanted polymerization for superior edge quality. The systems also implement a modified build platform with holes we introduced to improve resin flow and automated controls for refilling. Comparative testing shows our 50-inch LCD VPP system achieving a superior production rate compared to the commercially available VPP machines. The large build area and enhanced curing precision empower mass customization applications like simultaneously printing variable shoe sole designs. Our advances help transition LCD-based VPP techniques into higher speed, higher volume, mass-customizable industrial additive manufacturing.

## **Oral Presentations**

## Recyclable photoRDRP towards Dual Stimuli-Responsive Functional Diblock Copolymers

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### Abstract

Inspired by the natural responsivity of the biomolecules, researchers have developed various stimuli responsive polymers for applications in engineering and biomedical fields. These external stimuli includes temperature, pH, light, ultrasound, and electron transfer (redox changes).[1-3] Although there are multiple reports on single stimuli responsive polymers, till date, it is still extremely challenging to develop multi-stimuli responsive polymers with the essential response-specificity, tunability and control over their orthogonal and combinatorial response due to the absence of facile synthesis protocol, presence of color/odor/toxicity in the final polymer arising out of inefficient catalyst/chemical removal and scalability issues. This has severely limited their wider use.

In this work, we will present the development of magnetically recyclable iron-catalyst mediated photoRDRP of *tert*-butyl methacrylate (TBMA) and synthesis of well-defined dual-stimuli (pH/temperature) responsive poly(methacrylic acid)-*block*-poly(poly(ethyleneglycol) methacrylate) diblock copolymers via iron-mediated sequential photoRDRP, followed by post-polymerization modification. Both the catalyst and the polymerization media (ionic liquid) are recyclable upto multiple cycles making the protocol industry friendly.

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## **Large-area 2-D supramolecular polymers via controlled assembly**

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### **Abstract**

2-Dimensional (2-D) materials such as graphene, MoS<sub>2</sub> and others have unique features like high carrier mobility, superconductivity, good thermal conductivity, etc. which make them ideal candidates for optoelectronic applications.<sup>1</sup> However, achieving such a highly ordered arrangement over large area for organic systems is still challenging.<sup>2</sup> Here we have synthesized and studied a novel derivative of thiazolothiazole (TzTz),<sup>3</sup> an electronic and redox-active core as a central aromatic unit and amide group as a side group for hydrogen bonding interaction. This monomer was observed to assemble into micron sized, highly crystalline 2-D sheets in an appropriate composition of solvents. The combination of high crystallinity of the TzTz core and the directional hydrogen-bonding seems to dictate the formation of 2-D sheets. Finally, we have explored the potential of these 2-D sheets in optoelectronic application.

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## Liquid/liquid interface assisted in situ synthesis of conducting polymer/MnO<sub>2</sub> composites

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### Abstract

Liquid/liquid (L/L) interfaces provides a versatile platform for the manipulation of self-assembled nanoparticles (NPs). Particle-laden fluid interfaces gained immense attention for applications such as sensing, catalysis, optics and many more. Moreover, liquid/liquid interfacial techniques have been widely accepted for the synthesis of thin films of single or multi-component materials. The liquid/liquid interfacial synthesis strategy possesses an exquisite feature of the in-situ synthesis of thin films of complex materials that can be directly obtained from the reaction mixture without any post processing techniques. The immobilization of nanoparticle assemblies at liquid/liquid interfaces is primarily achieved by the aid of cross-linking agents or catalysts. An efficient method to develop nanoparticle assemblies at liquid/liquid interface is by in-situ synthesis of NPs embedded in polymer thin films. Thus, the potential capability of fluid interfaces in thinning the polymeric sheets to few nanometers can be utilized for the synthesis of composite sheets composed of high surface energy NPs with less particle agglomeration.

Herein, we report a mechanistic investigation of the self-assembly of in-situ grown ultra-thin polypyrrole/manganese dioxide (PPy/MnO<sub>2</sub>) sheets by a facile route of water/chloroform interface assisted method. The method confirms the successful encapsulation of ~6 nm MnO<sub>2</sub> NPs in ultra-thin PPy sheets devoid of any particle agglomeration. Hence, in the presentation, the unique synthesis strategy, interfacial polymerization and their capanbility in tuning the physico-chemical properites and their potential applications will be discussed.

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## Biocompatible Chitosan-Based Stimuli Responsive Nanogel for Drug Delivery

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### Abstract

Stimuli-responsive nanogels have attracted significant attention worldwide for biomedical applications, particularly for drug delivery systems. Nanogels are capable of high drug loading capacity and delivery of drug controlled and targeted manner into the affected sites. In current study, biocompatible and biodegradable nanogels based on chitosan (CS) and methacrylic acid (MAA) have been synthesized and characterized. The synthesized nanogels have been characterized by Fourier transform infrared spectroscopy (FTIR) for chemical analysis, field-emission scanning electron microscopy (Fe-SEM) for structural morphology, dynamic light scattering(DLS) for particle size distribution and particle stability, and X-ray diffraction (XRD) for crystal structure. Cytotoxicity study was done to detect the toxicity and biocompatibility of nanogels. It was observed that the nanogels are spherical in shape and in the size range of 100 – 150 nm. Moreover, nanogels are pH responsive due to presence of -COOH groups in MAA and -NH<sub>2</sub> groups in chitosan. High drug absorption capability, nano size, and stimuli-responsiveness (pH-sensitive) (to regulate drug delivery) of nanogels offer great potential for controlled and targeted drug delivery applications.

*Key words: nanogel, chitosan, pH-responsive, drug delivery*

## Development of Steric-Hindrance ROP Strategy for $\beta$ - Sheet Polypeptides and their Block Copolymers

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Synthetic polypeptides are typically made via ring opening polymerization of N-carboxy anhydride monomers of natural L-amino acids. Majority of the synthetic examples are reported based on  $\alpha$ -helical polypeptide owing to their excellent solubility and ability to form high molecular weights.<sup>1</sup>  $\beta$ -Sheet forming polypeptides are one of the least explored synthetic systems because to their uncontrolled precipitation during polymerization; thus, the resultant heterogenous ROP process inefficient to produce  $\beta$ -sheet block copolymer nanoarchitectures in the literature.<sup>2</sup> Recently, we have developed a steric-controlled ROP strategy by cleverly using *t*-butylbenzene unit as structure directing-cum-solubilizing agent and this methodology was successfully demonstrated to wide range of  $\beta$ -sheet L-amino acid residues<sup>3</sup>. In this new process, the growing polymer chains adapt  $\alpha$ -helical conformations in the propagating fronts to impart excellent solubility for homogeneous polymerization with excellent controlled over “living-characteristics”. The post-polymerization de-protection enabled the restoration of  $\beta$ -sheet secondary structures in the high molecular weight polypeptides. This ROP process was successfully demonstrated for three  $\beta$ -sheet forming polypeptides such as poly(L-serine), poly(L-cysteine) and poly(L-tyrosine). These new *t*-butylbenzene functionalized polypeptides were found to be readily soluble in tetrahydrofuran and chloroform, etc, and they were produced in high molecular weights having  $M_n = 32$  kDa with dispersity  $D \leq 1.3$ . ROP kinetics were studied by real-time FT-IR and <sup>1</sup>H-NMR to determine the actual content of the secondary structures in the propagating chains. This process was expanded to polymerization induced self-assembly (PISA) to yield stable polymer emulsions for in-situ encapsulation of different dyes such as curcumin, HPTS, Nile red, rhodamine B, near IR-780, and anticancer drug doxorubicin, etc for biomedical applications. The newly developed steric-hindrance ROP approach could be useful for exploring new polypeptide architectures for long-term impact in polymer science and technology.

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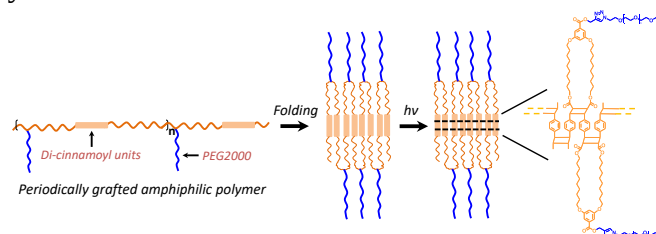
## Photo-cross-stitching of Folded Periodically Grafted Amphiphilic Polymers

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### Abstract

Periodically grafted amphiphilic polymers (PGAPs) are systems carrying hydrophobic alkylene backbone segments and hydrophilic polyoxyethylene (PEG) pendant segments, located at precisely periodic intervals. It was established in our lab that these PGAPs although have random coil conformation in good solvent, will undergo zigzag folding upon introduction of non-solvent for one of the segments, in a manner so as to collocate the alkylene segments at the center and the PEG segments on either side; it was observed that independent crystallization of both the backbone and pendant segments helped stabilize the folded structure.<sup>1</sup> Subsequently, we demonstrated that inclusion of mesogens either within the backbone or pendant segment also lead to the formation of folded chains permitting a precise control of the distance between the mesogenic layers;<sup>2,3</sup> these studies demonstrated that periodically grafted polymers could be an interesting design strategy to selectively locate desired functional units within well-defined layers in a bulk polymer



As proof for folding of PGAPs in solution, we first prepared a *periodically clickable polyester* carrying a di-cinnamoyl ester unit within the hydrophobic backbone segment; this polymer was clicked with PEG-azides of different molecular weights (750, 1000 and 2000), as depicted in the above schematic. Several studies were conducted to probe the formation of the folded conformation with increasing solvent polarity; the photodimerization process of the dicinnamoyl units within the polymer backbone is evidently *feasible only when the chain is folded in a zigzag fashion*, which brings the cinnamoyl units in close proximity to permit the reaction. Hence, we examined the photodimerization process as a function of solvent polarity to gain an understanding of the folding process, which provided us some valuable insights into solvent induced conformational transition in such PGAPs. Furthermore, we showed that, when PEG2000 segments are installed, the cross-stitched folded chains remain in solution even after complete cross-stitching, suggesting that they have transformed into single-chain polymer nanoparticles (SCNPs). I shall discuss the design, synthesis, and photo-cross-stitching of this interesting class of PGAPs and explore some of their potential applications.

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## A sustainable method for development of natural fibre based flexural composite: A step toward leather alternative

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### Abstract

A new method of manufacturing flexible composite has been developed by using cellulose-protein fibre blended needle punched non-woven structure and suitable chemical formulation of natural rubber, sulphur dispersion, accelerator, activator, stabilizer, natural filler antioxidant. Scoured proteinous wool fibre was used in different blend proportion with bleached cellulosic ramie fibre (ramie: wool= 80:10 and 80:20) for making non-woven structure having grammage of around 250 g/m<sup>2</sup>. One side of the developed fibre reinforced flexible composite was spray coated with optimised formulation of pigment and polyurethane in two phases (base coating and top coating), followed by hot-pressing and wax polishing. Physical properties like abrasion resistance, tensile strength, tear strength, puncture resistance, permeability and porosity of the developed product have been examined and compared with a marketed artificial leather and wet blue goat leather having same thickness and weight. The developed leather alternative presented tensile strength values 30% smaller than the natural goat leather, and both presented similar values of tear strength. Extensibility of the developed composites was within 23-27% whereas natural leather showed 70% extensibility. Ramie-wool reinforced rubberised flexible composites have shown 20-25% more thickness recovery as compared to the only ramie based flexible composites in dynamic loading test. Developed composite products were scientifically characterized by scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) analysis and compared with marketed synthetic leather. Biodegradability and antimicrobial property of the developed product were also examined as per standard test methods. Besides, commercialization prospect of the product with cost analysis also has been represented in the current context.

**Keywords:** Cellulose, Flexible composite, Natural leather, Natural rubber, Sustainability

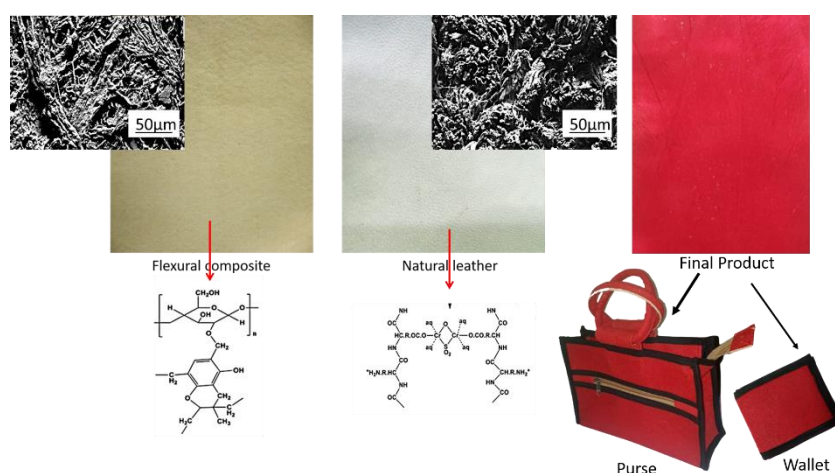


Fig 1. Developed Flexible composite and different product from it

## Fabrication, characterization and degradation of carbon dot modified electrospun scaffolds

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### Abstract

Development of fibrous and/or porous scaffolds from biodegradable and biocompatible polymers has played a significant role in advancing various fields in biomedicine. Here, we developed carbon dot modified cellulose acetate (CA)-scaffolds by electrospinning using a binary solvent mixture. The blended electrospun scaffolds were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetry (TGA) and water contact angle (WCA) to investigate the influence of carbon dot modification. The obtained scaffolds exhibited uniform, bead-free, and random orientation with an average diameter of 300 nm. The SEM micrographs showed that addition of CD benefits formation of well interconnected porous fibrous network structure. A study on degradation under UV irradiation and soil burial tests revealed that the carbon dot modified nanofiber scaffolds were more susceptible to degradation compared to plain CA scaffolds. This was especially shown by the great decrease in the degree of substitution (DS). This deacetylation is an important rate determining first step during degradation of CA. The degradation process was monitored by the changes in molecular weight and the decrement in degree of substitution (DS) was calculated using integral peaks from nuclear magnetic resonance (NMR) spectra. The hydrophobic nature of the scaffold was changed to hydrophilic due to surface erosion by aging and especially the deacetylation process. The carbon dot-modified porous CA scaffolds may, thus, provide a promising option for the production of biodegradable scaffolds suitable for multiple applications.

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## The Novel Indegenious Ziegler-Natta Catalyst for Ultra-High Molecular Weight Poly- $\alpha$ -olefins as Drag Reducing Agent

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### Abstract

Almost 93% of raw oil is transported by pipelines worldwide. Transporting oil through pipelines has some challenges like long distance, large pipe diameter, high energy consumption, corrosion and pressure drop. Pressure drop is caused by the flow turbulence. Currently DRA's (Drag Reducing Agents) are used for the transport of crude oil, light products and heavy oils worldwide through pipelines. DRA reduces the frictional pressure within the flow of pipeline. It decreases the amount of energy lost in turbulent formation which ultimately helps to increase the flow. Increasing the flow rate, throughput capacity and flexibility of pipelines makes DRA most valuable components in petroleum industry. Ultrahigh molecular weight poly- $\alpha$ -olefins (i.e., poly-1-hexene, poly-1-octene, poly-1-decene and poly-1-dodecene) are extensively used as a drag reducing polymers. The ultra-high molecular weight poly- $\alpha$ -olefins are synthesized by Ziegler-Natta catalyst.

This work represents synthesis of novel Ziegler-Natta catalyst comprising bio-based donor/modifier. The synthesized Ziegler-Natta catalyst has evaluated for alpha olefin polymerization. The Ziegler-Natta catalysts has non-toxic, environment friendly internal electron donor and afford production of ultra-high molecular weight poly- $\alpha$ -olefins. The obtained polymer formulation tested for drag reduction of hydrocarbon feed & it has shown 18 to 20 % performance.

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## Starch/Polyvinyl Alcohol (PVA) Blended Bio-Films from Potato Peels: Preparations and Physicochemical Properties

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### Abstract

Starch was extracted from peels of *Solanum tuberosum* (potato) and glycerol plasticized starch based bioplastic as well as its blends with polyvinyl alcohol (PVA). The physicochemical properties such as water absorption, biodegradable properties and acid-base resistance were investigated. The FTIR spectra of synthesized starch and commercial starch indicated the successful extraction of starch from the potato peels. The FTIR spectra of starch based bioplastics/PVA blend showed the peak at  $2924\text{ cm}^{-1}$  that showed the good compatibility between bioplastics and PVA. In the water absorption properties, pure glycerol plasticized bioplastic showed a high amount of water was absorbed in the concentration variation of plasticizer (glycerol). It showed short time degradation in soil burial tests as compared to the other concentration of glycerol plasticized bioplastics. Further, in the acid-base resistance test, it was resisted from complete degradation in acid and base at about 46 hours while the sample was dipped in the same concentration of acid and base solution. Likewise, the starch based bioplastic/PVA blend indicated that high composition of starch containing blend showed long duration (~50 hrs) in water absorption test.

**Keywords:** starch, bioplastic, polyvinyl alcohol, water absorption, blend



## Nitroxide free radical containing bis-indolyl polyurethane dendrimers as potential cytotoxicity for induces cell cycle arrest in breast cancers.

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### Abstract

Nitroxide free radical polyurethane dendrimers up to third generation were obtained through the end-capping of bioactive bis-indole based polyurethane dendrimers containing with stable 4-hydroxy-2, 2, 6, 6-tetramethylpiperidin-1-yloxy (TEMPO). The end-capping was achieved by a single-step urethane interchange reaction between blocked isocyanate end groups and TEMPO. The structural veracity of the radical dendrimers prepared were checked using <sup>1</sup>H NMR, <sup>13</sup>C NMR, FT-IR, and MALDI-TOF-MS spectral techniques. The absolute molecular weight of the dendrimers was determined by the SEC-MALLS technique. A triplet with a nitrogen hyperfine splitting constant of 15.7 G at g = 2.0046 exhibited by the TEMPO radicals in the EPR spectrum. On the other hand, to determine the role of the nitroxide radical polyurethane dendrimers effects in various cancer cell-lines for cytotoxicity and cell cycle analysis.

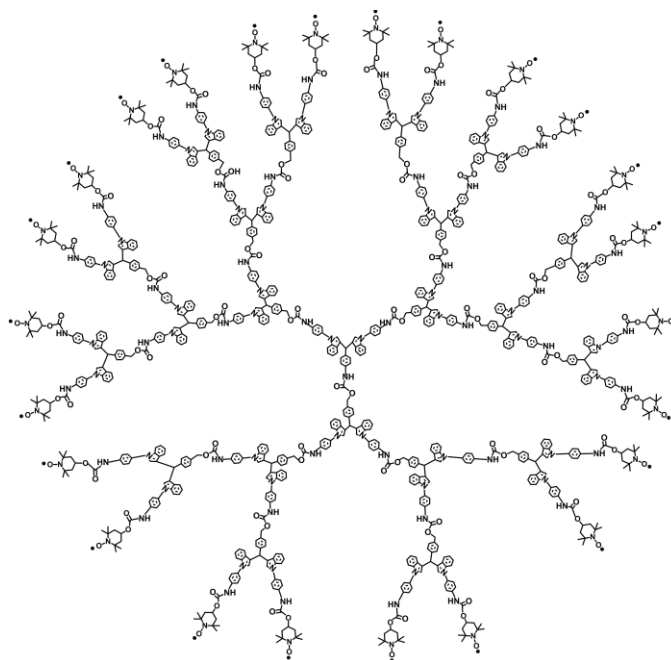


Fig.1. Structure of TEMPO end-capped bis-indolyl G3 polyurethane dendrimer.

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## Isothermal Crystallization Kinetics of Thermoresponsive Shape Memory PCL-PDMS-PCL Triblock Copolymer Films

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### Abstract

In this study, Polycaprolactone (PCL) of variable chain length and constant polydimethylsiloxane (PDMS) segment were used to synthesize the shape memory triblock photocrosslinked copolymeric films. The effect of PCL chain length on thermal and shape memory properties are analysed for PCL-PDMS-PCL triblock copolymeric films. Discrete crystal morphology is observed with increase in PCL chain length by optical microscope and X-ray diffraction. Differential scanning calorimetry (DSC), in both isothermal and non-isothermal modes, is used to assess thermal characteristics. With an increase in PCL chain length, triblock polymer crystallinity and melting point rise. Avrami and Lauritzen-Hoffman (LH) models are used to analyze the isothermal crystallization kinetics of triblock PCL-PDMS-PCL copolymeric films. Avrami model results instructed that PCL crystals were growing in three dimensions in copolymer films. Longer crystallization times, a greater energy barrier, and changes in the crystal growth rate of the PCL block were all caused by the inclusion of the PDMS block. These changes in turn affected the shape fixity and shape recovery ratio accordingly.

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## 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; fibbers 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 a useful tool for a successful failure analysis. A typical chromatogram obtained from a heart-cutting method is presented in Fig 1.

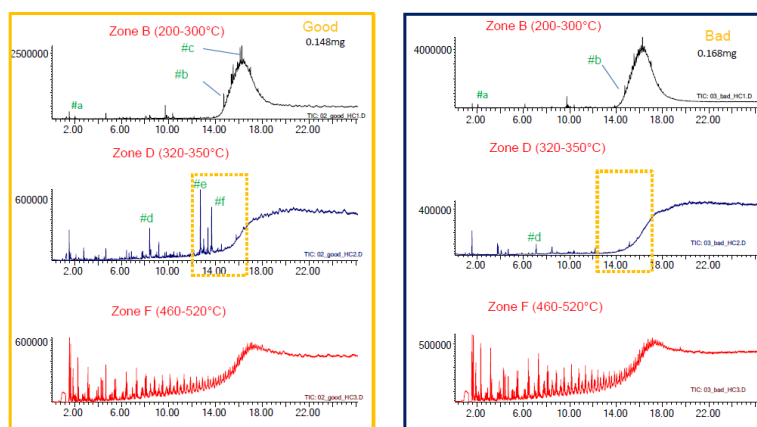


Fig 1 Heart-cut chromatogram of good and bad rubber from Diaphragm

## Tailoring of 3D Bioprinted PLA/MBG Scaffold with Rapid Apatite Crystallization and Enhanced Cytocompatibility for Bone Tissue Regeneration

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### Abstract

In recent years, bone tissue engineering has emerged as a promising solution for treating bone defects resulting from various factors such as trauma, infection, and surgical procedures. To overcome these limitations, our current study focuses on the development of hybrid scaffolds using poly (L-lactic acid) (PLA) and mesoporous bioactive glass (MBG) in a 30:70 weight ratio, mimicking the composition of natural bone. After preparation of bioink with suitable rheology, printing parameters were optimized for development of 3D printed PLA and PLA/MBG composite constructs with a hierarchical pore structure suitable for bone tissue engineering. The work provides insight into challenging aspect of 3D printing with such high content of inorganic component i.e, MBG. The obtained pore range of 500–700  $\mu\text{m}$ , indicating their macroporous nature is conducive to optimal bone cell growth. Mechanical analysis demonstrated that the PLA/MBG composite scaffold exhibits superior compressive modulus and yield strength compared to neat PLA, the mechanical characteristics obtained for the 3D printed PLA/MBG scaffolds tends to match natural cancellous bone. *In vitro* bioactivity assessment revealed the rapid formation of apatite crystals, achieving a Ca/P ratio of 1.66 equivalent to natural bone mineral within the 3<sup>rd</sup> day of simulated body fluid (SBF) treatment. The 3D bioprinted PLA/MBG composite scaffold demonstrated promising outcome in terms of cell attachment, proliferation, mineralization, and gene expression when assessed through *in vitro* biological evaluations using MG-63 osteosarcoma cells. Consequently, the 3D bioprinted PLA/MBG scaffold holds potential as an implant for applications in bone tissue engineering.

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## Isocyanate-Free Poly(hydroxyurethane)s from Vanillin-CO<sub>2</sub> derived Cyclic Carbonates

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### Abstract

Polyurethanes are an important class of polymers that finds numerous applications in various sectors.<sup>[1-3]</sup> The synthesis of these polymers entirely depends on fossil fuel and involves using hazardous chemicals such as isocyanates.<sup>[4,5]</sup> Herein, we report the synthesis of a series of polyhydroxyurethane (PHUs) via the polymerization of fully renewable cyclic dicarbonates derived from biomass and CO<sub>2</sub> with a series of diamine compounds. Kinetics of polymerization was studied and the chemical structure of synthesized cyclic dicarbonate and PHUs was confirmed by FTIR and NMR spectroscopy (<sup>1</sup>H, <sup>13</sup>C). Further, the molecular weights of the developed system were determined by gel permeation chromatography (GPC), and we have observed the highest molecular weight of M<sub>n</sub> is 5500 g/mol. Moreover, the thermal properties of PHUs were analyzed by differential scanning calorimeter (DSC) and thermogravimetric analysis (TGA) and found out all PHUs are thermally stable above 210°C. The current methodology, avoiding toxic reagents and using renewable resources from biomass and CO<sub>2</sub>, makes this approach an attractive and greener pathway to developing PHUs networks.

**Keywords:** Poly(hydroxyurethane), vanillin, CO<sub>2</sub>, cyclic dicarbonate.

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## Hierarchical GO-g-PANI Nanocomposites by Oligomer-Initiated Controlled Polymerization of Aniline for electrochemical Storage

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### Abstract

Presently, supercapacitors have gained an important space in energy storage modules due to their extraordinarily high power density, although they lag behind the energy density of batteries and fuel cells.<sup>1</sup> Electrodes are the most important component of a supercapacitor cell. The electrode performance significantly depends on the available surface area, porosity and conductivity of the component materials, and thus nano-structuring of the electrode is an elegant approach for fabrication of high performance supercapacitors. Recently we have synthesized hierarchical graphene oxide-g-polyaniline nanocomposites with a controlled nanostructure of uniformly oriented one dimensional (1D) polyaniline (PANI) nano cylinders over two dimensional (2D) graphene oxide (GO) surfaces.<sup>2</sup> PANI chains are grown from the GO surface attached oligoaniline units using oligomer initiated controlled polymerization (OICP) of aniline in aqueous acidic medium.<sup>3</sup> The developed method involves a generalized approach, which holds potential for applications on various nano surfaces irrespective of their dimensionality or nature. The synthesized nanostructured materials show further organization to generate unique, highly porous three-dimensional (3D) microstructures. These are presumably generated via supramolecular organization by the in situ developed higher oligoaniline nucleates, followed by controlled growth of polyaniline chains from them. Nanocomposites containing supramolecularly organized macroporous, three-dimensional microstructures have shown remarkably improved specific capacitance as high as 965 F/g (1 A/g) compared to 442 F/g (1 A/g) for the noncovalently attached uncontrolled nanocomposite under similar conditions.

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## Enhancing Properties of Poly(3-hydroxybutyrate) Aerogels Through Thermally Induced Structural Transitions

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### Abstract

Poly(3-hydroxybutyrate) (P3HB), a prominent microbial biopolymer in the polyhydroxyalkanoate (PHA) family, stands out for its rapid biodegradability, minimal toxicity, and biocompatibility. P3HB and its copolymer demonstrate two crystal modifications: the stable  $\alpha$ -form, achievable through melt or solution processing, and the metastable  $\beta$ -form induced solely by stretching P3HB films (Figure 1).<sup>1,2,3</sup> Herein, we fabricated P3HB aerogels by the freeze-drying process of P3HB gels prepared by both TIPS and NIPS methods. The as-fabricated aerogels exist in the  $\alpha$  form of P3HB. We investigated thermally induced crystal-to-crystal phase transition during the heating process of  $\alpha$ -form aerogel. DSC thermogram of P3HB aerogel showed an endotherm followed by an exotherm during heating prior to the melting. Around 120 °C, a significant alteration occurred in the SAXS pattern, accompanied by the emergence of a new scattering peak associated with the reorganization of the lamellar structure. The 2D WAXS patterns revealed the appearance of the  $\beta$  form above 120 °C and the lattice dimensions, crystallite sizes, and crystallinity were derived from the WAXS patterns. To further clarify the observed transition in the DSC thermogram, Raman and FTIR measurements were carried out. It is evident that the thermodynamically stable  $\alpha$ -form partially transformed into the  $\beta$ -form just prior to the melting temperature. Both  $\alpha$  and  $\alpha + \beta$  aerogels showed fibrillar morphology and the resultant  $\alpha + \beta$  aerogels exhibit remarkably improved mechanical, oil-water separation, and sound absorption properties.

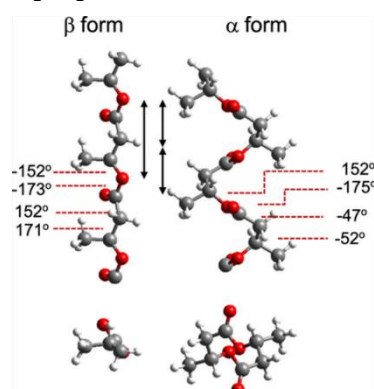


**Figure 1.** Chain conformations of  $\alpha$ - and  $\beta$ -forms of P3HB

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## A dual-functional smart coating to combat catheter-associated urinary tract infections

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### Abstract

Infectious diseases present a grave danger to human health and impose a substantial burden on the global economy. The rapid rise of drug-resistant pathogens, coupled with their contamination of hospital supplies and invasive medical equipment, has led to the proliferation of hospital-acquired infections (HAIs). Among these HAIs, urinary tract infections (UTIs) stand out as one of the most prevalent. Catheter-associated urinary tract infections (CAUTIs) alone affect a staggering 150 million individuals annually. To compound matters, bacteria can adhere to catheter surfaces and form resilient biofilms, leading to encrustation. Conventional treatment approaches have proven ineffective against CAUTIs due to the circulation of drug-resistant pathogens and their impenetrable biofilm formations.

In our research, we have devised a non-covalent antimicrobial dual-active smart polymer nanocomposite coating, known as Antimicrobial Polymer Nanocomposite (APN), specifically designed for urinary catheter surfaces. This remarkable coating is comprised of a two-component organo-soluble formulation consisting of a quaternary antimicrobial polymer and zinc oxide nanoparticles. Applying this coating to various surfaces proved simple and efficient. APN demonstrated the ability to eradicate a wide range of multidrug-resistant bacteria responsible for CAUTIs, including *E. coli*, MRSA ATCC 33591, and even highly pathogenic fungi such as *Candida* spp. Moreover, APN effectively inhibited the formation of bacterial biofilms on coated surfaces. The coating exhibited membrane disruption capabilities and triggered the generation of reactive oxygen species (ROS) within bacterial cells. Given the alarming prevalence of community-acquired and nosocomial infections, the development of effective coating strategies to combat deadly pathogens is an urgent necessity. In the light of this, our easy-to-apply antimicrobial coating, APN, represents a significant breakthrough in the field of coatings for tackling CAUTIs. Its development marks a substantial contribution to the fight against these infections, offering a promising solution for the future.

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## Terpene-Derived Sustainable Elastomers through RAFT-Mediated Miniemulsion Polymerization

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### Abstract

Elastomers and elastomeric materials are fundamental in various industries such as automotive, construction, electronics, footwear, adhesives, and biomedicine. Shifting from conventional petroleum-based elastomers towards sustainable options has become imperative. This investigation concentrates on producing eco-friendly elastomers using biosourced terpene monomers. The synthesis involves copolymerizing terpene monomers with glyco-based or bio-based (meth)acrylate monomers using RAFT-mediated miniemulsion polymerization. This method ensures precise control over molecular characteristics and a narrow range of resulting copolymer dispersities. The terpene element contributes elastomeric traits, while the glyco/(meth)acrylate part enhances material robustness. Mechanical scrutiny underscores the impressive performance and recyclability of these bio-based elastomeric materials.

Furthermore, the synthesized polymeric materials exhibit noteworthy film-forming abilities and transparency. An MTT assay evaluating biocompatibility indicates the material's potential in biomedical applications, such as patches and catheter pipes. This research showcases the feasibility of crafting terpene-derived bio-based elastomers through RAFT-mediated miniemulsion polymerization. By presenting an environmentally conscious alternative, this elastomeric material paves the way for sustainable and biocompatible biomedical uses.

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## Multifunctional nanogels to cure drug-resistant bacterial infections and attenuate bacterial antigen responsive hyper-inflammation

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### Abstract

Infections caused by bacterial pathogens remain a major threat in global healthcare. Emergence of antimicrobial resistance (AMR) to the available antibiotics, and the staggered status of development of new antibacterials compel newer paradigms for anti-infective therapy.<sup>1-3</sup> Such notorious infections are often reported to lead to sepsis, systemic inflammatory response to infection, with case made for the pathogenic role of excessive immunity, the so-called 'cytokine storm'.<sup>4</sup> These are often associated with numerous hospital acquired infections such as pneumonia, cystic fibrosis etc. with high morbidity worldwide. The bacterial co-infection and secondary infections were widely observed during the COVID-19 pandemic often accompanied by hyperinflammation owing to the presence of excessive proinflammatory factors, for instance, LPS.<sup>1,3</sup> To tackle these challenges, we have engineered modular antibacterial nanogels to treat the drug resistant infections and control associated hyperinflammation. These nanogels are able to scavenge bacterial antigens, neutralise them and therefore minimise the production of different pro-inflammatory cytokines. The optimised biocompatible nanogel due to their multifaceted mechanism of action, rapidly kills wide range of Gram-negative superbugs with >5 log reduction in the bacterial titre. Most importantly, it was able to eliminate difficult-to-treat infections such as intracellular infections and disseminate bacterial biofilms, unlike the conventional antibiotics. To the best of our knowledge, no such nanogels are reported with dual pronged ability to counter biofilm mediated complicated infections and regulate the cytokine storm associated with it. These therapeutic nanogels bear immense potential to be developed as intranasal or systemic therapy to treat different infections and attenuate hyperinflammation.

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## Development of MMT-cellulose-PVA films containing banana bract anthocyanins for smart milk packaging applications

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### Abstract

In the present work, an eco-friendly, smart material with pH sensitivity has been developed for milk packaging applications. Cellulose-Montmorillonite (CEL-MMT) reinforced PVA films have been made by adding different weight percentages of CEL-MMT to PVA films into which anthocyanin-rich banana bract extract (BBE) was added to develop pH-responsive films. The hydrogen bonding interactions between BBE and the modified cellulose matrix resulted in the formation of iceberg structures[1]. The films were characterized by FTIR, FESEM, TGA, XRD, and UV-Vis spectroscopic techniques. The hydrophilicity of the material was assessed by water contact angle measurements. The biological activity studies were performed to evaluate antibacterial behaviour against *E-coli* and *S. aureus*. The mechanical property measurements were done using Universal Testing Machine. The weight of CEL-MMT to be added to the PVA matrix to obtain desired characteristics such as high water contact angle and high elongation was optimised. The developed film material exhibited significant colour changes when exposed to different pH conditions, indicating its potential to reveal spoilage of the material packed. The colour change of the packaging material indicating spoilage of the material packed was also checked with real milk samples. The antibacterial behaviour of the packaging film was observed to be better than the commercial polythene ziplock packet. The results indicate the potential use of anthocyanin-rich banana bract extract-loaded CEL-MMT reinforced PVA as a green and sustainable alternative to commercially available petroleum-based packaging materials.

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## Investigation on PMMA-SiO<sub>2</sub> coating on SS316L using Sol-Gel method for biomedical applications

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### Abstract

Bio-material SS-316L coated using an organic and inorganic hybrid coating of polymethyl methacrylate (PMMA) and silicon dioxide (SiO<sub>2</sub>) is being attempted in the present investigation with crosslinking agent 3-aminopropyl tri-ethoxy silane (APTES). The solvent-gel method and dip coating with varying percentages of SiO<sub>2</sub> (i.e., 0.5, 1 and 1.5 wt.%) are used for surface modification. Fourier transform infrared spectroscopy (FTIR) at 1000-1250 cm<sup>-1</sup> reveals the crosslinking of silicon and PMMA. The coatings created on SS-316L are homogenous, transparent, free of defects when seen macroscopically. A good crystallinity and presence of coated material can be seen from the XRD and microstructure analysis of coated surface. The PMMA coating with 1.5 wt.% SiO<sub>2</sub> has the most apatite crystals deposited on surface as observed for seven days of immersion on simulated body fluid (SBF). These findings provide cogent link that coating SS-316L with SiO<sub>2</sub> promotes bone bioactivity, and that PMMA+1.5 wt.% SiO<sub>2</sub> coatings can be employed in biomedical applications. Results reveals that a sustainable coating solution for improved bioactivity in medical applications and surgical equipment.

**Keywords:** Bioactivity; Microstructure; PMMA-SiO<sub>2</sub> coating; Sol-Gel method; Surface modifications

## Development of Bio-based Polycarbonate: A Route towards Sustainability

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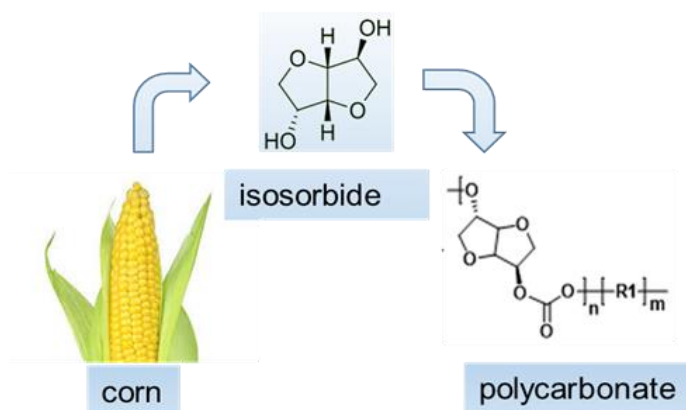
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### Abstract

The continuous depletion of fossil-based feedstock and excessive emission of carbon dioxide (CO<sub>2</sub>) has affected ecological environment and has become a significant concern. One way to overcome these problems is to adopt and develop novel green chemical processes based on renewable resources (biomass, CO<sub>2</sub>, etc.) and replace the conventional chemical processes with high energy consumption and pollution and realize the transformation and upgradation of the chemical industry. Traditionally, Polycarbonate (PC) is conventionally synthesized from phosgene and bisphenol A (BPA) and; the use of BPA has been forbidden in food packaging and medical equipment, especially in children's milk bottles, owing to its chronic toxicity.

The proposed work focuses on synthesizing isosorbide-based polycarbonates using a CO<sub>2</sub> derived carbonate molecule such as dimethyl carbonate, diphenyl carbonate, etc. having high molecular weight have been synthesized via non-phosgene route using newly found economically viable metal-containing homo- as well as heterogeneous catalyst systems. Notably, designed catalyst system showed better performance compared to other well-known metal catalyst even at mild reaction conditions. In addition, the synthesized polycarbonate shows better optical clarity reflected by its low haze value and high glass transition temperature. Overall, an effort has been made to develop a bio-renewable polycarbonate which is an initiative undertaken towards net zero emissions by 2070, the target set by Govt. of India.



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## **PVDF/TMDs-An Advanced Piezo-Polymer with High Piezoelectric Performance for Energy Applications**

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### **Abstract**

The development of wireless and MEMS technologies in contemporary life has resulted in an ongoing increase in energy consumption and environmental problems. These gadgets run on batteries, which might affect how well they work. So, it is becoming more and more important to have a green energy generating devices that can provide the energy without harming the environment. These gadgets have the ability to draw power from ambient sources that are already present in our surroundings. Numerous materials exhibit piezoelectricity, encompassing piezoelectric ceramics and piezoelectric polymers. However, each possesses distinct advantages and limitations. This research endeavours to address these challenges by developing and characterizing an energy harvesting device based on semiconductive filler-incorporated piezoelectric polymer. This approach aims to surmount the drawbacks associated with battery-operated portable and wearable electronics. The study focuses on PVDF, a preeminent piezoelectric polymer, and a 2D transition metal dichalcogenide as a semiconducting filler. This selection is motivated by their eco-friendliness, self-poling behaviour, and wide band gap. The research showcases the piezoelectric response of the resulting nanocomposite piezoelectric materials, fabricated using a spin-coating technique that eliminates the need of additional pre/post activation setups. This endeavour holds potential to contribute to the advancement of sustainable energy solutions for modern electronic gadgets.



## Acetabular liner made of UHMWPE and its composites with inborn plateau finish and their testing

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### Abstract

Ultra-high molecular weight polyethylene (UHMWPE) has been considered as the gold standard of acetabular liner in the metal-on-polymer total hip joint replacements (THR) since 1960. However, the life of a metal-on-polymer total hip arthroplasty (THA) is still limited to 15-20 years, mainly due to excessive wear debris generation during its operation, leading to osteolysis and aseptic loosening. Researchers attempted to improve the tribological characteristics of UHMWPE liners with better processing techniques, bio-compatible reinforcements and superior bearing surface finish. The objective of the present work is to design and develop medical-grade UHMWPE and UHMWPE-MWCNT composite based acetabular liners for THR by an ingenious manufacturing technique for their *in vitro* evaluation using a novel 'Ball-on-Cup' tribometer with a synthesized synovial fluid analogue as the lubricant, following the international guidelines. To achieve the same, processing parameters are optimized to obtain UHMWPE products having the relative density of  $\sim 98\%$  and Vickers hardness of  $\sim 5.0$ , where the latter is further improved by 77% with the reinforcement of 0.25 wt.% MWCNT. After achieving the desired mechanical properties of UHMWPE and UHMWPE-MWCNT samples, rubber moulds of novel design are employed to manufacture the machining-free acetabular liners having plateau finished bearing surface with  $R_a < 100$  nm. *In vitro* wear test of newly developed acetabular liners is performed against stainless steel femoral head using a 'Ball-On-Cup' tribometer, designed and fabricated as per the ISO-14242-3, under a synthesized solution of 2% w/v high molecular weight sodium alginate and 0.75% w/v Gellan gum to create a rheological environment similar to synovial joint. The wear debris obtained from the test rig has a significant morphological resemblance with those retrieved from human bodies while using THA and it is confirmed that adhesive wear and fatigue wear are the leading causes of material loss under *in vitro*. Total volume of wear debris generated from the UHMWPE-MWCNT liner is found to be 52% less compared to that of pure polymer liner with a 33% reduction in linear wear depth. After achieving a significant resemblance in recreating *in vivo* conditions under *in vitro*, it is concluded that UHMWPE-MWCNT may be considered as a potential aspirant for the bearing material in a next generation metal-on-polymer THR in order to increase its longevity.

## Development of Sustainable Smart Shape Stable Phase Change Materials (SSPCM) using Waste

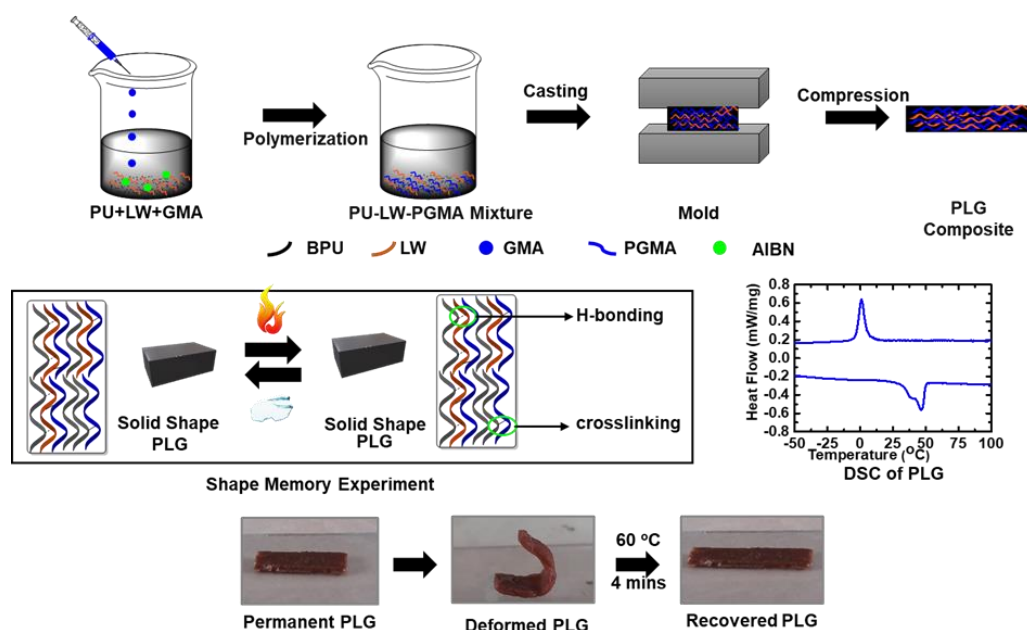
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### Abstract

The accumulation of leather waste (LW) is a global problem due to landfilling. The sustainable use of LW in biodegradable polymer matrices to produce valuable materials reduces landfill waste before and after application.<sup>1-4</sup> By synthesizing a biodegradable polyurethane (BPU) using eco-friendly polycaprolactone (PCL) diol and sustainable castor oil (CO) polyol, yielding 90%, and incorporating tolylene-2,4-diisocyanate (TDI), this study created PL and PLG composites where P, L, and G are BPU, LW, and poly(glycidyl methacrylate), respectively. The role of LW's was elucidated using FTIR and SEM for hydrogen bonding, chemical crosslinking, and interpenetrating network (IPN) formation. Self-healing and shape memory properties were examined in air and water. Thermal properties and shape stability were examined via temperature-responsive TGA, DSC, and leakage study. This research unlocks LW's direct utilization in energy materials, potentially finding application, with its self-healing and 100% shape recovery SSPCM, in sectors demanding high durability and flexibility, such as aerospace and footwear.



## Generation of multicellular tumor spheroids via 3D cell culture utilizing a hydrogel comprising chitosan and allylthiourea

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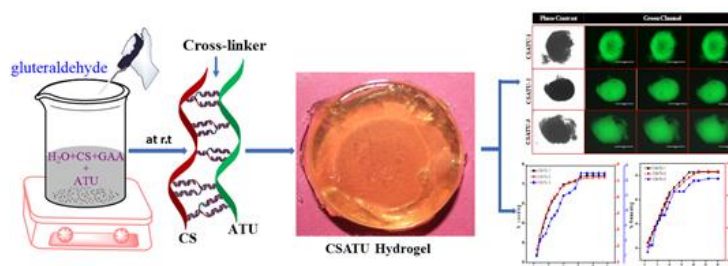
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### Abstract

Hydrogels made with chitosan (CS) biopolymer can undergo mechanical and chemical modifications that can lead to new properties and functions in the biomedical field, which can be used for 3D cell culture as well as the formation of tumor spheroids that mimic the microenvironment of a tissue or organ. Chitosanpoly(allylthiourea) (CSATU)-based hydrogels were synthesized, which exhibit self-healing properties, biocompatibility, nontoxicity, and reasonable mechanical strength. The ratio of chitosan was varied to synthesize a series of CSATU hydrogels viz. CSATU-1 containing (CS : ATU) in a (2 : 1) ratio, CSATU-2 containing (CS : ATU) in a (1 : 1) ratio, and CSATU-3 containing (CS : ATU) in a (1 : 2) ratio. The swelling of all CSATU hydrogels was found to be maximum in a neutral medium. The maximum mechanical strength was demonstrated by the CSATU-1 hydrogel among all hydrogels. However, the CSATU hydrogels were characterized using FT-IR spectroscopy. Furthermore, the CSATU hydrogels have been explored to investigate the biocompatibility of the cells. Our results revealed that the CSATU hydrogels were nontoxic to the T-cell lymphoma and MCF-7 cells. Additionally, all three hydrogels have successfully established the formation of multicellular tumor spheroids. Overall, our present study demonstrated that the synthesized CSATU hydrogels can be used as a promising platform for spheroid development, which has potential applications in tissue engineering and drug development.



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## Binotinylated Stimuli-triggered Degradable Polyurethane for Anticancer Drug Delivery

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### Abstract

Stimuli-responsive drug delivery systems (DDSs) have shown great potential in the diagnosis and treatment of various kinds of diseases worldwide. There are plenty of endogenous stimuli available in tumour cells microenvironment which can be utilized to fabricate smart stimuli-responsive polymers to eradicate cancer. Also, to reduce off-target drug accumulation in non-cancerous cells, receptor mediated targeted drug delivery is always preferred.<sup>[1]</sup>  $H_2S$  is an important signaling molecule which exists in higher concentration in cancer cells due to overexpression of cystathione- $\beta$ -synthase enzyme.<sup>[2]</sup> pH is another parameter which has been utilized extensively for the fabrication of pH-responsive drug delivery vehicle. In tumor microenvironment, intracellular organelles such as endosomes and lysosomes are among those region where pH is in acidic range (4.5 to 6.5). Here, we have developed a pH/ $H_2S$  responsive theranostic self-assembled polymer for cancer cell targeted drug delivery (Figure 1). Attachment of biotin in polymer chain end will enhance the cancer cell specific endocytosis of polymeric drug delivery vehicle. Dansylated segment of the polymer triggers the degradation of the polymer due to the action of  $H_2S$  which further stimulates the drug release from the polymeric micelle. In addition, the trafficking of the polymer in lysosome inside cell further degrades the polymer due to the lysosomal enzyme (esterase) triggered hydrolysis of urethane bonds. Hence, this biotinylated self-assembled pH/ $H_2S$  responsive degradable polymer can serve as a potential drug delivery vehicle for remediation of cancer.

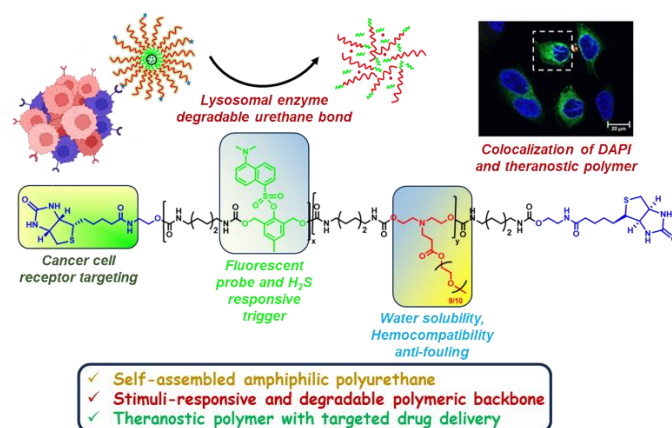


**Figure 1.** Schematic representation of functional polyurethane and its characteristic features.

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## Gels and Fibers of Cellulose ether derivatives for Biomedical Applications

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### Abstract

Smart bio-polymeric bio-materials are now developed at a prolific pace for their use in various biomedical applications like drug delivery, wound healing, scaffolds and implants for tissue engineering and regeneration. Natural polysaccharides (e.g., celluloses and proteins) are gaining an increased interest for researchers to develop newer and novel health care products. However, the major drawback of using bio-polymers is they lack good mechanical properties. In this work, we report synthesis of novel microgels using cellulose ether based derivatives for topical drug delivery of an anti-cancer drug for a site specific application on the skin using water in oil emulsion technique. The microgels were spherical in shape and uniformly distributed with a flower-like morphology. The 5-Fluorouracil drug was successfully incorporated into the microgel matrix. The microscopic images of drug loaded microgels exhibited cell death of cancer cells. Further we electrospun this bio-polymer into nanofiber mats and incorporated Halloysite nanoclay (HNT) into the matrix to understand their morphology, mechanical properties, *in-vitro* and *in-vivo* characteristics and release behaviour of an antibacterial drug. The Halloysite (HNT) loaded fiber materials exhibited very good mechanical properties and showed a potential in wound healing activity by slow and sustained release of the Gentamicin drug. The embedded nanofiber mats also showed very good stability with no scar formation on the wistar rats. These biomaterials provide outstanding properties such as high elasticity, strength, porosity and surface-area-to-volume ratio which can have a variety of applications in the biomedical area.

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## Biomimetic pH-Tunable Strain Stiffening Peptide-Polymer Conjugate: Replicating Biopolymeric Networks to Augment Myogenesis

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### Abstract

In biological system reinforcement due to the internal stress is of utmost significance and forms the foundation of numerous biomechanical pathways and tissue integrity. For example, cells strengthen their contiguous matrix by dragging on collagen and fibrin fibers and molecular motors promote rapid fluidization and dynamic stiffening of the cytoskeleton by pulling thin actin filaments associated with bundles of myosin. Human carcinogen *Helicobacter pylori* (*H. pylori*) controls the pH at the time of colonization in the epithelial layer of the stomach and cellular actin cytoskeleton to form stress fibers and deregulates adhesion complexes to induce changes in cell shape. Herein, we demonstrate a sophisticated synthetic method for creating stimuli-responsive stiffening network of peptide-polymer conjugates that exhibit numerous hierarchical controls. By modulating the pH, dynamic Schiff base crosslinking of semi-flexible peptide fibres with thermo-responsive poly(*N*-isopropylacrylamide) copolymer creates a covalent network. Owing to the lower critical solution temperature (LCST) of the polymer, the conjugates exhibit a macroscopic heat-stiffening response by producing inner stress through a coil-to-globule transition. Moreover, the covalently crosslinked network intensely stiffens in retort to applied shear stress that can be further ramped up in the peptide fibers. Additionally, the hydrogel network promotes enhanced proliferation and myogenic differentiation of C2C12 myoblast cells, suggesting its potential as a promising biomaterial for skeletal muscle tissue engineering. Overall, the synthetic network promotes myoblast differentiation owing to the non-linear mechanical attributes.

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## **Degradable Thiol-ene Networks from Ethyl Lactate-based Polymer for 3D Printing Applications**

**S. Pal<sup>1</sup>, Asha S.K.\*<sup>1</sup>**

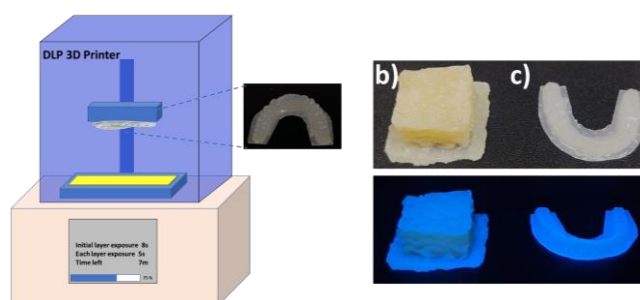
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### **Abstract**

Ethyl lactate is a biobased material obtained naturally or chemically in high yields in the form of ethyl ester of lactic acid.<sup>1</sup> Here, we report an efficient and scalable method for creating a biobased thiol-ene network from allyl poly (acrylate ethyl lactate) (PAEL) and multifunctional thiol via DLP 3D printing. The thiol used in this report is also synthesized from isosorbide, the dehydration form of D-sorbitol, contributing to the overall eco-friendly nature of the resulting thiol-ene network.<sup>2</sup> The properties of these networks can be customized based on the specific type and stoichiometric ratio of the thiol crosslinker employed. This customization allows for a wide range of tunability in both Young's modulus (ranging from 1.75 GPa to 1.03 GPa) and glass transition temperature (ranging from 44 °C to 54 °C) for the PAEL-based networks. Furthermore, these PAEL-based thermosets exhibit good thermal stability, with decomposition temperature ( $T_{d,10\%}$ ) above 350 °C for all the networks studied. Additionally, the research demonstrates the suitability of these resin formulations for resin-based 3D printing, producing 3D-printed parts with good resolution. The study also highlights the hydrolytic degradation properties of these 3D printed parts through ester hydrolysis, showing that PAEL-based resins are highly promising for sustainable rapid prototyping and mass production applications. Overall, this work demonstrates the immense potential of PAEL-based materials as a sustainable source of bio-based resins, providing the prospect of the development of specialized thermosetting compounds required for a variety of applications, such as 3D printing and biomaterials.



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## Resorbable PLA/nHAp composites for Orthopedic Fracture Fixations

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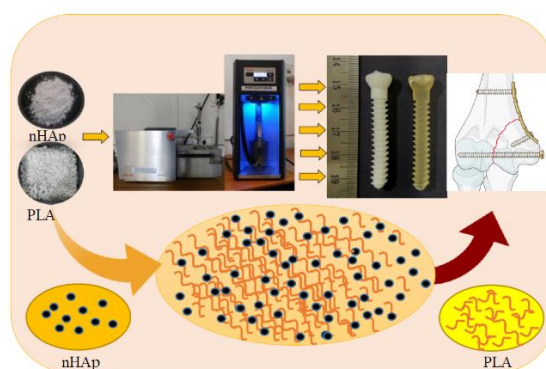
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### Abstract

The demand of resorbable implants is quite high due to many merits such as resurgery not required after bone fracture healing, tailored the combination of materials to customize the implants and after all prevention of underlying bone damages and stress shielding. Alone Polylactic acid (PLA) cannot fulfill all the properties required for the implants thus nano nanohydroxyapatite (nHAp) plays a vital role in order to encourage the neo bone regeneration and also provide sufficient mechanical strength. The present investigation discusses about fabrication and characterization of resorbable bioimplants based on PLA and nHAp composites. The implants were fabricated in twin screw extruder cum injection molding machine, designed and developed as per ASTM standard. The mechanical test along with degradation studies and bioactivity studies were performed using ASTM protocol. The mechanical strength of the fabricated implants were almost matches with the natural bone. The value of elastic modulus lies within the 3-4 GPa, flexural strength lies between 50-60 MPa. It was observed the fabricated implants were resorbable in nature and exhibit biocompatibility during the experiment. The degradation of the composites were completed in almost 8-10 months which validates the time period of the natural bone healing. Thus from this studies, new resorbable implants may be fabricated in order to have more functions and applications in coming days.



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## The role of enthalpy and entropy in the binding affinities of polyelectrolyte chains

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### Abstract

Polyelectrolyte chains are strongly correlated in dilute solutions in the absence of additional strong electrolytes. The interactions between polyelectrolyte chains depend on various physical variables, such as ion sizes, charge densities, temperature, polymer concentration, polymer length, and monovalent salt concentration. We focus on the interactions between single and many polyelectrolyte chain systems. The thermodynamics of a charged polymer system is characterized by the interaction potentials, the conformational entropy of the polymer chains, and the entropy of free counterions and salt ions. We have developed a theory that investigates the role of enthalpy and entropy in the complexation between oppositely charged polyelectrolytes. Our analysis shows that the complexation is driven by enthalpy in the weak electrostatic strength regime and by entropy in the strong electrostatic strength regime. We have also calculated the potential of mean force between oppositely charged polyelectrolytes as a function of charge density. Detailed numerical analysis suggests that, in general, the counterion-release picture is valid for a given range of Coulomb strength. This means that the released ions play a major role in the interactions between polyelectrolyte chains. Consequently, the significant binding affinities are governed mainly by the translational entropy of the released ions. Additionally, the counterion size plays an important role in the interactions between polyelectrolytes.

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## **Cold Atmospheric Pressure Plasma rapid Synthesis of Custom Peptide-Based Structures and Gaining Deeper Insights into the Enigma of Amyloid Formation.**

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### **Abstract**

The remarkable progress in designing and assembling biomaterials based on oligopeptides has opened up exciting possibilities for creating sophisticated and functional assemblies. Utilizing cold atmospheric pressure plasma (CAPP) for the production of peptide-based materials opens up a world of exciting possibilities for synthesizing custom-designed structures within few minutes. In this study, an inbuilt helium gas CAPP jet was used to fabricate fibrils from two oligopeptides - KLVFFA and GNNQQNY. These peptides serve as model systems for formation of self-assembled structures as they have higher propensity to form fibrils. The observed oligopeptide supramolecular entities exhibit distinct amyloid fibril characteristics, particularly in the KLVFFA peptide confirmed through FESEM, fluorescence microscopy, and thioflavin assay. Zeta potential, circular dichroism spectroscopy, and Fourier transform infrared spectroscopy measurements indicated an increase in attraction charges and no significant conformational changes in the self-assembled peptide aggregates. The combination of these techniques provides valuable information about the properties of the peptide aggregates and possible formation of biomaterials triggered by the nature of the amino acid sequence suggesting that they maintain their original secondary structure and do not undergo major conformational changes. This microscopic understanding will expand our comprehension of amyloid fibril formation in the brain thereby identifying key factors and mechanisms involved in the formation of these fibrils. Overall, the employment of CAPP and the characterization techniques deployed in this study offer a promising avenue for the development of peptide-based materials with tailored properties, bringing us one step closer to unravel the intricate mechanisms amyloidosis disorders.

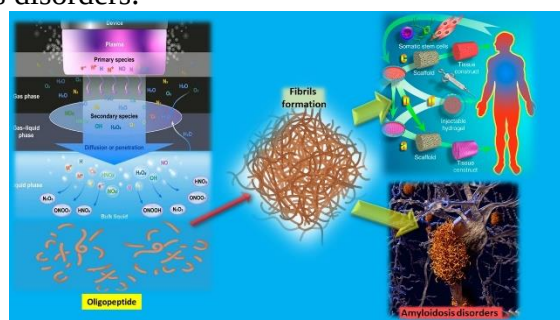


**Fig.- Graphical Abstract**

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## Development of Biodegradable Polymer Using Conventional Processing Equipments

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### Abstract

The global biodegradable plastic market size was estimated at US \$4.1 billion in 2021. During the fore cast period, it is expected to grow at a compound annual growth rate (CAGR) of 9.7%. Market growth is being stimulated by government bans on single use plastic and public awareness of the negative effects of plastic waste. The segment's growth is expected to be bolstered by the increasing use of bio degradable plastics in packaging and agriculture. Non decomposable plastics are a global concern. This problem is being addressed by governments around the world by prohibiting single use plastics and promoting the use of biodegradable plastics. In addition, consumers are willing to pay more for biodegradable plastics because of their eco friendly nature. Over the past two decades, the push for renewables and the future sustainability of materials and processes has continued. This has prompted further developments in the provision of environmentally friendly processes and products, both in terms of greater recyclability and greater use of renewable resources. Through HPGRDC, the Green Composites Initiative, we have developed polymer composites reinforced with natural fibres for various food packaging and cutlery applications. The developed green polymer composites are having higher natural fibre content with minimum polymer matrix. These green polymer composites are easily processable in conventional processing equipments without any design changes and it is bio compostable and bio degradable.

Keywords: Biogradable Polymer, Biodegradation, Single Use, Non biodegradation, Plastics, Processing, Natural Fibers, Polymer Composite.

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## Self-immolate Macromolecular Architectures for Drug Delivery In-vivo

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### Abstract

Poly(amino-ester)s are very good self-immolative cationic polymers known to undergo autodegradation into small non-toxic molecules at physiological pH=7.4. Despite their excellent biocompatibility, they failed to serve the purpose of ideal drug delivery nano-vector due to the uncontrolled and immature drug leaching under storage in PBS, cell culture media or blood plasma, etc. To circumvent this, we demonstrate the strategy to stabilize the self-immolative poly( $\beta$ -amino-ester)s by zwitterionic electrostatic interaction by carefully incorporating fully enzymatic-biodegradable carboxylic acid substituted PCL<sup>1,2</sup> units in the polymer backbone. We have designed well defined fully enzymatic biodegradable PCL based zwitterionic di-block and triblock copolymers by controlled ROP process and characterized by NMR, SEC, TGA and DSC. pH dependent self-assembly studies demonstrated excellent stability of triblock based nanocarriers in the entire pH range (pH 3-11) and these polymers exhibited outstanding DLCs for anticancer drug Doxorubicin and biomarkers (HPTS, IR-780) compare to anionic or cationic counterparts. These nanocarriers were spherical in shape with 200nm sizes characterized by DLS, FE-SEM and AFM with excellent stability in PBS, pH 7.4, FBS and cell culture media over 7 days. Release profiles demonstrated 90% drug release in presence of esterase enzyme in 24h. Nascent polymers were non-toxic to cells (WT-MEF, MCF-7, SKOV3 and RBCs) and DOX loaded nanoparticles were equally efficient to free DOX in killing cells. DOX loaded nanoparticles were taken up by cells via endocytosis pathway and underwent lysosomal biodegradation depicted by live-cell imaging and exhibited 3-4-fold higher cellular uptake compared to free DOX. *In vivo* biodistribution studies of near IR-780 loaded nanoparticles exhibited long blood circulation with longer retention in mice compare to free IR-780 over period of 72h. Thus, these zwitterionic polymers are proved to be excellent drug delivery candidates for *in vitro* and *in vivo*.

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## Ion Size Dependent Electrochromism in Air Stable Naphthalenediimide-based Conjugated Polymers

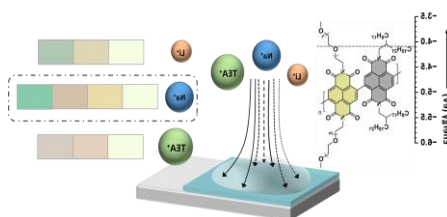
Dipanjani Giri, Shraman Kumar Saha, Ram Kumar Canjeevaram Balasubramanyam, and Satish Patil\*

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### Abstract

Conjugated polymers (CPs) that show stable and reversible cation insertion/de-insertion under ambient conditions hold great potential for optoelectronic and energy storage devices.<sup>1</sup> However, n-doped CPs are prone to parasitic reactions upon exposure to moisture or oxygen.<sup>2-4</sup> This study reports a new family of Naphthalenediimide (NDI) based conjugated polymers capable of undergoing electrochemical *n*-type doping in ambient air. By functionalizing the NDI-NDI repeating unit with alternating triethylene glycol and octadecyl sidechains, the polymer backbone shows stable electrochemical doping at ambient conditions. We systematically investigate the extent of volumetric doping involving monovalent cations of varying size ( $\text{Li}^+$ ,  $\text{Na}^+$ , tetraethyl ammonium ( $\text{TEA}^+$ )) with electrochemical methods, including cyclic voltammetry, differential pulse voltammetry, Spectro electrochemistry, and electrochemical impedance spectroscopy. We observed that introducing hydrophilic side chains on the polymer backbone improves the local dielectric environment of the backbones and lowers the energetic barrier for ion insertion. Surprisingly, when using  $\text{Na}^+$  electrolyte the polymer films exhibit higher volumetric doping efficiency, faster-switching kinetics, higher optical contrast, and selective multi-electrochromism when compared to  $\text{Li}^+$  or  $\text{TEA}^+$  electrolytes. Using well-tempered metadynamics, we characterize the free-energetics of side chain-ion interactions to find that  $\text{Li}^+$  binds more tightly to the glycolated NDI moieties than  $\text{Na}^+$ , hindering  $\text{Li}^+$  ion transport, switching kinetics and limiting the films doping efficiency.<sup>5</sup>



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## Thermo-responsive glycopolymer-grafted-nanoparticles via RAFT polymerization: Temperature responsive binding with lectin

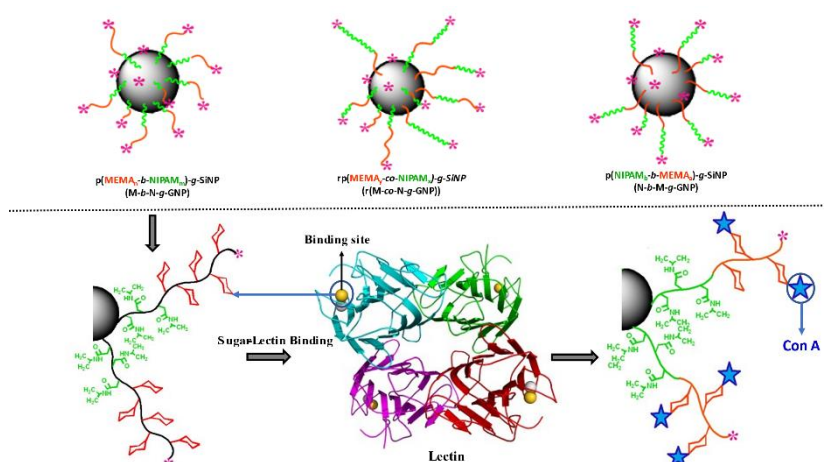
Somdatta Rudra, Saradmoni Mondal, Mithun Chakraborty, Musti J. Swamy\* and Tushar Jana\*<sup>1</sup>

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### Abstract

Thermoresponsive polymers are a category of stimuli-responsive polymers which have gained wide attention recently owing to their vast applications in controlled and targeted drug delivery, cell encapsulation and various bio-medical fields. In this work, we have synthesized a series of thermo-responsive glycopolymer-grafted-silica nanoparticles (GNPs) and glycopolymers (GPs) and investigated temperature dependent binding studies with a lectin namely Con A to understand the binding behaviour of carbohydrate and protein in presence of a temperature responsive polymer that undergoes volume phase transition at physiological temperature and has a lower critical solution temperature (LCST) of 32°C. The glycomonomer and the thermo-responsive monomer used in this work are  $\alpha$ -D-Mannose-HEMA ( $\alpha$ -MEMA) and N-Isopropylacrylamide (NIPAM), respectively. The series of polymers with mannose chains outside and far away from the silica core showed stronger binding activity with the lectin. This result reflects the greater accessibility of the polymer chains hanging outside away from the silica core to the lectin. The GNPs and GPs displayed stronger binding to the mannose specific protein, Con A at temperatures below LCST with high binding constant values while at temperatures above LCST, no proper binding activity is seen. Also, the GNPs show higher binding with Con A than the GPs owing to the positive entropic binding contribution which resulted in an association constant 800- and 400- times stronger than the mannose chains and GP chains, respectively.



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## **Fabrication and characterization of ternary biopolymer hydrogel crystals**

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### **Abstract**

This conference oral presentation explores the innovative development of a ternary hydrogel crystal system utilizing entirely environmentally-friendly polymers. The focus of this research is to create a hydrogel with exceptional swelling capacity while simultaneously incorporating potent antibacterial properties. By harnessing sustainable and biocompatible polymer materials (Chitosan, PVA, and Gelatine), this study aims to contribute to the growing field of green materials science. The presentation will provide insights into the synthesis, characterization, and performance evaluation of this novel ternary hydrogel system, shedding light on its potential applications in various fields, including medicine, agriculture, and environmental science.

## Coaxially Electro-Centrifugally Spun Core-Sheath Nanofibers With Dual Drug Loading For Use in Cancer Treatment

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### Abstract

Nanofiber fabrication techniques have witnessed considerable advancements, opening up innovative possibilities for biomedical applications. This study is primarily centered on the creation of core-sheath nanofibers using the highly efficient coaxial Electro-Centrifugal Spinning (ECS) method. The ultimate objective of this research is to fabricate a nanofibrous dual drug delivery system for cancer treatment. In this strategy, we employed Pullulan as the core material and Poly(lactic-co-glycolic acid) (PLGA) as the sheath material. This distinctive structure enables the simultaneous loading of two different drugs, with Ciprofloxacin (antibacterial drug) residing in the core and Paclitaxel (chemotherapeutic drug) in the sheath. This dual-drug configuration is expected to yield a synergistic drug release profile, potentially enhancing cancer treatment by addressing both the malignancy and the risk of secondary bacterial infections in patients. Furthermore, FTIR was employed to investigate the drug-polymer chemical interactions. The mechanical properties hold significant promise for its potential utilization in biomedical applications. Additionally, it was found that the mechanical properties and the drug release pattern could be tuned by varying the core diameter of the nanofiber. The findings of the work is expected to reveal the efficacy of the nanofibers to be used for cancer treatment.

**Keywords:** core-sheath nanofibers, Electro-Centrifugal Spinning, Pullulan, PLGA, drug release

## Amino acid-containing Thermoresponsive Hydrogel/MOF Composite for Atmospheric Water Harvesting

Sandeep kumar Sahoo, Bijay P. Tripathi\*

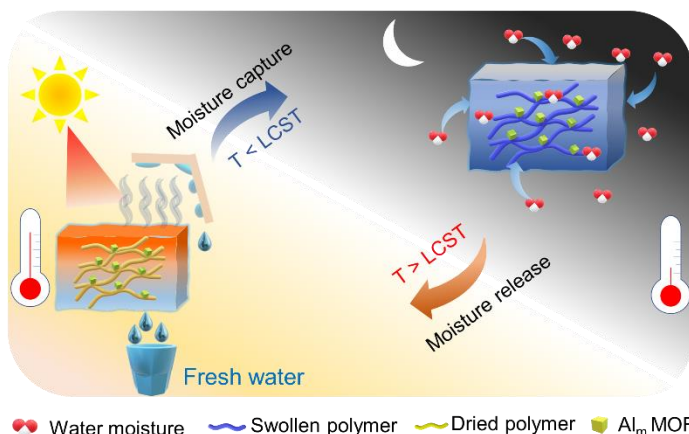
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**Keywords:** Sorption-based water harvesting, Thermoresponsive hydrogel, Atmospheric water harvesting

### Abstract

The innovative approach based on sorption-based water harvesting involves extracting moisture from the atmosphere, mitigating water scarcity, and establishing a sustainable means of obtaining clean water. The amino acid-based hydrogels are known for their ability to absorb and retain water effectively due to their hydrophilic nature, responsiveness, and biocompatibility, and the incorporation of Metal-Organic Frameworks (MOFs) into hydrogel matrices is a prevalent approach, resulting in a range of hydrogel/MOF composites exhibiting enhanced sorption characteristics. The combination of MOF's rapid hydration and superior breathability with hydrogel's hydrophilic properties and large water retention capacity



make these composites a promising alternative for extracting water from the atmosphere. The present study concentrates on the latest advancements in the techniques employed for the synthesis of MOFs, hydrogels, and hydrogel-MOF composites, and a comprehensive analysis of the advantages and disadvantages of each approach is presented and focused on its microstructure, moisture sorption capacity, and moisture sorption recyclability. The results indicate that the macro-porous hydrogel-MOF composite achieved high-performance atmospheric water harvesting (AWH) with the maximum capacity reaching 2.21 gg<sup>-1</sup> at approximately 90% RH and 30°C within 24 hours. The composite also exhibits outstanding durability, low desorption temperature (approximately 35±5°C, the lowest), and high water-releasing rate, releasing 98% of the sorbed water under 40 °C and 60% RH for only 2 hours. This hydrogel-MOF composite has the potential to significantly impact various industries, including water treatment, desalination, and moisture harvesting.

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## Stimuli triggered activation of heavy atom free photosensitizer and implications in targeted photodynamic therapy

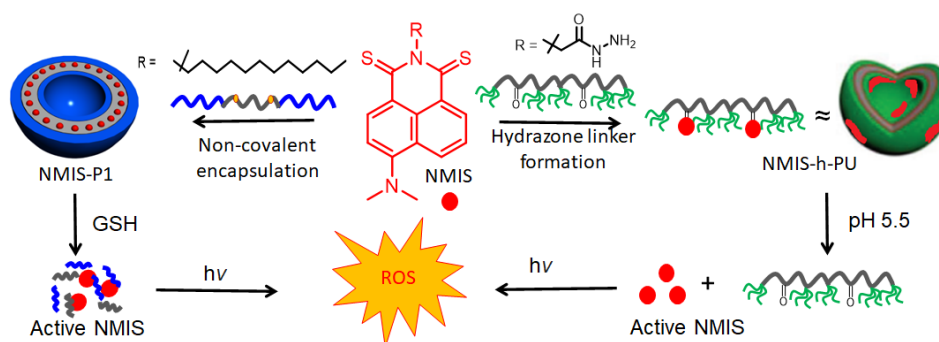
T. Banerjee,<sup>1</sup> K. Dan<sup>1</sup> and Suhrit Ghosh\*<sup>1</sup>

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### Abstract

Photodynamic therapy (PDT) has emerged as an attractive tool to treat skin cancer and other diseases. In PDT, a photoactivatable drug (photosensitizer, PS) is used to produce different reactive oxygen species (ROS) upon light irradiation which causes cell death. However, in most cases, the PS consists of heavy metals with high cytotoxicity even in the dark. Thus, in the recent past heavy metal free photosensitizer have gained significant attention.<sup>1</sup> We envisaged the scope and utility of such therapy would be enhanced if the PS can be delivered in a dormant state and activated selectively by a biological stimulus. With this broad objective, we have explored PDT using the naphthalene-monoimide based PS (NMI-S, Scheme 1). Initially, we encapsulated hydrophobic NMIS inside a redox responsive polymer that drastically reduces the ROS generation efficiency due to aggregation of the dye in the confined environment. In contrast, after GSH treatment the NMIS encapsulated bio reducible polymeric vesicle exhibits disassembly and release the NMIS in its active form that kills cancer cells effectively upon light irradiation (>70%).<sup>2</sup> Further a polyurethane (PU) -NMIS covalent conjugate was developed via acid labile hydrazone linker (NMIS-h-PU) which produced vesicular morphology in aqueous solution in which the NMIS remained in dormant state. In acidic pH, cleavage of hydrazone linker leads to the release of the NMIS in active form that results in reduced cell viability after photoirradiation of NMIS-h-PU treated cancer cells. Recent results from our group in this area will be discussed in the presentation.



Scheme 1: Schematic representation of stimuli responsive release of activatable NMIS. *Left*- redox triggered release of hydrophobic NMIS, *right* – pH triggered cleavage of hydrazone linker and release of NMIS in active form and ROS generation.

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## **Processing of Biopolymers into Value-added Products**

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### **Abstract**

Synthetic polymers have become ubiquitous in human activities. While they offer solutions to many of humanity's challenges due to their lightweight nature, specific strength, and ease of processing, they often suffer from the drawback of being non-biodegradable. Consequently, when these polymers are disposed of, they persist in the environment for many decades. Unlike synthetic polymers, biopolymers produced by or derived from living organisms are biodegradable and renewable. Although nature produces biopolymers in quantities of several billion tons per year, we have not been able to effectively utilize this resource, primarily due to issues with processability. As a result, billions of tons of biopolymers are lost to biodegradation each year. Our main focus is on transforming these biopolymers into value-added products using sustainable methods. We have successfully developed a range of value-added products, including foams, adsorbents, absorbents, and hydrogels using biopolymers. These products seamlessly integrate with the biodegradation pathways and contribute to a circular economy, once they are discarded after their service life. This presentation will delve into our recent investigations into biopolymer processing, with a particular emphasis will be on the development of haemostatic agents from chitosan and the production of packaging foams using gelatin as a base material.



Fig. Digital photographs of water-soluble and biodegradable foams prepared using gelatin.

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## Alkaline etching assisted polydopamine coating on 3D printed polylactic acid for enhanced bone regeneration

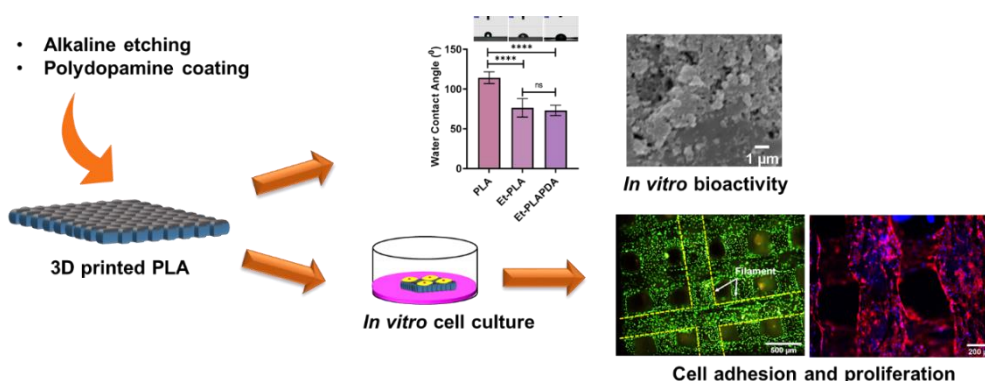
Athira Murali<sup>1</sup> and Ramesh Parameswaran\*<sup>1</sup>

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### Abstract

The ultimate success of tissue engineering relies on the design and development of efficient scaffolds to support osteoblast adhesion, proliferation and differentiation. Polylactic acid (PLA) is widely used in bone tissue engineering due to its biocompatibility. However, its non-bioactivity and hydrophobic nature makes it difficult to support new bone growth. The present work discusses the surface activation of 3D printed PLA scaffolds by alkaline etching mediated polydopamine (PDA) functionalization for enhanced cell-material interactions. It was observed that surface features such as wettability, surface roughness and porosity were significantly improved after alkaline etching. Moreover, alkaline etching assisted the PDA polymerization and deposition and further improved the wettability. Alkaline etching contributed to obtain a notable difference in the extent of PDA functionalization. The porosity and pore size of the samples varied significantly upon alkaline etching and subsequent PDA coating. The surface elemental analysis confirmed the PDA coating. The modified scaffolds showed enhanced *in vitro* mineralization compared to the bare PLA scaffold after 9 days of SBF immersion. Further, *in vitro* cell culture studies performed using human osteosarcoma (HOS) cell lines demonstrated the enhancement in cell attachment and spreading after two-step surface activation of PLA scaffolds.



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## Synthesis of High-Performance Polypropylene Products for Specialty Applications

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### Abstract

Olefin polymerization using magnesium dichloride ( $\text{MgCl}_2$ ) supported Ziegler–Natta (Z–N) system is a robust and preferred catalytic process for producing polyolefin (PP & PE) grades.<sup>1</sup> Herein, high performance polypropylene products synthesized using novel  $\text{MgCl}_2$  supported multidentate non-phthalate Ziegler-Natta pre-catalyst system and studied their properties.<sup>3</sup>

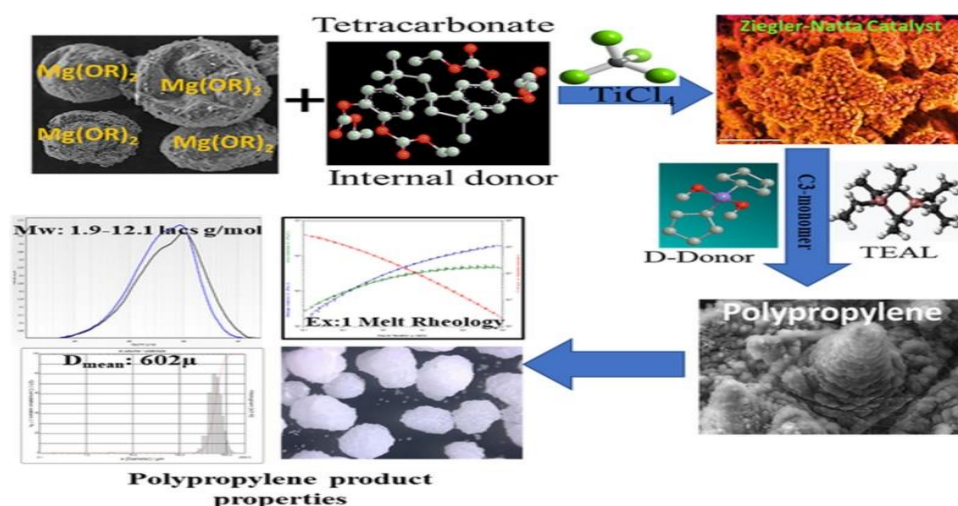


Figure 1. Polypropylene polymer synthesis & product properties<sup>3</sup>

Interestingly, the polypropylene products synthesized reactor-made with wide range of melt flow index (MFI) and controlled isotacticity compared to conventional bidentate Z–N pre-catalysts. In addition, the ultra-high molecular weight isotactic polypropylene (UHMWPP) product also synthesized with the same catalyst system. Further, GPC analysis reveal medium to broad unimodal molecular weight distribution (MWD) of PP products which can be used for specialty applications in defense, automobiles, aerospace, bio-medical sectors.<sup>2</sup>

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## Short-Peptide-Based Gel Nanofibers and Modulation of helicity

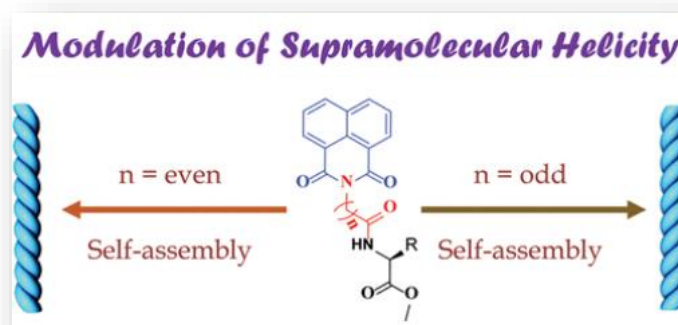
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### Abstract

Helical supramolecular architectures play important structural and functional roles in biological systems. The helicity of synthetic molecules can be tuned mainly by the chiral manipulation of the system. However, the tuning of helicity by the achiral unit of the molecules needs to be studied more. In this work<sup>1, 2</sup>, the helicity of naphthalimide-capped peptide-based gel nanofibers is tuned by the alteration of methylene units present in the achiral amino acid. The inversion of supramolecular helicity has been extensively studied by CD spectroscopy and morphological analysis. The density functional theory (DFT) study indicates that methylene spacers influence the orientation of  $\pi$ - $\pi$  stacking interactions of naphthalimide units in the self-assembled structure that regulates the helicity. This work illustrates a new approach to tuning the supramolecular chirality of self-assembled biomaterials.



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## Tunable Solvent-Induced Self Assembly in Luminescent Biodegradable Amino Acid based Polyurethanes

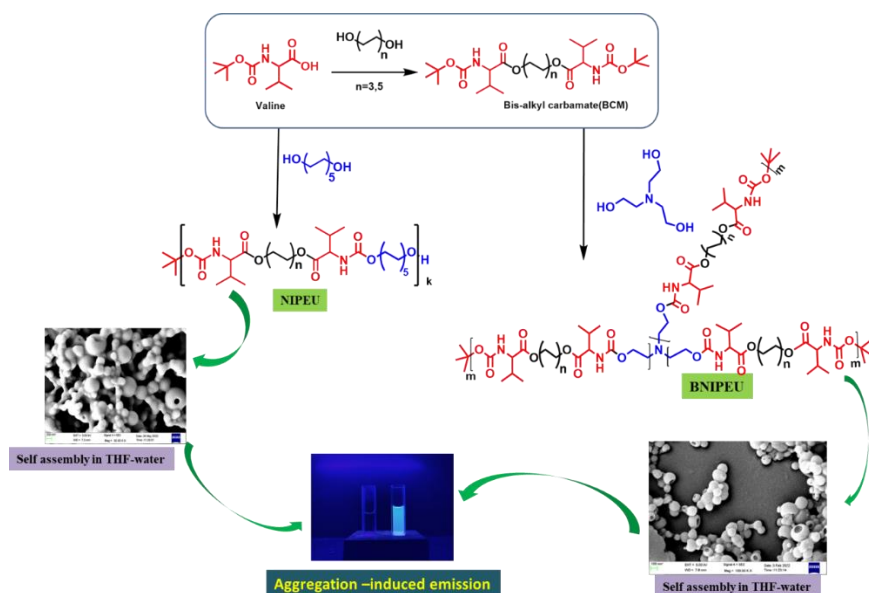
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### Abstract

Harnessing the intrinsic non-conventional luminosity of crystallised aliphatic amino-acids and their associated oligomers have gained a significant attention in recent times. In this work, luminescent vesicular self-assemblies *via* phase inversion route were generated from a range of amphiphilic bio-based poly (ester urethanes) (NIPEUs). Structural variations from linear to branched units were achieved for synthesized NIPEUs by varying different alcohol from diols to triols, showcasing a prominent impact on their self-assembled morphologies. By tuning the polarity of the co-solvent medium, polarity dependent morphological alternations from vesicles to large compound micelles (LCPs) were attained, giving the NIPEUs a taste of solvent-induced self-assembly. Moreover both enzymatic and hydrolytic degradation studies were incorporated to evident the biodegradability of the prepared NIPEUs. As a nutshell, this project is an amalgamation of four unique aspects that make it distinct in its own right: unconventional luminescence, distinctive solvent induced self-assembly, non-toxic non-isocyanate approach and *in vitro* enzymatic and hydrolytic biodegradability. Owing to their biodegradability and non-conventional luminescent self-assemblies, these unique NIPEUs can emerge as an effective tool in various bio-medical applications ranging from cell imaging to drug delivery.



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## Chain folding regulated self-assembly and antiviral activity of amphiphilic polyurethane

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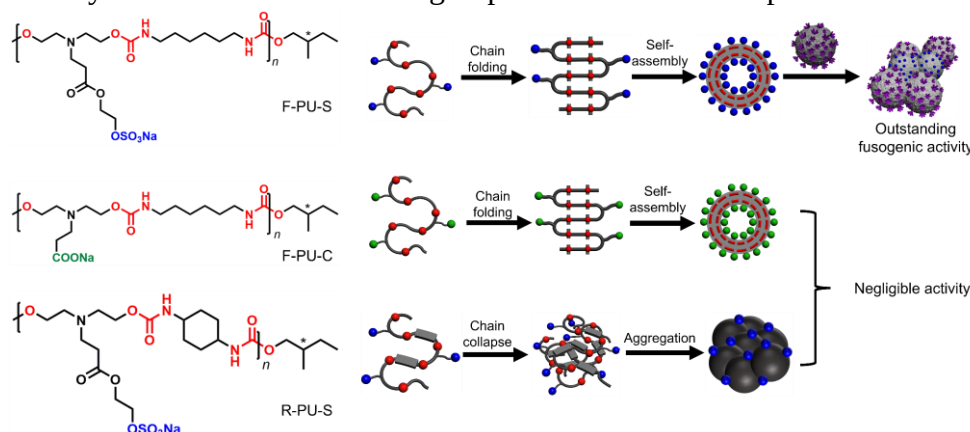
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### Abstract

Virus, a sub-microscopic agent lying at the boundary of living and non-living organism which can only replicate in living cells, has been the cause for various dreadful diseases worldwide.<sup>1</sup> Considering earlier reports showing flexible polyurethanes with pendant carboxylic acid groups forming vesicular morphology in water through intramolecular hydrogen bonding,<sup>2</sup> a polyurethane with sulfate groups as pendant has been synthesized with flexible backbone (F-PU-S) to form polymersome in which more sulfate groups are displayed at the surface for better interaction with the basic heparan sulfate receptors present on the viral capsid of Sendai virus. Whereas another polymer R-PU-S, with similar pendant sulfate groups but rigid backbone, forms irregular aggregates, leaving lesser number of sulfate groups at the surface to interact with the virus. The vesicular morphology formed by F-PU-S, creates a highly negatively charged surface in aqueous medium showing outstanding antiviral activity (scheme 1) in contrast to R-PU-S with negligible activity. On the other hand control polymer F-PU-C, in which carboxylate pendant group is attached instead of sulfate, does not show any notable antiviral activity. Recent results from our group<sup>3</sup> in this area will be presented in the poster.



**Scheme 1:** Schematic presentation on self-assembly and antiviral activity of sulfated PUs

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## Study on enhanced biofilm-formation of PHBHHx/PLA-based films by plasma treatment

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### Abstract

Enhanced hydrophilicity and bioactivity can make PLA and PHBHHx sufficiently interactive to enhance biofilm formation and cell attachment. To achieve this, PHBHHx/PLA-based films were irradiated with low-temperature inductively coupled Ar-plasma. Characterization of treated and untreated samples was carried out using X-ray photoelectron spectroscopy (XPS), contact angle, surface free energy (SFE), gel permeation chromatography (GPC), thermogravimetric analyser (TGA), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). Contact angle of modified films was measured just after the treatment and after samples were kept in air for 30 days in order to evaluate aging effect. A significant reduction in contact angle was observed from  $90^{\circ} \pm 2^{\circ}$  to  $25^{\circ} \pm 2^{\circ}$  which was found to be maintained at  $50^{\circ} \pm 2^{\circ}$  upto 30 days of plasma treatment (12 min, 100W). XPS results also confirmed the chemical modification on polymer surface as C1s spectra showed modified peaks of C-C(H), C-O, and O=C-O. Surface roughness and morphological changes were analyzed using atomic force microscopy (AFM) and field-emission scanning electron microscopy (FESEM). Finally, treated and untreated samples were evaluated to study initial adhesion and subsequent biofilm formation of *E. coli* and *B. megaterium*. Results exhibited significant enhanced potential of biofilm formation of plasma-treated surfaces. Furthermore, cell viability assay was performed using Baby Hamster Kidney (BHK-21) to evaluate cell proliferation and growth. Results showed a prominent impact on cell adherence due to improved hydrophilicity. In conclusion, the exposure of pure Ar-plasma could elevate the formation of polar groups and oxidation on the surfaces, thereby increasing wettability, roughness, cell proliferation, and degradability.

Keywords: Plasma treatment, biodegradation, chemical modification, wettability, cell proliferation.

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## Molecular Dynamic Simulation for Structure Property Relation of Polyolefin

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### Abstract

Polymers are critical class of materials, widely used in many different areas, from medicine to the aerospace industry. Polymers are macromolecules with a large variety of chemical structures and morphologies which determine their unique and various properties. The advances in Graphics processing unit (GPU) hardware and improved efficiencies of atomistic simulation programs facilitate the screening of polymers by running simulations for analysing and understanding the polymer interactions on atomistic scale. In recent years, molecular dynamics (MD) simulations have become a standard tool alongside experiments to understand the interaction of polymers with other molecules. These interactions are further related to the structural properties of the polymers, which in turn affect their macroproperties more specifically, physical, thermal and mechanical properties.

In HPGRDC, molecular simulation tools are being used as tool for prediction of structure-property relations. We have developed molecular model for polypropylene (PP) and polypropylene composite that has 10 polypropylene chains. MD simulations were performed for PP model using Schrodinger Material Science Suite which employs OPLS4 force field for optimization of molecular model at 1.01325 atm and 300 K for an NPT ensemble. The developed molecular model generated physical properties as per literature.

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## Development of Chitosan Nanostructures Reinforced Pectin/Pullulan Based Nanocomposites Assisted with Tea Tree Essential Oil for Sustainable Pouch Packaging

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### Abstract

In the current century, edible food packaging is considered as a sustainable packaging being developed using food grade ingredients such as protein, carbohydrates, lipids, bioactive compounds, etc. Edible films are a type of edible food packaging which is used as a sandwich material or wrapper on food products as a thin layer to provide protection against environment. Chitosan is a natural resource-based biodegradable, biocompatible polymer that is used in the creation of edible films and coatings. The study demonstrates the development of sustainable pouch packaging being edible in nature by incorporating chitosan nanostructures (NCS) in pectin/pullulan blend assisted by tea tree essential oil. NCS has antimicrobial property, and it is biocompatible, where pectin is a plant-based polysaccharide so it's part of human diet. The study aims to use ionotropic gelation method to develop NCS using sodium tripolyphosphate as a cross linking agent, which has been characterized using FTIR spectroscopy, XRD analysis and FETEM analysis. To prepare the films, NCS is incorporated in a ratio of 0%, 0.5%, 1% and 1.5% in the pectin pullulan blend and further, tea essential oil is added to the films to increase its antimicrobial properties. The developed films has been characterized in terms of FTIR spectroscopy, XRD spectroscopy, barrier property, non-toxicity, optical properties, mechanical properties, etc. The antimicrobial properties of the films has been measured against *S. aureus* and *E. coli*. Additionally, the developed film as a pouch packaging can be used for maintaining quality and shelf life of food products having good heat sealing property.

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## Nuclear Delivery of Molecular Drugs by Bio-Compatible Polymeric Micelle via Non-Endocytic Uptake

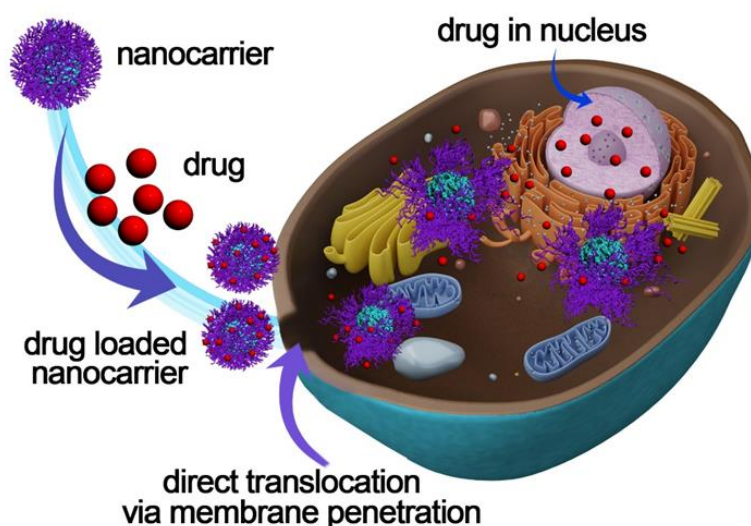
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### Abstract

Although sub-cellular targeting can enhance the therapeutic performance of most drugs, such targeting requires appropriate carrier-based delivery that can bypass endosomal/lysosomal trafficking. Recent works show that nanocarrier can be designed for direct cell membrane translocation and non-endocytic uptake, bypassing the usual endocytosis processes. Here we show that this approach can be adapted for rapid cell nucleus delivery of molecular drugs. In particular, guanidinium-terminated polymeric micelle based nanocarrier is used to create weak interaction-based carrier-drug nano-assembly for direct membrane translocation into cytosol. The rapid and extensive entry of drug loaded polymeric micelle into cell without any vesicular coating and affinity of drug to nucleus allows their nucleus labelling. Compared to endocytotic uptake that require more than hours for cell uptake followed by predominant lysosomal entrapment, this non-endocytic uptake labels nucleus within few minutes without any lysosomal trafficking. This approach may be utilized for polymeric micelle based subcellular targeting of drugs for more effective therapy.



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## Transition metal-based bimetallic oxides doped hydrocarbon-based polyelectrolyte composite membranes to induce high oxidative tolerance and enhanced performance in hydrogen fuel cells

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### Abstract

Utilizing the potential of transition metals to quench free radicals in hydrogen fuel cells, we prepare cerium-manganese and cerium-zinc bimetallic oxides ( $\text{CeMnO}_x$  and  $\text{CeZnO}_x$ ) nanostructures by alkali-aided deposition precipitation and utilize as fillers in hydrocarbon-based polymer electrolyte membranes (PEMs). In both the bimetallic oxides, Ce has been allowed to occupy the major portion, whereas Mn and Zn are doped into the  $\text{CeO}_2$  crystal lattice in different proportions. To improve the stability of the PEMs,  $\text{CeMnO}_x$  is used as filler in the blend of sulfonated poly ether ether ketone (SPEEK) and sulfonated poly (2, 6-dimethyl-1,4-phenylene oxide) (SPPO) with different weight ratios are employed as membrane backbone. Similarly,  $\text{CeZnO}_x$  is intercalated with the SPPO polyelectrolyte with varying filler loading of (1%, 2%, and 3% w/w) to construct stable PEMs. The interfacial adhesion and coupling configuration of three-dimensional  $\text{CeMnO}_x$  and  $\text{CeZnO}_x$  with sulfonic moieties of polyelectrolyte membranes enhances bound water content in the PEMs. It also constructs an extensive hydrogen bonding network with proton transport channels, uplifting the proton conductivity ( $K^m$ ) by promoting vehicular and Grotthuss-type transport. Reversible redox cycling of  $\text{Ce}^{3+}$ - $\text{Ce}^{4+}$  endorses the quenching of harsh radicals and augments the oxidative stability of the membranes, whereas  $\text{Mn}^{n+}$  and  $\text{Zn}^{m+}$  enhance the hydrogen pre-coverage and the overall  $K^m$  of the PEMs. Composite PEMs exhibit only 2-5% mass loss and 4-9%  $K^m$  loss after exploiting in harsh Fenton's solution. Representative SPZ-2 membrane (2%  $\text{CeZnO}_x$  loading in SPPO polyelectrolyte) showed an impressive power density of  $351.9 \text{ mW/cm}^2$  with a maximum current density of  $1104.6 \text{ mA/cm}^2$  at  $75^\circ\text{C}$  and 100% RH.

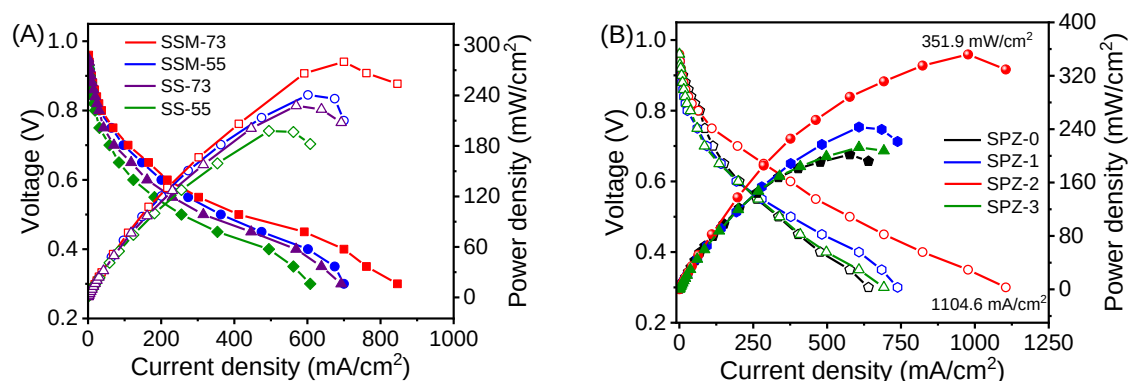


**Figure 1.** Single cell fuel cell performance for (A)  $\text{CeMnO}_x$  incorporated blend composite PEMs and (B)  $\text{CeZnO}_x$  doped SPPO composite PEMs.

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## Molecular Simulations of aggregation and complex formation between anionic polyelectrolyte and cationic surfactant in water: PAA - CTAB

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### Abstract

Polyelectrolyte-surfactant complexation in aqueous solution has wide applications in formulation of industrial, biological and household activities. We have investigated the complexation behavior of cationic surfactant cetyltrimethylammonium bromide (CTAB) with anionic polyelectrolyte poly(acrylic acid) in dilute aqueous solution using atomistic molecular dynamics simulation methods. Polyelectrolyte-surfactant complex (PSC) simulations of all systems as given in Table 1, were performed on an average of 400-800 ns of the simulation time and were found to be stable based on the calculation of radius-of-gyration ( $\langle R_g \rangle$ ) and potential energy of micelle, polyelectrolyte and complex. Complexation of polyelectrolyte with CTAB surfactants is purely driven by electrostatic interactions for ionized chains whereas hydrophobic (dispersion) interactions for unionized chains for entire range of surfactant aggregation number ( $N_{agg}$ ). The linear increasing behavior observed for radius of micelle with  $N_{agg}^{1/3}$ . The micelle attained more spherical shape with increase in  $N_{agg}$ . The ionized chain in PSC is adsorbed on the micellar surface from exterior headgroup-water interface side whereas unionized chain penetrates into hydrophobic core of the micelle. The presence of surfactant molecules disrupt the structure of water molecules in the vicinity of chain and shows the decrease in number of hydrogen bonds with increase in  $N_{agg}$ . Polyelectrolyte chain acts as shield on micellar surface which restrict the solvent interaction with micelle. Ionized chain efficiently acts as a polymeric counterion in oppositely charged PSC, leads to displacement of counterions ( $Na^+$  and  $Br^-$ ) into bulk solution via ion exchange mechanism. Detailed information about microscopic structures of PSCs will be present in conference presentation.

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## Mucin and Aminophenyl Boronic Acid Functionalised Zein/PVP Blend Electrospun Membranes: A Comparative Evaluation of Transmucosal Delivery of Propranolol Hydrochloride

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### Abstract

Functionalised polymers have been widely investigated for their supremacy in adhesion to mucosal surfaces. This piece of work proposes the design of fabrication of boronic acid and mucin functionalised electrospun membrane of Zein/PVP for transmucosal drug delivery. Boronate ester complex formation as well as the mutual interpenetration of mucin chains caused enhanced mucoadhesive properties. Mucin-functionalised membranes exhibited an eight-fold increase in adhesion over porcine buccal mucosal tissue. Boronic acid functionalised membrane showed  $5.68 \pm 0.47$  MPa tensile strength whereas mucin functionalised membrane had  $4.85 \pm 0.92$  MPa tensile strength. Boronic acid functionalisation was confirmed using FTIR, XPS, UV spectroscopy techniques and water contact angle analysis. Mucin functionalisation was confirmed using FTIR spectra and TNBS assay. Entrapment of propranolol hydrochloride (PL) in the membranes had resulted in poor entrapment for mucin-functionalised membranes due to a lack of compatibility in terms of pH. Cumulative release of PL from both membranes followed Korsmeyer-Peppas model of release kinetics at pH 7.4. The membranes were tested for cytocompatibility using RPMI 2650 cells and observed to be non-cytotoxic. F-actin staining and immunostaining of  $\beta$ -catenin proteins of adherens junction showed the absence of cell junction opening after treatment with the membranes. The mechanism of PL transport *in-vitro* through RPMI 2650 cells was analysed and found to be transcellular. TEER evaluation after treatment with the membranes showed no significant changes in the absolute value of TEER and confirmed the transcellular mechanism of transport. *Ex-vivo* evaluation of PL transport through porcine buccal mucosa also supported the transcellular transport mechanism.

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## Novel and Controlled Synthesis of hierarchical $\text{AgNi}_2\text{O}_4$ on Polypyrrole as an Advanced Electrode material for High performance Supercapacitor

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### Abstract

Production of renewable energy is of great significance due to an elevating crisis in the supply of fossil fuels. However, major emission of green house gases from fossil fuels accelerates the pollution levels that are detrimental to the atmosphere. To overcome this prime challenge, it is pivotal to build up devices with high power density, good capacity and extended life span. Ascribing to these key features, Supercapacitors have gained the attention of energy experts owing from its simplicity of use to its increased cycle stability. In this study, for the first time we have prepared an electroactive material viz.,  $\text{AgNi}_2\text{O}_4@\text{PPy}$  through a facile technique. It is necessary to mention that initially, spinel  $\text{AgNi}_2\text{O}_4$  was prepared and subsequently disseminated on Polypyrrole to produce the electrode material,  $\text{AgNi}_2\text{O}_4@\text{PPy}$ . The synthesized electrode material was characterized through microscopic and spectroscopic techniques. Additionally at varied scan rates and current densities the electrochemical properties of  $\text{AgNi}_2\text{O}_4@\text{PPy}$  were evaluated through cyclic voltametric and galvanostatic charge discharge techniques. On comparing,  $\text{AgNi}_2\text{O}_4$  and  $\text{AgNi}_2\text{O}_4@\text{PPy}$  electrode materials, the EIS results suggests that the polymer-based composite increased the specific capacitance ( $C_{\text{sp}}$ ) with high charge transfer and low resistance. Thus, the constructed electrode offers high energy density and increased retention percentage. Therefore, the above assessment indicates that  $\text{AgNi}_2\text{O}_4@\text{PPy}$  has the capability to be employed as a unique electrode material for the production of highly efficient and reliable energy storage device.

**Keywords:** Spinel compound, Conducting Polymer, Specific Capacitance, Electrical Properties.

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## Predicting Structural and Mechanical Properties of Biodegradable Copolymers using Molecular Dynamics Simulations

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### Abstract

Biodegradable and biocompatible elastomers have gained widespread attention in regenerative tissue engineering and drug delivery applications. Artificial 3D scaffolds of these polymers are expected to have tunable elastic properties, suitable biodegradation rates, and enhanced cell adhesion and proliferation. In this regard, Citric acid and diol-based copolymers are promising candidates as they combine high mechanical properties of synthetic materials and high degradability of biomaterials. The condensation polymerization between the inexpensive and water-soluble citric acid and 1,6-hexanediol leads to the formation of Polyester ethers (PEE). However, the correlations between PEE's mechanical properties, degradability, and molecular composition are poorly understood. Here we perform all-atom equilibrium molecular dynamics (EMD) and non-equilibrium molecular dynamics (NEMD) of Citric acid-1,6-Hexanediol copolymers and establish correlations between their structure and degradation for varying acid-to-alcohol ratio and the monomer sequence. The OPLS interatomic force field is used to model the copolymers. The data suggest a strong correlation between the elastic properties, solubility, and the composition of the copolymers. The work provides essential design rules of PEE for artificial scaffolding applications.

## Structure and property study of protein-based carbon dot incorporated seaweed biopolymer film for food packaging

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### Abstract

In this work, protein-derived carbon dots synthesized using the hydrothermal method were incorporated in Seaweed polymer film. Carbon dots were characterized using a Transmission Electron Microscope, UV-visible spectrophotometer, spectrofluorometer, and Fourier Transformed Infrared Spectrophotometer. The carbon dot-based seaweed biopolymer film was characterized using multiple instrumental techniques such as UV-visible spectrophotometer, Scanning Electron Microscope (SEM), Thermogravimetric analyzer (TGA), and contact angle measurement. The water stability of the edible film was examined using a water retention and solubility study. Transparency property was examined by color measurement of the film. The barrier property of the edible film was examined via water vapor permeability measurement. SEM image showed a dot-like structure present in the carbon dot-based seaweed biopolymer film. The anti-oxidant study of the film was also conducted which showed pronounced anti-oxidant activity in carbon dot film compared to the film without carbon dot. The prepared biopolymer nanocomposite film possesses good tensile strength (above 20 MPa). The film shows stability for several months in the air without any degradation or microbial growth. Hence, protein-based carbon dot biopolymer films are excellent for food packaging applications.



**Figure: Seaweed biopolymer film (a) without carbon dot (b) with carbon dot**

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## ***In-situ* synthesis of random networks of zirconium-doped manganese oxide nanoribbons and poly(3,4-ethylenedioxythiophene) flakes at water/chloroform interface**

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### **Abstract**

Owing to their magnificent chemical and physical properties, transition metal-based heterostructures are potential materials for applications ranging from point-of-care diagnostics to sustainable energy technologies.<sup>1</sup> The cryptomelane-type octahedral molecular sieves (K-OMS-2) are extensively studied porous materials with hollandite ( $2 \times 2$  tunnel of dimensions,  $4.6 \times 4.6 \text{ \AA}^2$ ) structure susceptible to the isovalent substitution of metal cations at the framework of  $\text{MnO}_6$  octahedral chains.<sup>1-3</sup> Here, we report a facile *in-situ* synthesis of framework-level zirconium (Zr) doped K-OMS-2 nanoribbons in poly(3,4-ethylenedioxythiophene) (PEDOT) nanoflakes at a water/chloroform interface at ambient conditions.<sup>4</sup> An oxidant system of  $\text{KMnO}_4$  and  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$  initiated the polymerization at temperatures ranging from  $5^\circ$  to  $50^\circ\text{C}$ .<sup>4</sup> The lattice distortions arising from the framework-level substitution of  $\text{Mn}^{4+}$  by  $\text{Zr}^{4+}$  in the K-OMS-2 structure were evidenced with powder X-ray diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy, and  $\text{N}_2$  adsorption-desorption studies.<sup>4</sup> Transmission electron microscopic and mapping images confirmed that PEDOT/Zr-K-OMS-2 comprises a highly crystalline random network of two-dimensional PEDOT flakes and Zr-doped K-OMS-2 nanoribbons.<sup>4</sup> In this regard, the proposed interfacial strategy affirms an *in-situ* method for the morphological tuning of heterostructures on polymer supports at low temperatures.<sup>4</sup>

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## Synthesis and characterization of BTCA/PANI/MoS<sub>2</sub> Ternary nanocomposite for energy harvesting as supercapacitor

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### Abstract

We report the formation of benzene 1,2,4,5-tetracarboxylic acid (BTCA) doped PANI nanostructures functionalized with MoS<sub>2</sub> to investigate and enhance the supercapacitive behavior of the ternary nanocomposite BTCA/PANI/MoS<sub>2</sub>. The reported work successfully synthesizes a novel ternary composite, BTCA/PANI/MoS<sub>2</sub>, utilizing an in-situ polymerization approach. BTCA serves as a soft template, dopant acid, and surfactant, aiding in composite formation. MoS<sub>2</sub>'s layered structure enables EDLC and pseudocapacitance, PANI enhances conductivity and pseudocapacitance, while BTCA acts as a template and surfactant, improving capacitance and stability. Synergy among MoS<sub>2</sub>, PANI, and BTCA holds promise for improved supercapacitor technology. BTCA plays the role of a dopant acid as well as a structure-directing agent. The system has been optimized and found BTCA: Aniline (An) to be 1:4 and An: APS (Ammonium persulphate) to be 1:1 (molar ratio). Electrochemical characterization indicates that the synthesized ternary composite BTCA/PANI/MoS<sub>2</sub> exhibits enhanced supercapacitive behavior, as evidenced by the increasing area under the cyclic voltammetry (CV) curve and increase in the maximum current with an increase in the scan rate. This behavior can be attributed to the capacitive properties of the composite. Furthermore, the conductivity of the ternary composite is found to be dependent on the molar ratio of BTCA to An and follows the variable range hopping mechanism, providing valuable insights into the electrical transport phenomena in the composite material. BTCA/PANI/MoS<sub>2</sub> suggests improved  $\pi$ - $\pi$  interchain stacking which results in increased conjugation length, longer mean free path and finally supports improved carrier transport because of less structural disorder of the PANI chain.

## **Solvent Based Waste Polyolefins Recycling: Challenges and Opportunities**

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### **Abstract**

Disposal of accumulated plastic waste and the associated environmental concerns have garnered significant attention. Transforming waste plastics into valuable resources by various technique such as mechanical recycling, pyrolysis etc. holds the potential to establish a circular economy and material recycling [1-2]. India recycles only 30% of 3.4-million-ton plastic waste generated annually with annual plastic demand of ~15 million tons [3]. Mechanical recycling involves the collection, sorting, and reprocessing of polyolefin while pyrolysis involves the thermal degradation of polyolefins to yield valuable products like fuels and chemicals. Colour of used plastics as well as inorganic additives added are not getting removed in mechanical recycling. To overcome the fundamental limitations of mechanical recycling, solvent based recycling technique is developed to purify contaminated polymers via chemical approaches. Solvent based recycling technique uses the extraction of impurities in solvent and the dissolution of polymers, which produce high-quality recovered plastics comparable to virgin polyolefin. Researchers and technologist are now focusing on development of cost-effective, scalable, and simple process. This talk will summarize the overview of polyolefins recycling techniques and its benefit and disadvantages along with commercial technology examples. Further challenges and opportunities are solvent based polyolefins recycling technologies will be discussed along with few examples. Solvent-based polyolefin recycling offers a promising pathway to manage plastic waste, promote resource efficiency, and contribute to a greener.

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## **Rapid evaluation of photo, thermal and oxidative degradation of high impact polystyrene by a xenon lamp-based online ultraviolet irradiation-pyrolysis-GC/MS system**

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### **Abstract**

Photo, thermal and oxidative degradation behaviors of high impact polystyrene (HIPS) containing butadiene rubber (BR) were evaluated by online ultraviolet irradiation-pyrolysis (UV/Py)-GC/MS system with a micro-UV irradiator. Volatile degradation products evolved during UV irradiation at 60 °C in air were identified and quantified through online GC/MS measurements. Formation of some typical volatiles from the HIPS sample during 1 h irradiation, such as benzaldehyde, acetophenone and benzoic acid originating from PS and 2-propenal from BR, clearly indicates the contribution of oxidative reactions in the polymer chains. Moreover, the residual HIPS samples after irradiation up to 12 h were characterized by evolved gas analysis-mass spectrometry (EGA-MS). The observed EGA thermograms clearly showed not only lower temperature shifts of onset and peak top of gas evolution, but also peak broadening compared with that of the original HIPS sample, reflecting some structural changes in HIPS polymer chains during the irradiation. Furthermore, the degradation behavior of HIPS by the micro-irradiator was compared with that obtained by the conventional accelerated degradation test using a Xe weather meter. The observed EGA profile of HIPS irradiated by the Xe weather meter for 300 h showed the equivalent temperature shift and broadening to that for the residual HIPS after 1 h irradiation by the micro-UV irradiator. This result suggests that the micro-UV irradiator in UV/Py-GC/MS system might achieve the comparable degradation processes of polymeric materials much more rapidly compared with the conventional accelerated degradation test methods.

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## **Cutting-Edge Solutions: Viability of Abrasive Waterjet Machining to Characterise Residual Stress using Contour Method in Polymer Composites**

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### **Abstract**

Residual stress in polymer composites is an often overlooked yet significant aspect that demands attention. These stresses, which result from the manufacturing processes, can significantly affect the structural integrity, durability, and dimensional accuracy of polymer composites. By providing precise stress distribution data, it aids in assessing the structural integrity, predicting material failure, and optimizing manufacturing processes.

The contour method involves carefully severing the sample and then analysing the resulting deformation contours. The contour represents 2-dimensional distribution and magnitude of displacement profile due to the release of residual stress in the cut plane. By measuring the surface deformation and applying the Bueckner's principle [1] one can accurately determine the residual stress present in the material. With its ability to provide detailed 2D bulk residual stress, it is emerging as a most common technique to characterise residual stress in the components of aerospace and automobile industries. However, the method is widely applied on only metals, as the conventionally used wire- Electric Discharge Machining as a cutting technique relies on the conductivity of the sample of interest. And hence poses challenging in applying the method on polymer composite due to its non- conductivity [2]. The present study aims to explore the suitability of abrasive waterjet cutting technique for the application of contour method to characterise residual stress in polymer composites.

### **Acknowledgements**

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## Effects of antibacterial ZnO nanoparticles on the performance of a mucilage edible coating for post-harvest fruit preservation

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### Abstract

The potential application of ZnO nanoparticles have been extensively used as a antibacterial agents in edible coatings to protect food from deterioration by viruses, fungi, and bacteria. In this work, ZnO nanoparticles were synthesized by *Dillenia indica* sepals extract and characterized by X-ray diffraction (XRD), fourier-transform infrared spectroscopy (FTIR), field emission scanning electron microscope (FESEM) and energy dispersive X-Ray analysis (EDX). The size distribution of ZnO nanoparticles observed in the FESEM micrographs ranged from 40 to 70 nm and the analysis of EDX spectra confirmed the presence of zinc and oxygen in the ZnO nanoparticles with atomic composition percentages of 52.67% and 47.33%, respectively. Furthermore, the antibacterial effects of ZnO-NPs were determined by measuring the minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) against *E. coli* and *S. aureus* respectively. The ZnO nanoparticles as an antibacterial agent were incorporated into a mucilage extracted from the gelatinious pulp of *Dillenia indica* for edible coating of fruits. The effects of mucilage/ZnO coating on quality attributes and shelflife of fruits were studied. Therefore, ZnO nanoparticles prepared by the green method has great potential in food packaging application.

## Impact Analysis of the Forward Osmosis Process Combined with Ultrafiltration Pretreatment in Coconut Water Concentration

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### Abstract

Coconut water is one of the most popular drinks worldwide due to the nutritional benefits offered by it<sup>1</sup>. The demand for packaged coconut water is increasing day by day. Several Membrane technologies are utilized to process the coconut water before packaging. Few of these processes are used for clarification, whereas Reverse Osmosis (RO) and Forward Osmosis (FO) are used for concentration. Due to Lower energy requirements during processing and lower transportation costs associated with the concentrated product of coconut water, the FO process offers superiority over other membrane processes. However, flux during the process is difficult to maintain throughout the FO process, which limits its application in Industrial products<sup>3</sup>. In this study, an attempt has been made to increase the flux by using Ultrafiltration (UF) hollow fibre membrane for the pretreatment step before the FO process, and in retentate of UF process has been added again in the concentrated product of the FO process. It is observed that pretreatment results in increased water flux for all three draw solutions (i.e., 1M NaCl, 2M NaCl, and 4 M NaCl) used in our study. Also, this two-step treatment process can achieve higher concentration factors while utilizing retentate as the first step for nutritional preservation. Thus, it can be concluded that pretreated coconut water has higher flux in the FO membrane process, and with the addition of UF retentate, nutritional values of coconut water are also preserved.

**Keywords:** Membrane process, Forward osmosis, Concentration, Pretreatment, Flux enhancement

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## Metal-Catalyzed Depolymerization and Upcycling of Polyethylene to Value Added Chemicals

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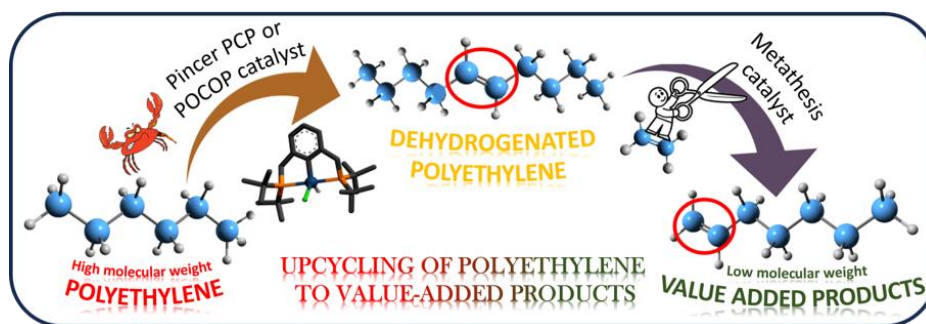
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### Abstract

The mounting environmental concern posed by the accumulation of non-degradable waste plastic, particularly polyethylene, demands innovative solutions. To address this challenge, we introduce a breakthrough technique to convert waste polyethylene into valuable long-chain mono- and bis-functional olefins. This approach comprises two key steps: the first step involves iridium PCP or POCOP ligand-driven dehydrogenation, which generates dehydrogenated polyethylene (DHP) with around 1% double bonds. The second step employs Grubbs catalyst-mediated cross-metathesis, enabling the transformation of DHP into long-chain olefins. Rigorous optimization of metathesis reaction conditions, including time, temperature, and pressure, yielded 50-77% overall yield of these valuable olefin products. This marks a pioneering achievement in the direct conversion of waste polyethylene, necessitating further research and scale-up endeavors to combat plastic pollution.



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## An experimental study on lubricating behaviour of pectin-based gel by rheological and tribological measurements

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### Abstract

The utilization of biopolymer-based lubricants has garnered increasing attention due to their biodegradability, safety, and potential applications in various industries. Pectin, a water-soluble polysaccharide found in the cell walls and intercellular tissues of certain plants, is well known for its gelling ability, thickening and stabilizing properties. Depending on degrees of acetylation, methylation and contents of galacturonic acid in it, pectins demonstrate gelling properties and can form complexes with divalent cations like  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$ . Although several other gels have found a large number of applications as a lubricant in every day medical, food products and cosmetics industries, but lubrication behaviour of pectin-based gel is still not understood. This study focuses on characterizing the lubrication properties of a pectin-based gel lubricant through a combination of rheological and tribological measurements. The rheological properties of the pectin-based gels were investigated using steady shear, large amplitude oscillatory shear (LAOS), small amplitude oscillatory shear (SAOS), measurement of stress and normal stress difference as a function of shear rate and complex modulus over the time at low and high shear strain. Tribology measurements were carried out in order to examine the coefficient of friction of the gels in dependence of the concentration. Rheological insights provided a comprehensive understanding of the gel's mechanical behaviour, while tribological measurements underscored its potential in reducing friction and wear. The findings can contribute to the development of sustainable lubrication alternatives and open avenues for further exploration in various industries.

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## Clay based Polyaniline/Acetylene Black nanocomposite for fabrication of symmetric supercapacitor

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### Abstract

Investigating new electrode materials is one of the most important steps in creating high performance energy storage systems to effectively utilize renewable energy. Clay minerals, notably montmorillonite (MMT), could be a possible candidate for electrode materials due to their naturally porous structure, strong ionic conductivity, high specific surface area, and environmental friendliness. However, due to their poor electrical conductivity, MMT cannot be used as a sole electrode material for supercapacitors. Therefore, to change the surface conductivity, conducting polymers would be a good choice. In this study, we have developed a novel ternary nanocomposite by in-situ chemical oxidative polymerization employing polyaniline (PANI) as the conducting polymer, acetylene black (AB), and MMT with varying mass ratios. The electrochemical performance of all the composites as electrode material for supercapacitors were examined, the ternary composite PANI/AB/MMT (16:1:1) displayed the highest electrochemical performance. Further investigation has been done on the constructed symmetric capacitor based on the PANI/AB/MMT (16:1:1) nanocomposite in both aqueous and solid polymer electrolytes (viz., PVA/H<sub>2</sub>SO<sub>4</sub>). In the solid electrolyte, the device generates specific capacitance of 772 F/g, energy density of 107.2 Wh/kg, and power density of 2000 W/kg at a current density of 1 A/g. Moreover, after 6000 cycles at a current density of 5 A/g, the device shows the capacity retention of ~ 98%. The increased performance of electrode material is attributed to the synergistic interaction of the three components, which results in an improved electroactive sites, increased surface area, mesoporous structure, reduced internal resistance, and high chemical stability.

## Cellulose Nanofiber-incorporated High-Solid Siloxane Acrylic Latex by Mini-emulsion Polymerization for Hydrophobic Coating and Wood Adhesive

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### Abstract

In order to contribute to the thriving research on bio nanocomposites for sustainable future, here we developed a cellulose nanofiber (CNF)-based siloxane acrylic nanocomposite aiming to the application as hydrophobic coating and wood adhesive. CNF was incorporated in a copolymer matrix of poly (methyl methacrylate-co-butyl acrylate) [P(MMA-co-BA)] cross-linked with methacrylate-terminated siloxane (MTS). The copolymer was prepared by mini-emulsion polymerization at a high solid content of about 57 wt%, where CNF was incorporated to the latex both by *in-situ* polymerization and *ex-situ* mixing process. The impact of the process of CNF incorporation and its content in the copolymer matrix were evaluated by measuring the thermal, mechanical, water repelling and adhesion properties. All the nanocomposites showed improved mechanical properties (tensile strength: upto 3.9 MPa) and wood adhesion strength (upto 1178 N) compared to the pristine copolymer. In addition, they showed significantly high water-repelling properties on spray-coated cotton (water contact angle: 110°–124°). Such siloxane acrylic/CNF nanocomposite has the potential as a sustainable material in the application area of hydrophobic coatings and adhesives.

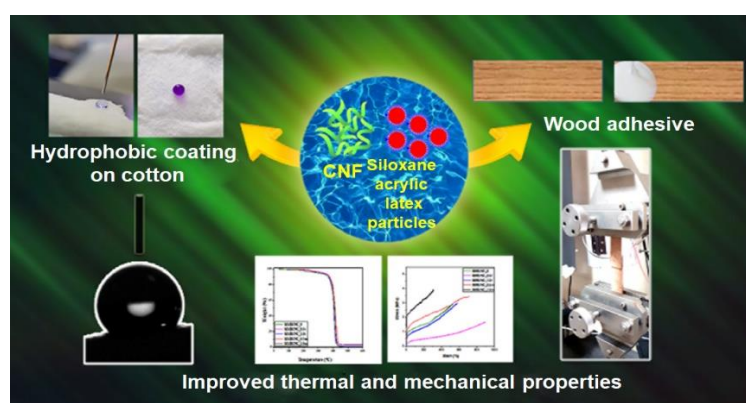


Fig 1. Siloxane acrylic polymer/CNF nanocomposites showing Improved properties and multifunctional applications.

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## Influence of chemical pretreatment on the degradation profile of epoxy resins, a precursor to fibre reinforced polymer composites

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### Abstract

The remarkable material properties of fiber reinforced polymer (FRP) composites attracted a huge applicability in various industries.<sup>1,2</sup> The widespread application resulted in a tremendous volume of 'End-Of-Life' (EOL) materials. The manufacture of virgin carbon fibre is a high-energy demanding high-temperature process (>1000°C).<sup>3</sup> These challenges demand a sustainable recycling process to recover the fibers from EOL composite. Incorporating two or more traditional recycling approaches (Mechanical, Thermal or Chemical) enhances overall efficiency by eliminating the drawbacks of individual methods. The present study adopts an idea of chemical pre-treatment followed by pyrolysis and examines the effect of chemical pre-treatment on degradation profile of the epoxy resin (ER) used for the fabrication of FRP composites. The cured ER was pre-treated with a solvent-metal salt system and the degradation profile was analysed using thermo gravimetric analyser. The pre-treatment of epoxy resin with 10% (w/v) ZnCl<sub>2</sub>-Ethanol system at 75°C for 120 min gives a reduction of 27.2°C in the degradation profile (Figure 1). Therefore, the chemical pre-treatment proved efficient in reducing the degradation temperature of the ER and so will aid same for FRP composites. The ethanol in the pre-treating solution acts as a swelling agent for the ER allowing the Zn<sup>2+</sup> ions to penetrate through it.<sup>4</sup> The penetrated Zn<sup>2+</sup> ions create organometallic linkages with the C-N bond in ER, promoting catalytic ER breakdown.<sup>5</sup> The study will be extended with other metal salts to compare the influence on the degradation temperature profile of the ER.

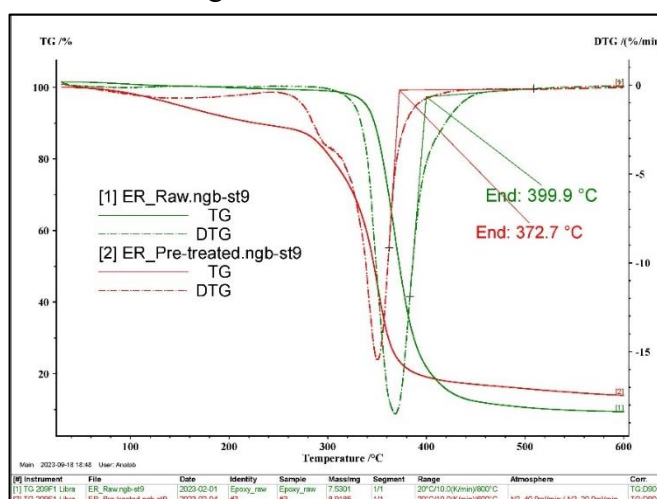


Figure 1. TGA and DTG curves of raw and pre-treated ER

### Acknowledgment

Financial support provided by Tata Steel Limited is gratefully acknowledged.

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## Development of Novel Nucleating Agent for Polypropylene

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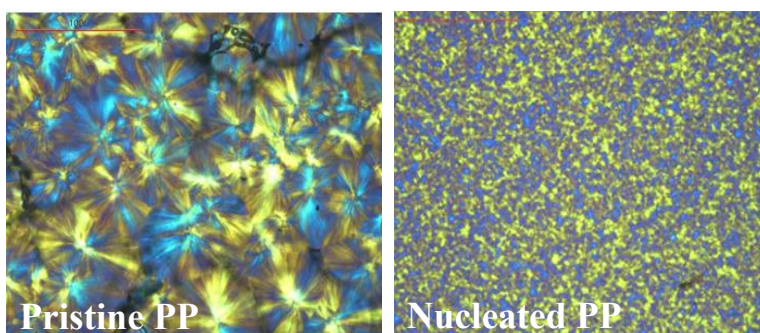
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### Abstract

Nucleating agent (NA) is used as an additive during the polypropylene processing to initiate the crystallization and augments the speed of overall process by providing faster crystallization rate. NA offers heterogeneous surface to polymer mix and finally can affect the properties of the end product. The NA is largely employed in enhancing the mechanical properties and improving the clarification of product. The nucleating agents are currently much more in demand than ever before as it gives higher productivity during processing of polypropylene at minimum dosage.

In-house synthesized urea-based novel nucleating agent was mixed with polypropylene then processed in twin-screw extruder within desirable processing temperature window to make nucleated PP. The nucleated PP was characterized by DSC, XRD and TGA to study the crystallization behavior and thermal stability. Further, the ASTM test specimens of nucleated PP were prepared by injection molding machine to analyze the mechanical properties, color index and haze.

In-house developed NA incorporated into PP possess higher crystallization temperature as compared to pristine PP. The nucleated PP shows better thermal stability, shrinkage and mechanical properties in terms of flexural modulus and tensile properties, as compared to pristine PP. The developed NA showed comparable performance as commercially available nucleating agents. So, these set of properties of NA can be provided marked benefits over commercial nucleating agents.



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## N-doped Carbon Nanofiber, Coated with PEDOT:PSS-Polyvinylpyrrolidone and their PDMS Composites as Flexible, high-performance Electromagnetic Interference Shielding Material

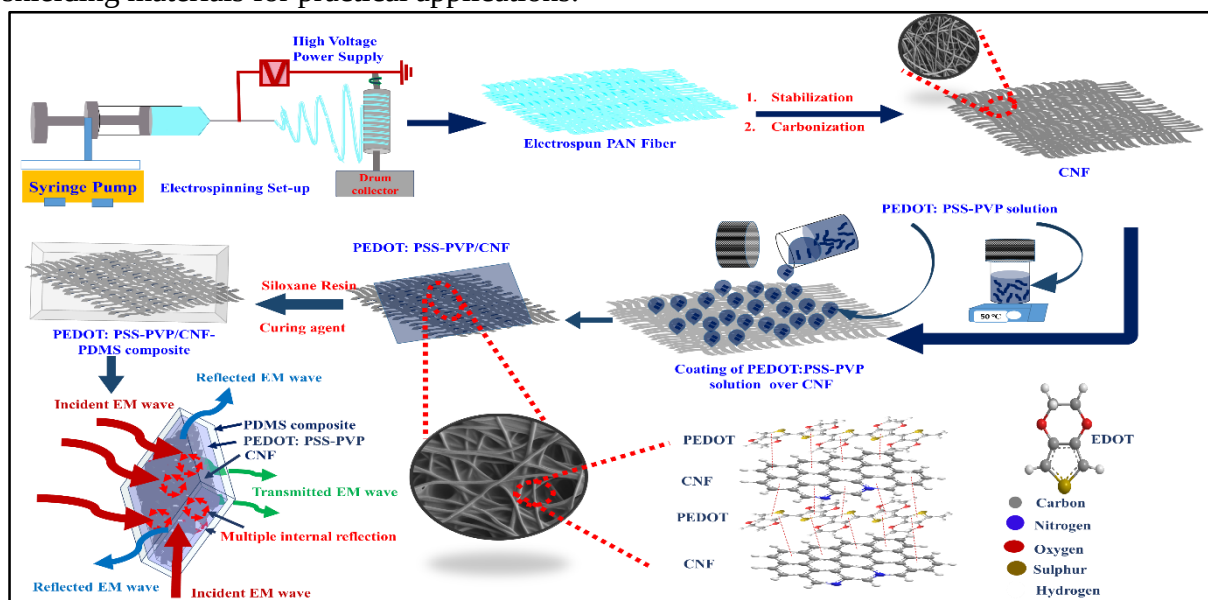
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### Abstract

Fast growth in the usage of lightweight, flexible, and portable electronics and wearable devices have contributed to and will continue to enhance electromagnetic interference (EMI) or EM pollution in an unprecedented level. Consequently, huge attention is being given to development of efficient, lightweight, hydrophobic, and flexible EMI shielding materials. The current work concerns with fabrication of poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT:PSS) and polyvinylpyrrolidone (PVP) coated, carbonized electrospun polyacrylonitrile (PAN) nanofiber (CNF) and their flexible polydimethylsiloxane (PDMS) composites. The material exhibited a high EMI shielding effectiveness of 44 dB in the frequency range of 8–26.5 GHz with a thickness of 0.06 mm. The high performance of the material is due to the combined effect of CNF matrix, PEDOT: PSS, and PVP. The material also showed excellent absolute EMI SE of  $5678 \text{ dB cm}^2 \text{ g}^{-1}$  with low loading of PEDOT:PSS-PVP. It is observed that PEDOT:PSS-PVP/CNF showed EMI shielding through an absorption-dominated mechanism rather than reflection. The results of the work imply that these composites are promising to be explored as thin, flexible, hydrophobic, and lightweight EMI shielding materials for practical applications.



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## Flexible and High Temperature Stable Polybenzoxazine Adhesive for Fire Proximity Clothing

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### Abstract

Benzoxazine linkage forms due to the Mannich-like condensation reaction between an amine group and phenolic -OH group which has encountered enormous interest among material chemists in the past 30 years.<sup>1</sup> However, polybenzoxazine formation induces hardness in the material which is a major challenge in using benzoxazine materials as a laminating adhesive between different material layers.<sup>2</sup> A number of reports with different modifications can be found in the literature to incorporate flexibility in the cured material although proper investigation of the process and systematic testing of the final material towards different applications is still missing.

To address this issue molecular tailoring of the benzoxazine molecule and the different curing techniques were taken into account to prepare a flexible, high-temperature resistant material in order to form the crosslinked polybenzoxazine chains. Flexible polybenzoxazines are particularly interesting in order to create a next-generation adhesive material that can withstand high temperature. As a possible application of this prepared adhesive material, the benzoxazine material was used for laminating glass fabric and one-sided aluminized PET film for use as the outermost layer of a fire proximity suit.<sup>2</sup> Also, the NFPA 1971 requirements were taken into account in order to validate the usability of the material as a better adhesive to be used in the fire proximity suit. For this purpose, BAP benzoxazine resin was synthesized and different formulations with amine-containing curing agent (ATBN) were investigated for fast curing at low temperature. DSC technique was utilized to examine the curing of the benzoxazine with amine, and TGA was used to examine the thermal stability of the cured benzoxazine adhesive. A temperature sweep rheology experiment was also conducted to examine the viscosity increase with temperature to determine the processing window of the synthesized adhesive. Furthermore, different testing methods such as peel adhesion testing, wet flex testing, radiation protective performance testing, and thermal protective performance testing were performed. Upon formulation of BAP benzoxazine monomer with ATBN the prepared material qualified all the standard tests for the adhesive characterization and all the formulations proved to provide better thermal protectiveness when compared with the commercial material GENTEX. However, 50:50 ratio of BAP and ATBN proved to be the better adhesive for the fire protective suit.

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## Functionalized jute: A biodegradable material with high charge, swellability, flame retardancy, and thermal stability

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### Abstract

Plastic-based packaging materials, being non-biodegradable, pose detrimental effects on the environment, human health, and wildlife. To address this issue, jute, a naturally occurring plant-based fiber with a historical use in storing fruits, vegetables, grains, and cereals, has been utilized to fabricate functionalized jute. The present study uses discarded jute bags to produce functionalized jute, which shows outstanding properties including superior water absorption and retention capacity, flame retardancy, thermal stability of up to 700 °C, and biodegradability. The modified jute displays a remarkable characteristic of rapid swelling when exposed to water. The functionalized jute exhibits high water absorption capacity when compared to normal jute, a negative charge, a minimal evaporation rate, biodegradability and has the potential to be utilised efficiently in the preservation of perishable fruits and vegetables. Thus, the functionalized jute has the potential to serve as an eco-friendly, sustainable, and biodegradable alternative for plastic-based food packaging materials.

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## Polyester Additives for Bitumen Modification

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### Abstract

In recent years, an increase in traffic load on road-building materials has led to a search for binders regarding the improvement in the performance of the base bitumen [1]. In the course of bitumen quality improvement, bituminous binders are often used before being utilized in the paving application [2-4]. The present study demonstrated the synthesis of sixteen colorless polyester-based additives to improve bitumen's mechanical and rheological properties. The polyesters were synthesized by polycondensation of maleic anhydride and glycerol in different molar ratios and reaction times. All sixteen polyesters were screened and optimized for bitumen modification using a dynamic shear rheometer study, and M3G1H5 was chosen as the bitumen modifier as it showed the least phase angle at 65 °C and a better fail temperature of 65.25 °C at shear modulus of 1.1 kPa compared to other polyesters. The M3G1H5 polyester is blended with conventional bitumen with varying concentrations of 6 to 15 wt% to make three modified bitumens, M3G1H5VG10-I, M3G1H5VG10-II, and M3G1H5VG10-III. These modified bitumens were physiochemically characterized for penetration, softening point, kinematic viscosity, dynamic viscosity, ductility, penetration index, and rheological analysis as per standard ASTM test procedures. The results revealed that except absolute viscosity, M3G1H5VG10-I and M3G1H5VG10-II meet the specification of VG30 and VG40 bitumen, respectively. The rheological study showed that M3G1H5VG10-I and M3G1H5VG10-II have better deformation resistance, complex modulus, and rutting resistance over conventional bitumen. The fail temperature at  $G^*/\sin\delta$  1.1 kPa for M3G1H5VG10-I and M3G1H5VG10-II were found to be 69.52 and 73.13 °C, respectively. Both the storage and loss shear modulus were significantly improved for M3G1H5VG10-II, indicating that M3G1H5 polyester increases the resistance to rutting and deformation.

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## Nanofibrillated Polymeric Composite Membranes using Electrospinning for Particulate Matter Removal from Ambient Air

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### Abstract

Increasing lifestyle and industrialization lead to continuously growing ambient air pollution in this modern era. Increased air pollution became a significant threat to human health as well as the ecological system. In modern day, people spend most of their time indoors, so it is very necessary that the breathable air should be clean and free from pollutants. To achieve a clean indoor environment, we are focused on the development and application of electrospun nanofibrillated composite membrane using nano structured inorganic oxides and cellulose acetate polymer for efficient removal of particulate matter from the surrounding ambient air. Through electrospinning, we fabricate membranes with intricate nano-scale fibrillar structures, optimizing surface area and filtration efficiency. These membranes are systematically characterized using SEM, XRD, and UTM and tested for their particulate matter removal capabilities. The study investigates factors such as membrane composition, morphology, and operational parameters, assessing their influence on filtration performance. Our findings demonstrate the exceptional potential of these nano-fibrillated membranes as advanced filtration media for mitigating ambient particulate matter pollution, we have observed high filtration efficiency and low pressure drop across the membrane at serve air quality (200  $\mu\text{g}/\text{m}^3$  concentration of particulate matter ( $\text{PM}_{2.5}$ )), offering a promising solution for enhancing air quality and environmental well-being.

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## Exploring the Structures, Growth and Spectral Properties of Some Polymers: *Ab Initio* Quantum Chemical and Density Functional Theory Perspective

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### Abstract

During the past few decades, the field of 'Computational Simulations' has become an indispensable approach in handling the challenges of modern times in all branches of science, including polymer science, both in academia and industry. Thus, it is no wonder that the application of quantum chemistry, in particular density function theory (DFT), has become a fundamental tool for pre-emptive determination of properties as well as gauging its role, prior to actually doing an experiment in the laboratory.

Polymers and their nanocomposites have received attention due to their diversified applications resulting from their unique characteristics, viz., exceptional strength and stiffness-to-density ratios and superior physical properties. The results of the quantum chemical study of some industrially important polymers (modeled by the oligomers) with reference to the structures, growth, and spectral properties within *ab initio* quantum chemical and DFT frameworks will be presented.

**Keywords:** Polymer conformers, Polymer nanocomposite, *Ab initio* quantum chemistry, Density functional theory, Structural Properties

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## Drug Eluting Mucoadhesive bandage for Localized Oral Drug Delivery Applications

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### Abstract

Multiple gel formulations for the treatment of various oral disease conditions are available in the market. However, the retention of these drugs in the target gingival region is challenging as those common gel formulations can be easily wipe down from the oral moist environment by food, liquids and even saliva. There is a massive need for formulations that can enhance the retention of drugs in the disease site. Various mucoadhesive systems in the form of microparticles, tablets, and paste containing drugs such as bethamethasone disodium phosphate, mycophenolate mofetil, hydrocortisone acetate, clobetasol propionate, curcumin, triamcinolone acetonide, and licorice has been reported. To overcome these challenges, we have developed mucoadhesive drug eluting bandage that can enhance the retention of drug in the dynamic oral environment. The mucoadhesive bandage showed an excellent mucoadhesive properties with a force of adhesion of > 350 g.

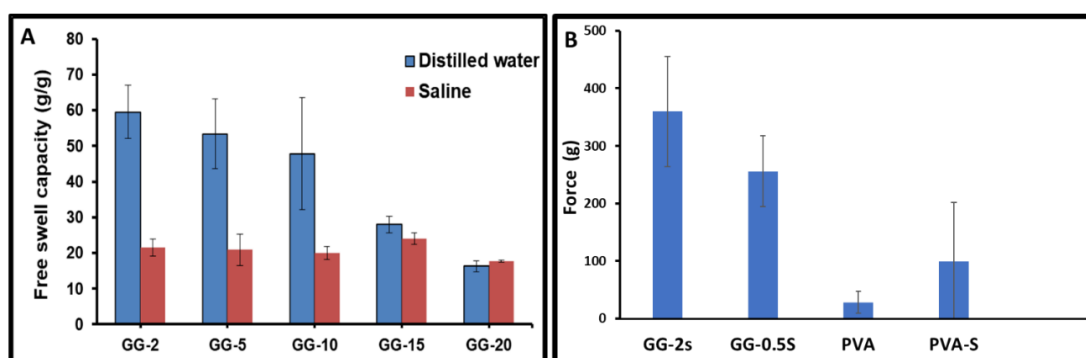


Figure 1: (A) % swelling polymer film at different crosslinking density in different media (B) force of adhesion of mucoadhesive layer of the bandage along with the control film of polyvinyl alcohol.

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## Biodegradable, hydrophobic, antibacterial, self-cleaning and sustainable drinking straws from rice crop waste

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### Abstract

The Rice cultivation has grown considerably in recent decades globally, leading to large amounts of rice straw (RS) waste production. The disposal of RS by burning generates significant amounts of toxic greenhouse gases, leading to severe harm to the atmosphere and living beings. The current work proposes a facile, scalable, and low-cost strategy for preparing all cellulose-based, adhesive-free, antibacterial, self-cleaning, drinking straws from rice crop waste (culm and leaf sheath) via delignification, crosslinking, and silane functionalization. The prepared straws showed high water stability (~5 days), solvothermal stability (0-95°C), tensile strength (128 MPa), low component leaching (>60 mg/kg), biodegradability (~126 days) and reduced wettability (105° water contact angle). The single-use plastic straws are the commercial standard which due to its non-degradability and toxic effects on the ecosystem and life forms is a significant concern. Paper straws as an alternative possess several limitations including the use of non-degradable adhesives, low water stability, and generation of odor in beverages. Compared to current commercial sustainable straw alternatives such as stainless steel (SS) and polylactic acid (PLA) straws, rice waste-based drinking straws with minimal processing, generate significantly lower carbon footprints (99.8% and 53.34% less GWP than SS and PLA straws, respectively) with enhanced straw features.

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## A study on the effect of rice husk ash addition on dimensional stability of glass fabric reinforced epoxy hybrid composites

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### Abstract

Rice husk ash (RHA) a source of silica was synthesized by burning the rice husk in muffle furnace at 550 °C for 5 h and subsequently used as filler material in glass fabric reinforced epoxy (EP/GF) composite. The EP/GF/RHA hybrid composite laminates with varying amount of RHA (0, 5, 10 and 15 wt.%) were fabricated by cost effective hand layup technique followed by compression moulding. The density, fiber volume fraction and void volume fraction of EP/GF/RHA composites were measured. The phase analysis of composites was done by using X-ray diffraction technique (XRD). The scanning electron microscopy (SEM) was used to see the dispersion of RHA particles and the coefficient of thermal expansion (CTE) was determined by dilatometry. The density of all the composites was found in the range of 1.6 - 1.66 g/cm<sup>3</sup> while the void volume fraction was increased with increasing RHA content. No sharp peaks were observed in XRD patterns of EP/GF composites with and without RHA indicating amorphous nature. The SEM revealed uniform dispersion of RHA particles all over the matrix. The CTE of neat epoxy was significantly reduced when reinforced with glass fabric as well as RHA and found close to the metals. The composite with 10 wt.% RHA showed lowest CTE. These results show that all composites are light weight with better dimensionally stability and could be recommended for applications where low CTE is of prime importance.

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## Influence of Spin Bath Parameters and Spinning Speed on Mechanical Properties of Viscose Filaments

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### Abstract

To convert Cellulose into usable textile material it must dissolve/derivative and convert it into other form. One of old method is to convert Cellulose by preparing Viscose solution and spun it form Viscose fiber. In this process cellulose derivatization performed of using CS<sub>2</sub> and Cellulose derivative is subsequently dissolved in NaOH. Then it is regenerated in a coagulation bath, of form Cellulose fibers/filaments. In general, the coagulation bath consists of H<sub>2</sub>SO<sub>4</sub>, ZnSO<sub>4</sub> & Na<sub>2</sub>SO<sub>4</sub> wherein H<sub>2</sub>SO<sub>4</sub> & Na<sub>2</sub>SO<sub>4</sub> plays the role of converting cellulose xanthate solution into regenerated cellulose. The ZnSO<sub>4</sub> retards the reaction to slower down the regeneration process and play critical role in fiber/filament structure formation. In this study different concentration of acid and zinc were studied along with varying spinning speed and its effect on the physical and mechanical properties of the yarn was evaluated. The yarn morphology and cross section was studied using Scanning Electron Microscopy (SEM), the orientation of cellulose in yarn was studied using Birefringence & X-ray Diffraction (XRD). From this study it was observed that with lower ZnSO<sub>4</sub> concentration tenacity of yarn increased by ~9% with the increase of ~35% H<sub>2</sub>SO<sub>4</sub> concentration in coagulation bath. Whereas at higher ZnSO<sub>4</sub> concentration the opposite trend was observed with tenacity decreasing by ~21% with similar increase bin acid concentration. In this study the effect of spinning speed was also studied, and it was observed with decreasing the speed by ~31% the average tenacity decreased by ~6.5%.

## Plant extract-loaded biocompatible, biodegradable, and bioactive polymeric films for potential biomedical applications

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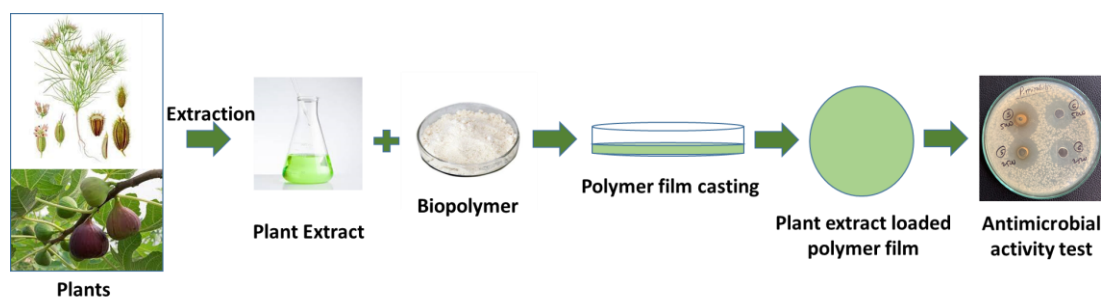
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### Abstract

The present study was aimed at obtaining natural biomaterial-based polymeric films loaded with plant extracts to exhibit antibacterial activity based on selected plants with biological activity for potential biomedical applications. The extracts were obtained from various comparatively less studied and promising plants by direct and successive extraction methods using a series of solvents. These extracts were studied for their biological activity against various microorganisms. The biologically active extracts were then mixed with a biopolymer such as polysaccharide—a bioactive, biocompatible, and biodegradable polymer—to obtain plant extract-loaded natural polymeric films for antibacterial activity. The plant extracts and the films were characterised by various techniques such as HPLC, HPTLC, LC-MS, antimicrobial studies, etc. As hypothesised, the natural polymer films behaved excellently as drug carrier mediums and exhibited improved antimicrobial activity against *P. mirabilis* and *S. aureus*, responsible for skin and urinary tract infections. It is noticed that the plant extracts obtained in certain solvents that did not show any biological activity showed considerable improvement in activity after combining with the polymeric materials. The increase in activity suggests the synergy between biopolymer and plant extract polyphenols, resulting in enhanced bactericidal properties. Thus, the plant extract-loaded biocompatible, biodegradable, and bioactive polymeric films obtained in the present study have the potential to find biomedical applications, such as in skin and soft tissue infections.

**Key words:** polymers, bioactive, biodegradable, antimicrobial, biomedical applications, plant extract.



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## Toughened Thermoset Blend of Epoxy with Glycidyl Terminated Polyurethane Exhibits Simultaneous Scratch-Healing and Shape-Memory Properties

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### Abstract

Integrating multifarious functionalities as well as stimuli responsiveness in a polymer matrix is highly desirable but remains an ongoing challenge. We report, glycidyl terminated polyurethane (GPU) induced simultaneous tunability of glass transition temperature, toughening, crack-healing and shape memory effects in a widely used epoxy thermoset. The GPU was synthesized by a two-stage end-capping process of isocyanate functionalization of polyols followed by glycidation. Blends of GPU and epoxy resin were cross-linked with a polyether diamine and characterized by a combination of complimentary analytical tools to delineate the hydrogen bonding interactions, phase morphology and segmental dynamics of the networks. The networks exhibited GPU induced tunable  $T_g$  and  $\alpha$  relaxation characteristics over a temperature range of 30-80 °C. Significant improvements in fracture toughness values for the thermoset blends were observed (20 % increase in  $K_{1C}$  and 270 % increase in  $G_{1C}$  at 15 wt. % GPU content) compared to the pristine epoxy network. Scratch-healing ability of the networks was evident from complete disappearance of wider scratch after thermal treatment at 80 °C for only 5 minutes. The blends showed dual shape memory effect (SME) with near perfect shape fixity of 99% and progressively increasing shape recovery (70-88 %) with increased GPU content. A triple shape memory effect was shown by 20% GPU containing network with shape fixity and shape recovery values > 90%. We posit the present study contributes towards design and development of multifunctional smart epoxy resins through a facile blending approach without resorting to the time and cost intensive dynamic covalent bond chemistries.

**Key Words:** Glycidyl polyurethane, epoxy, toughening, scratch-healing, shape memory, vibration damping.

## Efficient Optically Tunable Photoluminescent Polymeric Membrane

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### Abstract

The stretchable optoelectronic device derived from polymer represent one of the core research area.<sup>1,2</sup> The solvent dependent aggregation induced emission (AIE) will soon be replaced with polymeric membrane showing energy tunable emission. The thermal stability, water contact angle ( $\theta_c$ ) and viscoelasticity ( $\tan\delta$ ) represent certain crucial properties for optoelectronic material essential to improve quantum efficiency ( $\Phi$ ). Such selective properties within the membrane has potential to minimize or neutralize the mechanical and electrical damage.<sup>2</sup> The switch in contact angle( $\theta_c$ ) can cause switch in water flux. The contact angle ( $\theta_c$ ) monitor the percent of hydrophobicity and hydrophilicity for the synthesized membrane. This influences the stabilization of the  $\pi$ -stacked aggregates of polynuclear aromatic hydrocarbons (PAHs). Such phenomena is possible with switch in monomer for membrane synthesis. The PAHs used for tunable emission are simple. The tunability in emission was observed from ultraviolet (UV) to visible region. The energy tuned emission with simple PAHs showed low, moderate and high value of correlated color temperature ( $T_{cp}$ ) which can be a remarkable observation. The membrane with high  $T_{cp}$  values are crucial for the study of marine ecosystem. The membrane derived using simple PAHs changing the backbone showed improvement in quantum efficiency ( $\Phi$ ).<sup>3-5</sup> The incorporation of chirality influences the optical parameters such as fluorescence polarizance ( $\beta_{L/C}$ ) and fluorescence diattenuation ( $\alpha_{L/C}$ ). The polymeric membrane with all essential properties has scope to develop energy tunable promoter for catalysis to green synthesis and for dye degradation Therefore, such material has bright future towards catalysis and as efficient sensor.

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## Carbonated Castor Oil - Bioplasticiser and Toughening Agent for Amine Cured DGEBA Epoxy Resin

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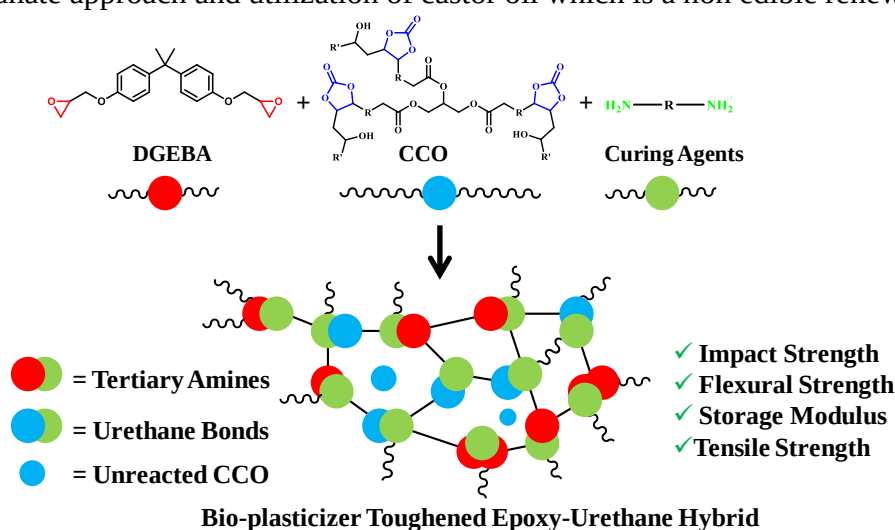
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### Abstract

Diglycidyl ether of bisphenol A (DGEBA) is commonly employed as the intermediate for the synthesis of epoxy resins, primarily because of its advantageous characteristics such as strong adhesion strength and excellent processability. The properties which make epoxy resins highly suitable are its excellent mechanical, thermal, and dielectric properties, along with corrosion resistance and minimal shrinkage upon curing. Epoxy resin, being a thermosetting material, possesses a notable level of crosslinking density, which imparts beneficial properties to it. However, the inherent brittleness and susceptibility to cracking, resulting from the highly cross-linked structure, impose limitations on the utilization of epoxy in advanced applications. In this work, carbonated castor oil (CCO) containing 5-membered cyclic carbonate rings has been used as toughening agent for DGEBA cured with 4,7,10-Trioxa-1,13 tridecanediamine. The inclusion of 10% CCO resulted in improvement in the tensile strength, storage modulus, flexural modulus and impact strength of the epoxy-urethane hybrid. The formation of hydrogen bonds between hydroxyl-urethane groups and other polar functional groups was the reason for the improvement in the mechanical properties. Moreover, the epoxy-urethane networks had reduced crosslinking density imparted by the fatty acid units of CCO and the presence of unreacted carbonate groups facilitated molecular movement, thereby contributing to energy dissipation during the deformation process. Thus, the development of high-performance epoxies with favorable properties has been achieved using carbonated castor oil as a toughening agent. Several advantages of the work includes its ecofriendliness, CO<sub>2</sub> utilisation (fixation), non isocyanate approach and utilization of castor oil which is a non edible renewable resource.



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## Direct Synthesis of Janus Hyperbranched Polymers using $AB_2 + A-R + A-R'$ Copolymerization

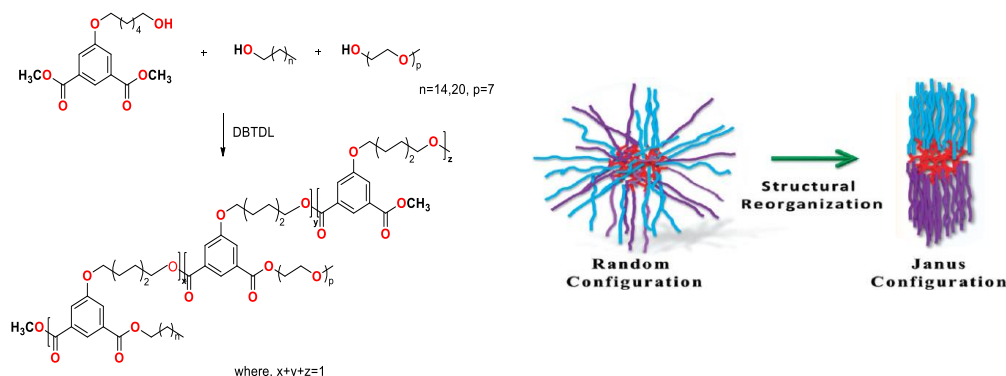
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## Abstract

*Janus* polymeric systems are very interesting and have been prepared using different strategies, most of which involve multi-chain aggregated systems;<sup>1</sup> single chain *Janus* polymeric systems are relatively rare<sup>2</sup> and hold the potential to reveal several interesting properties. Some years ago, we showed that simultaneous co-clicking of two immiscible segments, such as PEG and long alkyl chains, on to the periphery of hyperbranched polymers (HBP) can lead to self-segregation of the segments in bulk to generate *Janus* structures, thereby leads to the formation of bilayer lamellar ordering.<sup>3</sup> AB<sub>2</sub> type monomers carry one equivalent excess of B-groups, and hence can undergo direct copolymerization with any molecule carrying a single A-group; likewise, if two different molecules, carrying a single A-group each, are taken, it would lead to the formation of a HBP carrying two types of segments on their periphery. Here, we explore this concept for the preparation of *Janus* HBPs directly in a single step; thus, we have copolymerised 5-( $\omega$ -hydroxyalkoxy) isophthalate (AB<sub>2</sub>) along with various *n*-alkanols (A-R) and polyethylene glycol monomethyl ethers (MPEG-350) (A-R'), under melt transesterification conditions. The self-segregation of the alkyl and PEG segments in these functionalised HBPs was examined by DSC, X-ray scattering and Langmuir isotherm studies; further, we compare the efficacy of self-segregation with alternate strategies to access such *Janus* systems, such as sequential orthogonal clicking and co-clicking.



**Schematic representation for the direct preparation of amphiphilic Janus HBPs**

This direct approach to the preparation of *Janus* HBPs should render them readily scalable and therefore could find potential applications as emulsifiers, compatibilizers, multi-functional surfactants, etc.

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## Hydrophilic Enhancement of Cellulose Nitrate Polymeric Membrane Through Plasma Treatment and Identify the Role of Process Gas on it

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### Abstract

Plasma assisted surface modification of polymeric membranes are effective and charming approach for the improvement of antifouling and adhesive properties. A comparative study on the effect of low-pressure Nitrogen (N<sub>2</sub>) and Argon (Ar) plasma on surface morphology and structure for the cellulose nitrate (CN) polymeric membrane are studied in a view to improve the hydrophilicity of the membrane. The plasma characterizations are carried out with the help of a cylindrical Langmuir probe and Optical Emission Spectroscopy (OES). The surface characterisations are done for untreated and both N<sub>2</sub> and Ar plasma treated membranes. From the SEM characterization macro void creation and pore enlargement effects have been observed due to surface etching. The AFM analysis shows a prominent enhancement of the surface roughness after plasma treatment as compared to untreated one. Wettability of treated and untreated membranes are studied as a function of plasma treatment time. From the contact angle measurement, it is found that the hydrophilicity of the plasma treated membranes increases with increase in the plasma treatment time. A significant amount of pore size and pore area enlargement effects have been observed from BJH analysis of treated membrane. The recent experimental finding shows that the Ar plasma treatments are found to be more effective than N<sub>2</sub> plasma treatment to enhance the hydrophilicity of the membrane. It might be due to the higher etching rate during Ar plasma treatment as a result of higher atomic weight and ionization degree of Argon in comparison to Nitrogen.

**Keywords.** Cellulose Nitrate, Hydrophilicity, Low pressure Plasma, Wettability, Process Gas, Etching.

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## Evaluation of bioadhesive properties of boronic acid- functionalized electrospun polycarbonate urethane membranes

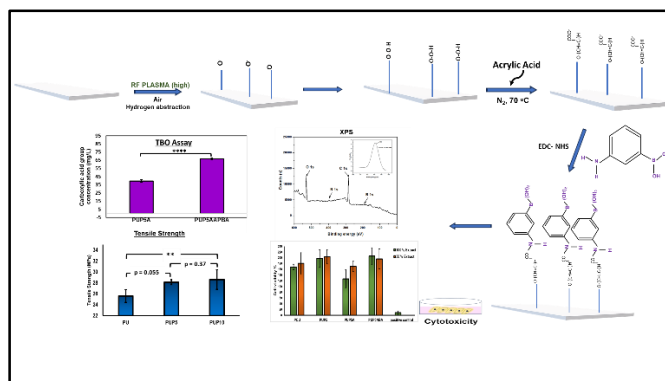
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### Abstract

Polycarbonate urethane (PU) is a thermoplastic and biocompatible polymer, ideal for developing matrices for biomedical applications. This work focuses on imparting tissue adhesive properties on the hydrophobic surfaces by plasma-treating PU membrane surfaces with subsequent grafting of adhesive molecules. The highly hydrophobic polymer was electrospun into nanofiber membranes, and modified by air plasma treatment at 18 W. This was followed by the 1-Ethyl-3-(3-dimethyl aminopropyl) carbodiimide (EDC)- mediated immobilization of 3- aminophenyl boronic acid (3-APBA) onto the membrane surface after graft polymerization of poly (acrylic acid) (PAA). The surface was characterized by dynamic contact angle, Fourier Transform Infrared Spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS). The results showed that at the plasma treatment time of 5 min, the surface densities of peroxides and PAA reached maximum value. The concentration of surface-bound carboxylic acid groups was estimated using the o- toluidine blue method (TBO). The XPS spectra showed the appearance of signals of boron at 193 eV confirming 3-APBA grafting. The O1s signals were deconvoluted and a small peak at 530.5 eV was found indicating the presence of carboxylic acid groups. The impact of plasma treatment on mechanical strength was evaluated using a universal tensile machine (UTM). The cytocompatibility of the modified membranes was evaluated using L929 mouse fibroblast cells and the results showed > 90 % cell viability. The bioadhesion studies of the functionalized membranes were carried out using a texture analyzer.



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## Development of Novel Bio-based Primary Antioxidant for the Thermo-Oxidative Stabilization of Polyolefins

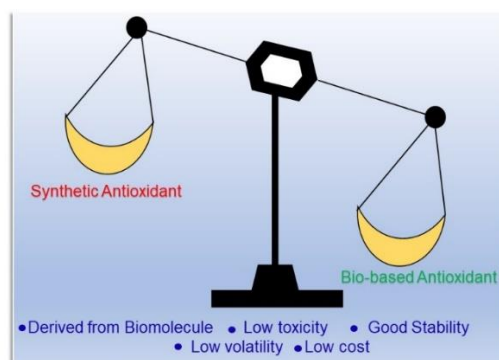
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### Abstract

Primary antioxidants is one of the most vital additives; used in polyolefins industry to stop the oxidative damages and degradation while processing and/or fabrication at higher processing temperature. To inhibit the oxidation and thermal damages, various types of primary antioxidants have been incorporated in polyolefin matrixes at ppm level. Markedly, most of the conventional primary antioxidants are derived from synthetic organic molecules. However, beyond a certain concentration, such synthetic antioxidants can migrate to the surface of the polymer article, and may contaminate food and serve as a source of unknown cytotoxicity, which makes them unsuitable for food contact applications. The aforementioned shortcoming as well as economic and environmental factors, re-searchers are putting their effort to replace the convention synthetic molecules with greener biomolecules. Such greener replacement not only saves the cost but also reduce carbon foot print. To investigate the efficiency of the designed antioxidant towards the stabilization of virgin polyolefins (most precisely polyethylene and polypropylene etc.), some typical characterizations have been accomplished such as oxygen induction time, melt-flow rate, yellowness index, thermal ageing, mechanical, thermo-gravimetric analysis etc. Notably, the newly designed antioxidant shows brilliant performance compared to traditional primary antioxidant. Due to its unique structure and physical characters, the resulting polyolefins did not show any notable color and property changes even after high temperature ageing experiments.



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## Proximity and Interlocking in Covalent Organic Framework for Diverse Photocatalytic Cross-Coupling Reactions

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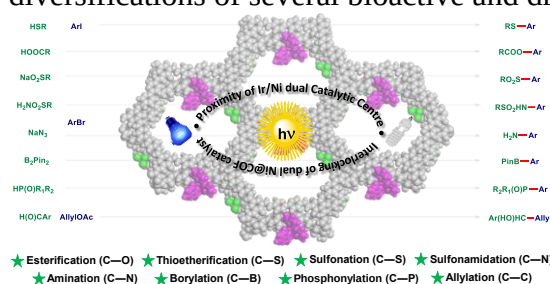
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### Abstract

Over recent years, heterogeneous photocatalysts created a sustainable kingdom compared to the typically known precious metal-derived homogeneous photocatalyst.<sup>1</sup> In particular, placing the photoactive and redox catalytic units in proximity enhances their photoredox communication compared to Brownian motion-limited homogeneous and semiheterogeneous counterparts. Covalent organic frameworks (COFs) are a promising toolbox in this field of heterogeneous catalysis. In this inclining field, we recently reported a dual metallation (iridium and nickel) strategy in a single 2D-COF TpBpy to perform a variety of C–N cross-coupling reactions.<sup>2</sup> The controlled metallation and recyclability without deactivation of both catalytic centers are unique with respect to previously reported coupling strategies.<sup>3</sup> We also prepared a nickel metal decorated highly conjugated Ni@Bpy-sp<sup>2</sup>c-COF to enable metallaphotoredox catalysis for light-harvesting cross-coupling reactions.<sup>4</sup> The interlocking of Ni metal in the COF backbone helped to explore eight different cross-coupling reactions towards C–X (X = B, C, N, O, S) bond formation.<sup>5</sup> These developed protocols enable selective coupling of a wide range of amines, carbamide, sulfonamide, thiol, acid, and electron-rich -neutral, and -poor (hetero)aryl halides and for late-stage diversifications of several bioactive and drug molecules.



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## Development of photocurable benzoxazines from renewable biophenol for low dielectric and photoluminescence applications

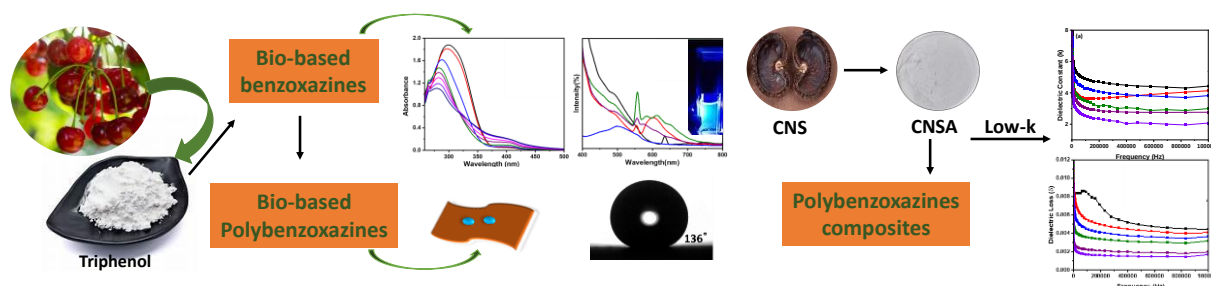
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### Abstract

In the present work, 3,5,4'-trihydroxy-trans-stilbene, a sustainable bio-phenol derived from biosources and five structurally different natural amines were used to develop photocurable bio-based benzoxazines. Molecular structure of the benzoxazines (TTS-od, TTS-dd, TTS-ff, TTS-ol, and TTS-le) was confirmed from spectral analyses. The five different benzoxazine were cured to get polybenzoxazines by thermal ring opening polymerization. The lowest curing temperature was noticed at 191°C for TTS-dd. Thermal stability of the developed polybenzoxazines was analysed using TGA. Among them, poly(TTS-ff) possesses the highest char yield value of 66% with LOI of 50.4. It was observed that the benzoxazines undergo photoinduced trans-to-cis isomerization and dimerization of olefinic bond through  $2\pi+2\pi$  cycloaddition reaction to form a cyclobutane ring under UV irradiation, which in-turn leads to crosslinking. Photoluminescence of benzoxazines was studied using fluorescence spectrophotometer and TTS-od has Stokes shift value of 318 nm. The cotton fabrics coated separately with two different bio-based benzoxazines (TTS-ff and TTS-ol) were thermal and photocured. Utilizing the sustainable concept strategy, bio-ash (CNSA) derived from cashew nut shell cake (CNS) was employed as a filler for the fabrication of biopolybenzoxazine composites for low dielectric application. The 10 wt% CNSA reinforced with poly(TTS-ff) composites has low k value of 2.07 and dielectric loss of 0.0017. The values of WCA observed for CNSA reinforced poly(TTS-ff) composites possess 147°, which is considered almost close to that of superhydrophobic behaviour. Data obtained from different studies suggest that polybenzoxazine matrices and composites developed in the present study can be considered for applications in the field of microelectronics insulation and water repellent uses.



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## Sulfonated Poly (vinyl alcohol)/MoS<sub>2</sub>-based Composite Proton Exchange Membranes with Higher Selectivity

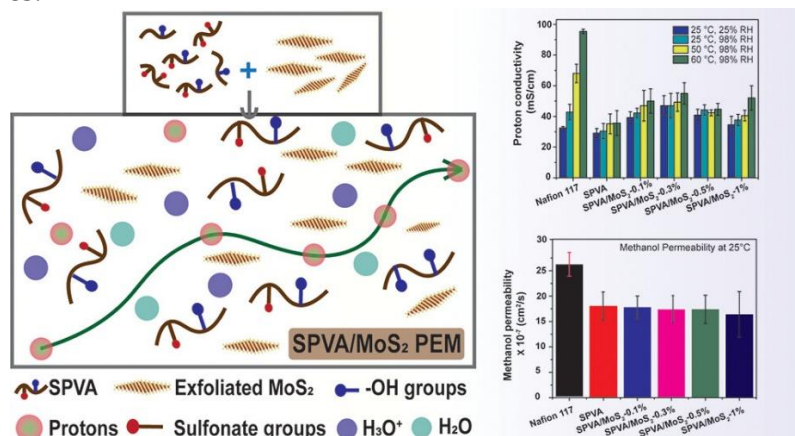
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### Abstract

Selectivity, the ratio of proton conductivity to methanol permeability, is an essential criterion of proton exchange membrane (PEM). A good PEM should exhibit a higher proton conductivity and lower methanol permeability with higher thermomechanical stability as direct methanol fuel cells (DMFCs) efficiency depends on it [1-3]. In this work, we developed sulfonated poly (vinyl alcohol) (SPVA)/MoS<sub>2</sub>-based composite proton exchange membranes (CPEMs) with different loadings of exfoliated MoS<sub>2</sub> as filler for higher selectivity. The synthesized CPEMs were characterized for their water uptake, ion exchange capacity, proton conductivity, methanol permeability, and thermomechanical stabilities to assess their physicochemical properties. The SPVA/MoS<sub>2</sub>-0.3% PEM exhibits a proton conductivity of  $48 \pm 7.5$  mS/cm at 25 °C and ~ 98 %RH, having nanoclusters and methanol permeability of  $1.72 \times 10^{-6}$  cm<sup>2</sup>/sec at 25 °C resulting 80% higher selectivity as compared to Nafion 117 (Scheme 1). The SPVA/MoS<sub>2</sub>-0.3% membrane is mechanically stable up to 60 °C and ~ 98 %RH, having  $54 \pm 5$  mS/cm proton conductivity. Further, the membrane was cross-linked with 1.5% and 3% glutaraldehyde solution for 12, 24, 36, and 48 hrs. to improve their performance for higher temperature applications. The optimized membrane 24X3.0SPVA/MoS<sub>2</sub>-0.3% showed the best results, displaying thermomechanical stability up to 80 °C with  $51 \pm 5$  mS/cm of proton conductivity [4]. The optimized membrane has 37 times higher selectivity at 60 °C and considerably higher selectivity at 70 and 80 °C than Nafion 117 and is suitable for DMFC applications at moderately high temperatures.



Scheme 1. Proton conduction mechanism, proton conductivity, and methanol permeability of the membranes.

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## Regulating the Polyethylene Microstructure by Increasing Steric Crowding in Naphthoxy Imine Ligated Ni(II) Complexes

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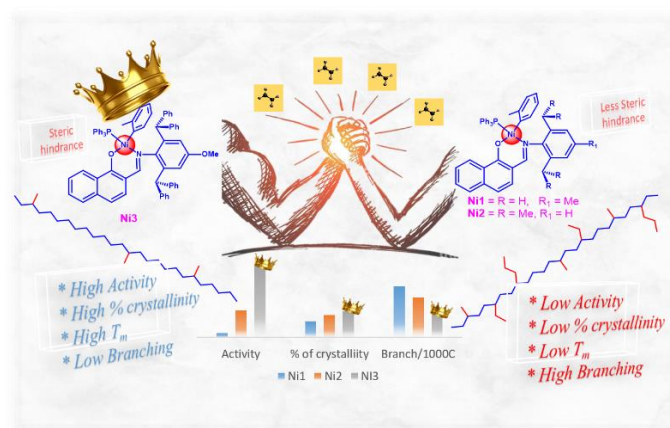
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### Abstract

Polyolefins are indeed the largest volume polymers produced globally. The annual production of polyolefins, specifically polyethylene and polypropylene, has consistently increased over the years due to their broad applications across sectors such as packaging, automotive, construction, textiles, and more. Controlling the polymer microstructure and molecular weight is important as it decides the application of the resultant polymer. Here we report synthesis of nickel complexes featuring naphthoxy imine ligands with systematically tuned steric properties. These complexes, namely **Ni1**, **Ni2**, and **Ni3**, were developed with a one-step procedure and exhibited excellent yields (ranging from 73% to 93%). These complexes were well characterized using <sup>1</sup>H, <sup>13</sup>C, 2D NMR spectroscopy, mass analysis, and single-crystal X-ray diffraction. The buried volume data indicates **Ni3** was the most bulky of the three. When the three nickel complexes **Ni1**, **Ni2**, and **Ni3** were exposed to ethylene, they generated polyethylene with high activity. The sterically bulky **Ni3** catalyst outperformed over sterically less crowded **Ni1** and **Ni2** catalyst.



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## Hyperbranched poly-beta-thiopropionate esters

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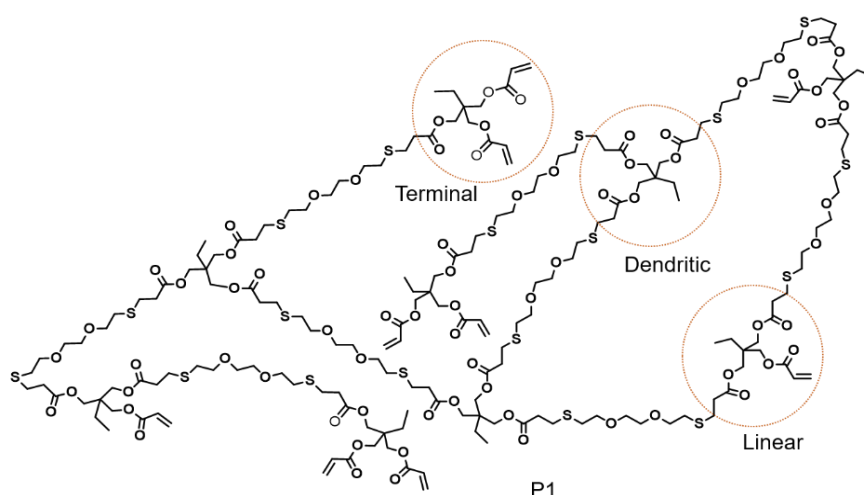
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### Abstract

Hyperbranched polymers (HP) are three dimensional highly branched macromolecules with distinct properties such as low viscosity, high solubility large number of terminal functional groups and others<sup>1</sup> Hyperbranched poly-urethanes, poly-ethers, polyesters, poly-silanes, polyphenylenes, polydisulfides and others have been developed in recent past, which have applications in coating, additives processing, nano- template for catalysis as well as therapeutic delivery vehicle. Generally, these polymers have been synthesized by self-condensation reaction of  $AB_n$  ( $n \geq 2$ ) type monomer or poly condensation reaction between  $A_2 + B_3$  type of monomers.

We have explored  $A_2B_3$  type of nucleophile catalyzed thiol acrylate Michael addition reaction for synthesis of a hyperbranched polyester. The synthetic ease of thiol acrylate Michael addition reaction and the formation of pH responsive linker “beta thiopropionate ester” makes it promising tool for developing pH responsive biodegradable materials for different applications.<sup>2</sup> This presentation will describe our recent results in this area including the synthesis of pH responsive beta-thiopropionate ester containing hyperbranched polymer (P1), its characterization using suitably designed model compounds, post-polymerization functionalization of the terminal acrylate groups by different functional hydrophilic thiols, as well as the pH responsive degradation of the resulting polymers in water.



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## Covalent Organic Frameworks as Porous Pigments for Photocatalytic Metal-Free C–H Borylation

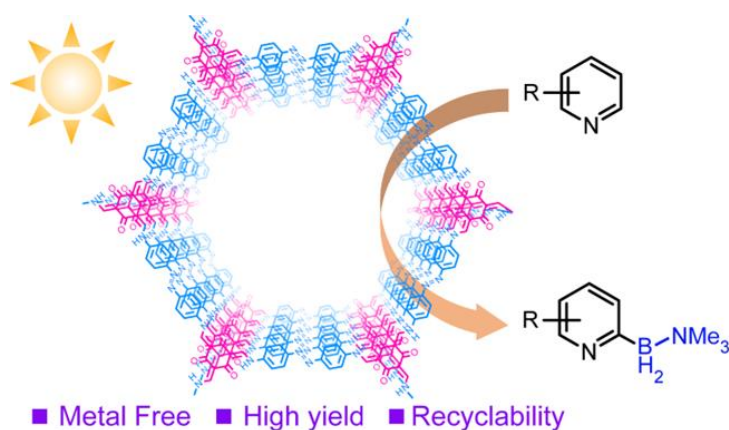
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### Abstract

Covalent organic frameworks (COFs) are highly promising as heterogeneous photocatalysts due to their tunable structures and optoelectronic properties. Though COFs have been used as heterogeneous photocatalysts, they have mainly been employed in water splitting, carbon dioxide reduction, and hydrogen evolution reactions. A few examples in organic synthesis using metal-anchored COF photocatalysts were reported. Herein, we report highly stable  $\beta$ -keto-enamine-based COFs as photocatalysts for metal-free C–B bond formation reactions. Three different COFs have been availed for this purpose. Their photocatalysis performances have been monitored for 12 different substrates, like quinolines, pyridines, and pyrimidines. All the COFs showcase moderate-to-high yields (up to 96%) depending upon the substrate's molecular functionality. High crystallinity, a large surface area, a low band gap, and a suitable band position result in the highest catalytic activity of TpAzo COF. The thorough mechanistic investigation further highlights the crucial role of light-harvesting capacity, charge separation efficiency, and current density during catalysis. The light absorbance capacity of the COF plays a critical role during catalysis as yields are maximized near the COF's absorption maxima. The high photostability of the as-synthesized COFs offers their reusability for several (>5) catalytic cycles.



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## Simple and effective anti-corrosive additives in polyurethane coatings for mild steel protection

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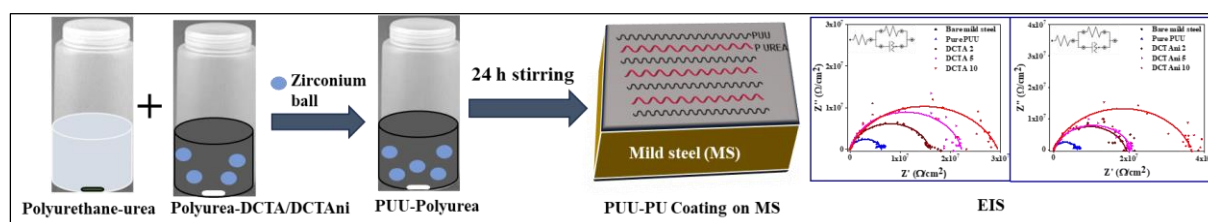
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### Abstract

Novel electroactive polyureas (EPU)s were synthesized by incorporating aniline oligomeric Trimer (DCTA) and tetramer (DCTAni) into IPDI and characterized with FT-IR, NMR, UV, and XPS. PUU were synthesized with PTMG-2000 as a polyol, IPDI, and dihydrazide adipate used as a chain extender. This PUU served as the polyurethane matrix for dispersing powder particles of polyurea EPU-DCTA and EPU-DCTAni as anti-corrosive additives. Coatings were formulated with EPU-DCTA dispersed within the PUU matrix with weight percentages of 2, 5, and 10, denoted as DCTA-2, DCTA-5, and DCTA-10, respectively. A similar procedure was followed for EPU-DCTAni, resulting in coatings and named as DCTAni-2, DCTAni-5, and DCTAni-10. The redox activity of DCTA, DCTAni, EPU-DCTA, and EPU-DCTAni were characterized using CV and UV-Vis spectroscopy. Anti-corrosion studies were studied by electrochemical impedance spectroscopy (EIS) and Tafel potentiodynamic polarization measurements. The obtained results designated an impressive  $R_p$  value of 122.15 MΩ and a low corrosion rate ( $C_R$ ) is  $2.38 \times 10^{-6}$  mm/year. Furthermore, an accelerated salt spray test was performed on all coatings using a 5% NaCl salt smog for a duration of 500 h. FE-SEM images reveals the smooth film surfaces. TGA revealed the polymer degradation, with a maximum  $T_{5\%}$  observed at 304.1 °C. Additionally, the glass transition ( $T_g$ ) of films was determined through DSC and DMTA analysis. Thus, the overall results forward the synthesized EPUs as a potent corrosion resistance polymeric coating material.



Representation of synthesis flow and analysis of EPU dispersed EPUU coatings

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## Mechanistic insights on the incorporation of higher alpha-olefins into acrylate copolymers via photoATRP

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### Abstract

Light is a widely accessible, non-harmful, and eco-friendly reagent that offers possibilities for temporal and spatial control required for ATRP process <sup>1-2</sup>. Therefore, photomediated polymerization utilizes light as an external stimulus to conduct polymerization under mild reaction conditions <sup>3</sup>. During the photoinitiated polymerization, monomers such as acrylates, methacrylates, and styrenes are polymerized by using UV-Vis light radiation either in the presence or absence of photosensitizers (PS) or photoinitiators (PI). The present research is focussed on visible light-induced simultaneous reverse and normal initiation (SR & NI) photoATRP of acrylates and higher alpha olefins ( $\alpha$ -olefins) (C<sub>8</sub>-C<sub>12</sub>) using Cu<sup>II</sup>Br<sub>2</sub>/L catalytic system. The polymerization has been initiated by generating of radicals from PI, i.e. phenyl bis (2,4,6-trimethyl benzoyl) phosphine oxide (BAPO). The kinetic analysis revealed the first-order, controlled, and living radical behavior of the polymerization using <sup>1</sup>H NMR spectroscopy. Moreover, the catalytic system provided good temporal control ability using light as the external stimulus.

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## Enhance Thermal Properties of Polycarbonates with Bisphenol-A Recovered from Waste Plastic via Polycondensation Process

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### Abstract

The escalating issue of plastic waste and the urgent need for resource efficiency have spurred innovative research in the fields of plastic recycling and sustainable material synthesis. This study presents a comprehensive investigation into the recovery of bisphenol-A (BPA) from waste compact disk polycarbonate (CD-PC) using a solution depolymerization approach. Additionally, the recovered BPA is employed in the synthesis of high thermal stability polycarbonate. The solution depolymerization method entails the dissolution of waste CD-PC in a methanol solvent under an organocatalyst (1,5,7-triazabicyclo[4,4,0]-dec-5-ene) at 50° C for 90 mins, which leads to the breakdown of the polymer into its constituent monomers, including BPA. The recovered BPA is subsequently subjected to purification and utilized in the synthesis of polycarbonate through a high-temperature polymerization process. Functional groups of synthesized materials were characterized by FT-IR and NMR analysis. The thermal properties of polymers were performed by DSC and TG analysis. The resulting polycarbonate exhibits enhanced Tg and decomposition temperature, which could be suitable for applications demanding elevated temperature resistance. The conversion of low-molecular-weight polycarbonates to high-molecular-weight polycarbonate study contributes to the circular economy paradigm by reducing waste, conserving resources, and fostering the development of value-added materials.

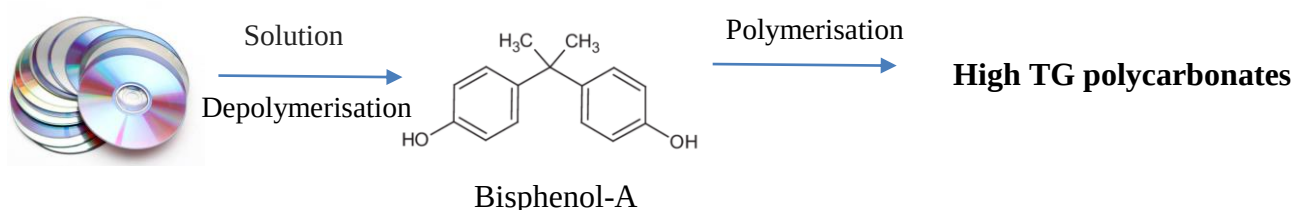


**Fig: Schematic representation of conversion of low-molecular-weight polycarbonate into thermally stable high-molecular-weight polycarbonates**

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## Antimicrobial water-based ink for active packaging application

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### Abstract

This study aimed to develop antimicrobial water-based ink suitable for printing on food packaging materials. The acrylic resin was synthesized for water-based ink and curcumin was added as an antimicrobial agent and a bio-based yellow pigment. Finally, the water-based ink with and without the active antimicrobial agent was printed on PET films. The physicochemical characteristics of the ink were also investigated. The thickness of the coated antimicrobial water-based ink was measured at 0.02 mm, and varying the curcumin concentration in the ink did not affect the printed thickness. The viscosity of the medium and the antimicrobial ink were determined to be 4.1 p and 3.4 p, respectively. The ink's drying time decreased from 10 sec to 8 sec in the case of curcumin-loaded ink. At the same time, the gloss increased from 30% to 50%. The antimicrobial water-based ink exhibited superior antimicrobial activity against *S. Aureus* and *E. Coli* compared to the regular water-based ink. These results demonstrated that the antimicrobial water-based ink possessed favorable storage stability, improved gloss, and a shorter drying time. Using curcumin with low volatile organic compounds (VOCs) emissions may hold significance for the printing applications of active food packaging materials (Dao et al., 2022; Sharma et al., 2021, 2022).

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## Development of photocurable benzoxazines from renewable biophenol for low dielectric and photoluminescence applications

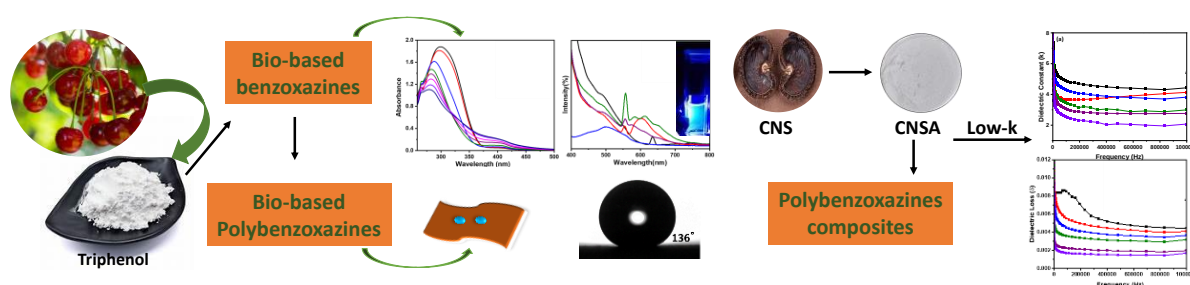
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### Abstract

In the present work, 3,5,4'-trihydroxy-trans-stilbene, a sustainable bio-phenol derived from biosources and five structurally different natural amines were used to develop photocurable bio-based benzoxazines. Molecular structure of the benzoxazines (TTS-od, TTS-dd, TTS-ff, TTS-ol, and TTS-le) was confirmed from spectral analyses. The five different benzoxazine were cured to get polybenzoxazines by thermal ring opening polymerization. The lowest curing temperature was noticed at 191°C for TTS-dd. Thermal stability of the developed polybenzoxazines was analysed using TGA. Among them, poly(TTS-ff) possesses the highest char yield value of 66% with LOI of 50.4. It was observed that the benzoxazines undergo photoinduced trans-to-cis isomerization and dimerization of olefinic bond through  $2\pi+2\pi$  cycloaddition reaction to form a cyclobutane ring under UV irradiation, which in-turn leads to crosslinking. Photoluminescence of benzoxazines was studied using fluorescence spectrophotometer and TTS-od has Stokes shift value of 318 nm. The cotton fabrics coated separately with two different bio-based benzoxazines (TTS-ff and TTS-ol) were thermal and photocured. Utilizing the sustainable concept strategy, bio-ash (CNSA) derived from cashew nut shell cake (CNS) was employed as a filler for the fabrication of biopolybenzoxazine composites for low dielectric application. The 10 wt% CNSA reinforced with poly(TTS-ff) composites has low k value of 2.07 and dielectric loss of 0.0017. The values of WCA observed for CNSA reinforced poly(TTS-ff) composites possess 147°, which is considered almost close to that of superhydrophobic behaviour. Data obtained from different studies suggest that polybenzoxazine matrices and composites developed in the present study can be considered for applications in the field of microelectronics insulation and water repellent uses.



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## Polyazomethines: Emerging Electroactive Material for High-Performance Supercapacitors

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### Abstract

Researchers have previously shown significant interest in the exploration and utilization of semiconducting polyazomethines, primarily driven by their distinct properties encompassing redox capabilities, thermal resistance, mechanical strength, hydrophilicity, and metal-binding capacity. Particularly, conjugated aromatic polyazomethines exhibit remarkable attributes relevant to electrical and optical conductivity. The potential applications for polyazomethines encompass electrochromic displays, battery cathodes, supercapacitor electrodes, and various electronic devices. A room temperature polyazomethine series (PAZ-1 to PAZ-5) has prepared via polycondensation route using 5-[4-(5-formylfuran-2-yl) phenylfuran-2-carbaldehyde (III) and diamines. Polymer series was confirmed by spectroscopic techniques; its structural, morphological and compositional properties were examined using XRD, FESEM, EDAX, TEM and wettability techniques. The  $-\text{CH}=\text{N}-$  peak at  $1600\text{ cm}^{-1}$  in FTIR spectra indicate the successful conversion of dicarbaldehyde (III) and diamines into polyazomethine. The amorphous nature of PAZ series is shown by XRD diffractograph. The nanoflower kind of morphology of polyazomethines has observed in FESEM and TEM images. The EDAX and elemental mapping study revealed the required plentitude compositions in prepared polymers. The electrochemical activity of polyazomethine electrodes have studied using Cyclic Voltammetry (CV), Galvanostatic Charge Discharge (GCD) and Electrochemical Impedance Spectroscopy (EIS) techniques. The detailed study of PAZ-1 to PAZ-5 electrodes in various electrolytes at various concentrations exhibits the PAZ-2 electrode with elevated specific capacitance ( $C_p$ ) of  $831.50\text{ Fg}^{-1}$ , specific energy (SE) ( $22.99\text{ Whrk}^{-1}$ ), specific power (SP) ( $82.87\text{ KWkg}^{-1}$ ) in 1 M NaOH electrolyte. The stability of PAZ-2 was found to be 71.65 % after 500<sup>th</sup> cycles in 1 M NaOH.

**Keywords:** Dicarbaldehyde; Conjugated Polyazomethine; Electrochemical performance; Impedance; Stability.



## Studies on impact of biocarbon reinforced sustainable polybenzoxazine composites derived from biophenol for superhydrophobic and dielectric applications

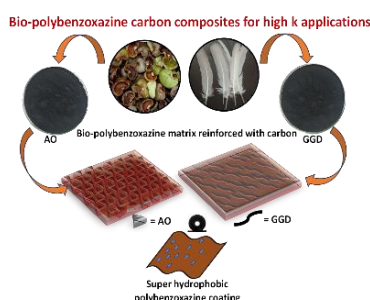
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### Abstract

To minimize the possible usage of petroleum resources in the production of benzoxazines, sustainable biophenol precursors 5,5-diallyl-[1,1—biphenyl]-2,2-diol (DBD) and bio-amine furan-2-yl methanamine (fma) have been utilized to synthesize biobenzoxazine<sup>1</sup>. DBD-fma benzoxazine was reinforced with two different types of carbon derived from poultry waste chicken feather<sup>2</sup> (*Gallus gallus domesticus*) (GGD) and agricultural waste cashew nut shell residue (*Anacardium occidentale*) (AO). TGA results indicated that poly(DBD-fma) possesses an excellent thermal stability with a char yield of 60%. The thermal stability of GGD and AO reinforced poly(DBD-fma) improved to a significant extent when compared to neat-poly(DBD-fma). The dielectric constant (k) of poly(DBD-fma) was found to be 5.52 which was further improved on reinforcement of GGD and AO. Among the different wt% of biocarbon reinforced composite, 15% GGD carbon reinforced poly(DBD-fma) possesses k value of 8.9 and 15% AO carbon reinforced poly(DBD-fma) possesses 7.8. The synthesized biopolybenzoxazine (DBD-fma) matrix exhibits an excellent hydrophobicity<sup>3</sup> with WCA of 143° which is close to superhydrophobic behavior. The durability of poly(DBD-fma) was studied by coating on cotton fabric. The WCA value of cotton fabric coated with poly(DBD-fma) possess the same value that of its matrix. It was also observed that poly(DBD-fma) coated cotton fabric retains hydrophobic nature even after 10 times of n-hexane washes. It is suggested that the sustainable biobased benzoxazine reinforced with biocarbon can be utilized for thermal resistant, insulation and water repellent applications. This work is considered to be cutting-edge concept in the field of development of environment friendly biobased precursors to replace fossil based polymeric materials.



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## Wound Infection Healing Properties of Nanoparticles Coated Natural Fibers

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### Abstract

Healing from a wound is an intricate procedure that can be slowed down by an assortment of circumstances. The irregular scarring and chronic condition that is more prone to infections occur from an interruption in the normal wound healing process. Wounds can result from various causes, including scratches, cuts, splinters, and more. While our bodies have exceptional healing capacities, there are times when wounds fail to recover within the expected timeframe, among the failure of wound healing bacterial infection is one of the main reasons. This study attempts to identify bacterial infection resistance by synthesizing copper oxide nanoparticles (CuO-NPs) and zinc oxide nanoparticles (ZnO-NPs) coated on agave fiber using a co-precipitation technique. ZnO-NPs and CuO NPs were synthesized via the chemical coprecipitation method and coated onto Agave fibers via the In-situ method of coating successfully. SEM and XRD analysis revealed the shape and size of the coated ZnO and CuO Nanoparticles on fibers. Scanning electron microscopy images of the textiles showed that the treated fibers were covered with uniform ZnO-NPs and CuO-NPs. We experimented with a variety of gram-positive and gram-negative bacteria, including *Escherichia Coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, and *Bacillus subtilis*, to investigate each bacterium's resistance to the nanoparticles and commonly used antibiotics (gentamicin). The antibacterial test showed that the ZnO-NPs coated on fibers had high antibacterial activity against the gram-positive bacteria, bacteria, *Staphylococcus aureus*, and *Bacillus subtilis*. CuO-NPs had shown quite high antibacterial activity against the gram-negative bacteria, *Escherichia coli*.

**Keywords:** wound healing, natural fibers, nanoparticles, electron microscopy, X-ray diffraction

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## Studies on enhancing shelf-life of cut apple using polysaccharide based edible packaging

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### Abstract

The shelf-life of cut-apple is limited due to deterioration of its quality and safety during storage by several physical, chemical and microbiological factors. Biopolymer-based edible coating formulation is a promising sustainable preservation technology which can enhance the shelf-life, improve the nutritional quality and reduce the food waste. This research study aimed to enhance the shelf-life of apple slices using polysaccharide-based edible packaging by dip coating method at ambient storage conditions. Initially, an effective coating formulation was screened out on the basis of water loss %, browning index, firmness and visual appearance on 3<sup>rd</sup> day of storage. After that, apple slices were dip coated using best formulated coating solutions and stored for 15 days at room temperature along with control sample. The weight loss, browning, firmness, total soluble solids, titratable acidity, antioxidant capacity and yeast & mold counts were analyzed and compared with control apple slices. The results depicted reduced % weight loss, browning and fungal growth, and higher firmness, total soluble solids, titratable acidity and antioxidant capacity of developed coating solutions for whole 15 days at room temperature than control. The formulated coating solutions were tested against *E. coli* and *S. aureus* and the solutions were effective against gram-negative *E.coli* whereas only one solution effectively inhibited gram-positive *S. aureus*. The cytotoxicity analysis against BHK-21 cell lines was also done to assess the adverse effects on human cells due to consumption of edible packaging material with fruit materials and found to be safe and biocompatible. The coating solutions were analyzed for their rheological and functional characteristics. The coating solutions exhibited shear-thinning behavior having almost similar viscosity at 25 and 50 °C and showed vibration peaks of various functional group which confirmed presence of active agents of the additives used in the formulations. Thus, the current research work presents a dip coating formulation which can able to preserve ready-to-eat cut-apple for a longer duration of storage time without altering much of the quality attributes as compared to untreated cut-apple.

## Microbial Fuel Cells: A transition tool towards circular economy

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### Abstract

Microbial Fuel Cells (MFCs) are promising sustainable energy technology integrating power generation with waste remediation, forming an important tool in the transition towards circular economy. However, its practical application is mainly hindered by its low power density and the cost of membranes. The uniqueness of the work is the validation of the experimental study with comprehensive Classical Molecular Dynamics (MD) study complementing the experimental studies with new information about the system assembled with the indigenous membrane components. Environmentally benign polymers, poly (vinyl alcohol) (PVA) crosslinked with glutaraldehyde (GA) and Chitosan (CS) have been developed and its performance evaluated against the commercial membrane in real wastewater fed MFCs. The membranes developed demonstrate potential as separator in future MFCs based on its enhanced performance and low cost of installation. Low power density owing to poor bacterial adhesion and electron transfer efficiency between bacteria and anode is addressed by development of flexible electrodes using conducting polymer polyaniline (PANI) with sustainable polymer polylactic acid (PLA) demonstrating excellent biocompatibility, outperforming the flat graphite anode with increase in maximum power density and COD removal efficiency. An attempt to delve deeper into the atomic level to investigate the proton transport mechanism across the developed PVA membrane using MD study demonstrates presence of multi-hydrated protons observed from MD trajectories suggesting that the proton transfer in the PVA polymeric membrane system occurred via vehicular mechanism. Thus the design of sustainable anode material and low-cost indigenously developed membranes demonstrate the enormous potential of scale-up of MFCs for wastewater treatment in the future.

**Keywords** Microbial Fuel Cell, wastewater treatment, power generation, mixed culture bacteria, polyvinyl alcohol membrane, biobased electrode

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## Development of green ceramic membranes from waste coal fly ash and bottom fly ash waste via stereolithography technique

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### Abstract

The continuous combustion of coal has resulted in raising environmental concern due to its byproduct, coal fly ash (CFA) and bottom coal fly ash (BCFA). In this study, utilization of coal fly ash material, zero-solid waste reduces the environmental impact by fabrication of CFA/BCFA-based membranes. The parts were fabricated in a 3S system that was custom developed. The 3S system consists of the stereolithography (SLA) technique with a novel adaptable membrane formwork, that is based on the layer-by-layer fabrication process. It was set to project blue light that has a visual spectrum range 800 nm. The exposure time of light set to 1.5 seconds for the CFA and 4 seconds for the BCFA and at optimized specific slurry viscosity of 2.81 Pa.s and 2.1 Pa.s respectively resulted in development of disc type ceramic membrane with diameter size of 3.2 cm and thickness 0.3 cm. The green parts have a linear shrinkage of almost 4 % after sintering at 1100°C. It can directly influence the packing morphology and the pore area that can be obtained post-sintering in the nano-scale range. The favourable sintering temperature for the CFA and BCFA ranges from (850-1000) °C and (850-1050) °C respectively and beyond which membranes begin to crack and molecules of the CFA and BCFA start shrinking. Furthermore, the membrane surfaces which were originally super hydrophilic in nature were successfully modified to hydrophobic porous ceramic membranes expanding its horizon of application of the membranes from microfiltration to pervaporation application.

**Keywords:** Coal fly ash, Bottom coal fly ash, 3D printing technology. Stereolithography, Pervaporation

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## **Poster Presentations**

## Effect of SiO<sub>2</sub> nanofibers on the electrical properties of cellulose acetate based gel polymer electrolytes

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### Abstract

In the present study, synthesis of a nanocomposite gel polymer electrolyte (NCGPEs) is formed by imparting SiO<sub>2</sub> nanofiber in different weight percentage with lithium hexafluorophosphate (LiPF<sub>6</sub>) salt solution and adding plasticizer propylene carbonate (C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>) and diethyl carbonate (C<sub>5</sub>H<sub>10</sub>O<sub>3</sub>) in immaculate biodegradable cellulose acetate (CA). It has been observed that addition of nanofiber and plasticizer greatly influence in the ionic conductivity and mechanical strength of the resulting NCGPEs with advanced electrochemical properties [1]. Ionic conductivity of the NCGPEs exhibit its maximum value with 7.5wt% of nanofiber concentration. Thus, the increase concentration of nanofibers in NCGPEs have improved conductivity and can transfer energy more efficiently that allows for better control over the movement of ions within the electrolyte solution [2]. This has exciting implications for various applications like batteries and fuel cells. SEM, XRD, FTIR, XPS, DSC and TGA have supported the enhanced electrical and electrochemical properties of the synthesized nanocomposites gel polymer electrolyte.

Keywords: Biodegradable, Cellulose Acetate, Nanofiber.

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## Unraveling the role of solvophobic sequences grafted on hyperbranched polymer in their self-assembly behavior and stimuli-responsiveness

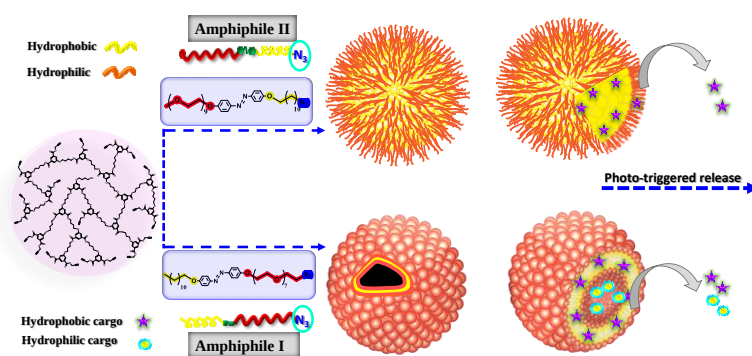
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### Abstract

The self-assembly of amphiphilic polymers represents a multidimensional platform for engineering and tailoring nanomaterials with diverse structures, versatile functionalities, and wide-ranging applications.<sup>1-3</sup> Versatility of self-assemblies is governed by primary polymer structure, including pendant composition, chain length, degree of polymerization, and sequence distribution.<sup>4</sup> The incorporation of hydrophilic/hydrophobic blocks in the copolymers allow precise control of the interactions between these blocks, thereby engendering a wide array of self-assemblies.<sup>4</sup> Herein, we have investigated the effect of 'anchoring the solvophobic sequences' on the hyperbranched polyester (HBP) self-assembly. Two solvophobic segments were designed with identical hydrophobic/hydrophilic balance. A hydrophobic dodecyl and a hydrophilic octaethylene glycol chain (OEG) are connected by a photosensitive unit. The parent HBP was post-functionalized with these two solvophobic segments to form HBP-1 (OEG-interior) and HBP-2 (OEG-exterior). Regardless of the same hydrophobic/hydrophilic balance, the self-assemblies exhibited disparity in size and morphologies. HBP-1 gave rise to vesicles, whereas HBP-2 yielded smaller spherical micelles, as verified by TEM, DLS, and high-resolution confocal microscopy techniques. These findings highlight the importance of attachment points and molecular arrangement in shaping the resulting nanostructures. Owing to its distinctive bilayered structure, vesicles were suitable carriers of hydrophilic and hydrophobic guests within their aqueous lumen and lipid bilayers. However, micelles exhibiting core-shell structures proved excellent hydrophobic guest carriers. The photo-triggered release from both vesicles and micelles further highlights the potential of designed systems for smart and controlled drug delivery. These insights show how slight variations can lead to significant differences in self-assembled nanostructures' formation, stability, and properties.



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## Super-stretchable, Self-Healing 2D MXene-Based Composites for Thermal Management and Electromagnetic Shielding Applications

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### Abstract

Due to the pressing need to mitigate current electromagnetic wave pollution (connecting to the 5 G era), lightweight, stretchable, thermally, and electrically conductive nanocomposite materials have attracted significant scientific interest. In this study, using successive wet cum melt mixing, MXene-based carboxylated nitrile butadiene elastomeric (XNBR) based nanocomposites were fabricated for outstanding electromagnetic radiation shielding efficiency, healing capability, thermal management, and recyclability. The composites exhibit excellent stretchability and mechanical strength with a desirable shielding effectiveness of -27.4 dB (in the frequency range of 8.2-12.4 GHz) and a thermal conductivity of 1.24 W/mK while retaining electrical conductivity of 0.5 S/cm, room temperature self-healing ability of 46.8%, and 100% recyclability. Notably, the continuous conducting network is unaltered even after chemical treatment, stretching, bending, prolonged exposure to sunlight, and reprocessing, which verifies the material's overall chemical and mechanical performance. Our multifunctional elastomeric composites collectively supply a prominent directive for establishing high-performance elastomeric composites with outstanding shielding efficiency, self-healing ability, thermal management, recyclability, and excellent mechanical behaviour.

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## Flexible Covalent Organic Framework Membranes with Linear Aliphatic amines for Enhanced Organic Solvent Nanofiltration

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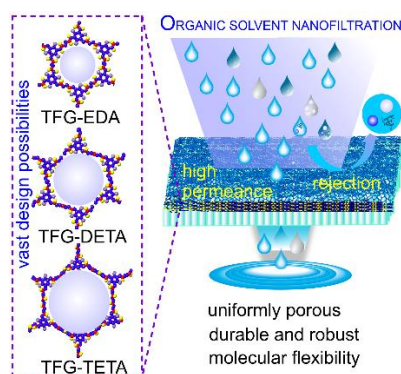
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### Abstract

Covalent organic framework (COF) based membranes hold great promise for organic solvent nanofiltration (OSN) due to their unique molecular arrangement, well-defined porous network, and broader solvent tolerance. However, scaling up their fabrication on porous supports without compromising these properties presents many challenges. In this study, COF membranes are fabricated on a porous support using liquid-liquid interfacial polymerization. The pore size and chemistry of the COF membranes are rationally modified by covalently bridging different aliphatic diamines with varying amine groups. The growth process of the COFs nanofilm is thoroughly studied using morphology and chemical structures analysis, which confirms imine bond formation between both monomers. Next, the COFs film is transferred to a porous support and thoroughly investigated before its application in OSN. The fabricated COF membranes display superior solvent permeance and precise molecular separation compared to conventional nanofiltration membranes. They also demonstrate substantial fouling resistance in both static and dynamic conditions. Furthermore, the COF membranes show good operational stability when subjected to continuous solvent permeation for 24 h without any surface defects or disruption in permeation activity. These results demonstrate the potential for synthesizing linear aliphatic diamine-based COFs and their membranes via facile liquid-liquid interfacial polymerization for various membrane filtration applications.



## Physical, Morphological, Thermal and Micromechanical Properties of *Allo* Fiber Loaded Resorcinol Formaldehyde Resin Composites

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### Abstract

The study focuses on developing composite materials based on thermosetting polymers such as resorcinol formaldehyde using locally available *Girardinia diversifolia* (commonly called *Allo*) fiber as filler that helps to explain the structure-property correlations with a special focus on morphology and deformation behaviors. Firstly, the resorcinol formaldehyde (RF) resin was synthesized by *in situ* polycondensation from the reaction of resorcinol and formaldehyde. The microcellulose was extracted from the *Allo* fibers by different chemical treatments such as mercerization and bleaching followed by acid hydrolysis to prepare nanocellulose. Thus produced micro- and nanocellulose were then *in situ* incorporated into the RF matrix to prepare the composites with different compositions (such as 0%, 2%, 4%, 8%, and 10% by weight of fibers). Later, the differently composed *Allo* fiber composites were subjected to characterization by different techniques. Structure, morphology, mechanical, and thermal properties of matrix, filler, and composites were studied. The results demonstrated that the chemically treated fibers showed significant differences in their properties as compared to the neat fibers. The composites prepared with treated *allo* fiber were found to be more compatible at the fiber-matrix interfaces suggested by FTIR spectra and SEM images of cryo-fractured surfaces of the composites. The indentation and compressive strength of the composite was found to increase with the filler loading in treated fiber-loaded composites and these distinctions were also evident in their mechanical properties and water absorption behaviors.

**Keywords:** Natural fiber, thermosetting resin, polycondensation, microcellulose, nanocellulose 42-51.

## Valorization of Waste Fish Scales for Development of Vegetable Oil Based Composites

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### Abstract

In recent years, research on bio-based fiber reinforced polymer matrix is of great interest due to properties like biodegradability, low cost, eco-friendliness and availability.<sup>[1]</sup> The disposal of fish scale, a waste product from fish processing industries, causes serious problem to the environment. These scales can be made value added by forming composites with bio based thermosetting resins.<sup>[2]</sup> Vegetable oils are an important fatty acid material, which contains high unsaturation making them an attractive starting raw material for the synthesis of bio based resin.<sup>[3]</sup> But the unsaturation and ester bonds present in the vegetable oils are not reactive enough for crosslinking purpose. So in order to convert vegetable oil into useful resin and to enhance their reactivity, further modification by introduction of functional groups can be done. We have modified epoxidised soybean oil with acrylic acid and maleic anhydride to form the resin MAESO. In this study, efforts were made to prepare composites using MAESO as resin, itaconic acid-glycidyl methacrylate (IG) adduct as reactive diluent as well as crosslinker and waste fish scale fibers as reinforcing agent<sup>[4]</sup> via compression molding technique. The resin MAESO was characterized by Fourier transform infrared (FT-IR) spectroscopy. The physico-chemical properties of the prepared composite were studied by different analytical techniques like FT-IR, thermogravimetric analyzer, water uptake, chemical resistance, LOI and hardness studies.

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## Impact of Nanoclay on the Properties of Citric Acid Crosslinked Green Composites Based on Coconut Fiber and Modified Vegetable Oil

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### Abstract

The use of renewable and sustainable resources in the production of materials and products is imperative in order to tackle ecological and environmental concerns effectively. Layered silicate nanoclays have been extensively debated for their potential in nanocomposite technology to improve material strength and durability<sup>[1]</sup>. Due to their high aspect ratio, silicate nanolayers are a perfect choice for enhancing and strengthening materials, making them an excellent option for various applications<sup>[2]</sup>. In this study green composites based on coconut fiber as a reinforcing agent, modified epoxidized vegetable oil as resin, citric acid as crosslinker and various percentage of nanoclay as nanofiller were prepared via compression molding technique. Nuclear magnetic resonance and Fourier transform infrared spectroscopy confirmed the modification of the resin. X-ray diffraction analysis was done to study the delamination and distribution of silicate layers. The thermal and mechanical properties of the composites were assessed using Thermogravimetric Analyzer and Universal Testing Machine. The morphological structure was examined by Scanning Electron Microscopy. The chemical resistance and water uptake capacity of the composites were also evaluated. The findings demonstrated that the inclusion of nanoclay had improved multiple properties of the composites, indicating potential for biodegradability and diverse structural applications.

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## Nitrone functionalized green silica; polymer grafting and reinforcing potential in styrene-butadiene rubber compound

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### Abstract

Nitrone (Figure 1) is a versatile compound containing a nitrogen and oxygen double bond, widely used in organic synthesis for diverse reactions leading to complex molecules<sup>1</sup>. The nitrone functionalities are also proven efficient in polymer grafting techniques such as enhanced spin-capturing polymerization (ESCP)<sup>2</sup> and nitrone-mediated radical coupling reactions (NMRC)<sup>3,4</sup>. In this study, we gave grafted nitrone functionality over silica derived from rice husk ash via co-condensation, and the potential of polymer grafting via ESCP using styrene and 1,3-dipolar cycloaddition using polystyrene macromonomers has been investigated. The nitrone-functionalized silica samples were further subjected to the compounding studies with elastomers where the radicals formed during mixing and mastication, as well as the alkene functionality on the elastomer chains, can be covalently bonded with the surface nitrone functionalities resulting in better silica-elastomer interaction. The nitrone functionalities were further introduced to commercial precipitated silica and commercial RHA silica via post-modification. The samples were subjected to polymer grafting and compounding studies with elastomer, and the polymer grafting densities, as well as the curing and mechanical properties, were determined. The data obtained for various silica systems with different functionalization approaches and different nitrone grafting densities can be tuned to optimize the curing and mechanical properties of nitrone-functionalized silica-elastomer compounds.

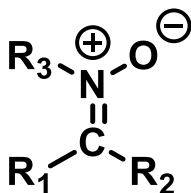


Figure 1. General structure of nitrone.

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## Natural Dye Extracted from Marigold Flower for Fabric Dyeing Using Natural Mordants

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### Abstract

Nowadays, the scopes of natural dyes have been widening due to their eco-friendly, renewable, and non-hazardous properties. The aim of this study is to extraction and characterization of natural dyes from Marigold (*Tagetes erectus*) for fabrics dyeing. The extracted dyes had been characterized through ultraviolet-visible (UV-Vis) spectroscopy, scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy. Natural mordants such as Chuk (concentrated lemon juice), Fitkiri, and Chun and metallic mordants (ferrous sulfate) were used for cotton fabrics dyeing. Natural dyes contained flavonoids and ether group which gives a variety of colors and effective towards gram-positive bacteria as compared to gram-negative bacteria and fungi. The yellow dye extracted from the flowers of *Tagetes erectus* for fabric dyeing was found effective in presence of natural mordants as compared to metallic salts as commercial mordants.

Keywords: Natural dyes, *Tagetes erectus*, mordants, dyeing

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## Role of compatibilizer on the various properties of bio-filler based synthetic polymer composites

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### Abstract

Replacing the petroleum-based polymer materials with bio fillers and materials in a sustainable manner provides a competitive advantage as they possess unique properties which cannot be emulated by conventional polymers. The drawbacks of synthetic polymers can be partly overcome by using naturally derived materials. In this work, High Density Polyethylene (HDPE)-Polypropylene (PP) based composites were prepared by using Epoxidized soybean oil (ESO) and Polyethylene-co-Glycidyl Methacrylate (PEGMA) as compatibilizer, Calcium oxide as heat stabilizer and bamboo fibres. The materials were first melt-mixed and then compression molded to get the composites. The composites were prepared by varying the different ingredients. The interaction among the materials was revealed by Fourier Transform Infrared Spectroscopy (FTIR). Surface morphology of the samples was studied by Scanning Electron Microscope (SEM). Thermal stability of the composites was analysed by Thermogravimetric Analysis (TGA). Mechanical properties, flame retardancy, chemical resistance, water uptake and dimensional stability were also studied. Further optimisation are to be carried out in order to achieve an overall improvement in properties.

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## Effect of modified cellulose nanofiber on the thermomechanical properties of cardanol based benzoxazines

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### Abstract

Polybenzoxazines are a new class of high- performance thermosetting resins with improved features over traditional thermosets, in terms of molecular design flexibility, dimensional stability, and thermomechanical properties. However, high curing temperature, low crosslinking density, and brittleness are the major shortcomings that limits their application[1-2]. The present work aims to address these challenges by developing sustainable, eco-friendly, and high- performance polybenzoxazine nanocomposites using cardanol as the biobased phenol and modified cellulose nanofiber (MCNF) as the reinforcing filler. The effect of different weight loading of MCNF on the curing kinetics of cardanol- aniline based benzoxazine (Ca-A) was studied using non-isothermal differential scanning calorimetry (DSC) at various heating rates, and apparent activation energy ( $E_a$ ) was calculated using Kissinger and Ozawa methods. The results revealed that the addition of MCNF up to 2% showed a marginal decrease in the activation energy and thereby reduce the curing time. Further FT-IR was used to analyse the difference in hydrogen bonds in the cross-linked structures of Ca-A and Ca-A-MCNF composite. It was observed that the addition of MCNF suppress the formation of Type I – OH $\cdots$ N hydrogen bonds, which ensures high degree of polymerization and simultaneously improve the properties. The results are further analysed using tensile and Dynamic Mechanical Analysis (DMA).

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## **Synthesis and Development of Surface Modified Cellulose Nanofiber Composites for High Performance Materials**

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### **Abstract**

Nanocellulose is gaining greater interest for its use in environmental remediation solutions as a result of its appealing properties, which include excellent mechanical strength, high specific surface area, good biocompatibility, and strong barrier properties. The presence of hydroxyl rich groups on its surface made it suitable for preparing polymer composites for various applications. However, despite its many advantageous characteristics, its intrinsic hydrophilicity poses a significant challenge as a reinforcing filler. It hinders its dispersion in hydrophobic host polymer often results in aggregated structures, which could be an impediment to mechanical performance of composites. TEMPO oxidation<sup>1</sup> and nitro-oxidation methods<sup>2</sup> were effective chemical routes for the preparation of surface functionalized cellulose nanofibers (NCF). Herein, surface modified NCF was obtained by chemical treatment followed by high-pressure homogenization to produce uniform sized banana-cellulose nanofiber (B-CNF). Further, the fiber surface was made hydrophobic using silanization<sup>3</sup> method and benzoxazine composites were prepared. The fibrillated morphology of B-CNF were analysed using HR-TEM and further characterized by ATR-FTIR, XRD and XPS techniques. One of the objective of this study is to understand the effect of surface modified B-CNF on the curing kinetics, kinetic behaviour and mechanical strength of cardanol-derived benzoxazine - B-CNF composite coatings for surface coatings, and adhesives applications.

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- [3] Ghasemlou, Mehran, FugenDaver, Elena P. Ivanova, Youssef Habibi, and BenuAdhikari. Progress in Polymer Science 119, 101418, 2021

## Performance and characterization of PLA-biowaste-based composite for FDM 3D printing

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### Abstract

Ecofriendly plastics present viable alternatives to harmful non-degradable polymers/plastics. Polylactic acid (PLA), a bio-resin derived from corn starch is one of the commonly employed thermoplastic polymers in the realm of three-dimensional printing due to its exceptional ease of use, and biodegradability, leading to its widespread applications.<sup>1</sup> Nevertheless, the mechanical and biological attributes of PLA need further refinement. Biocarbon derived from biowaste has emerged as a promising eco-friendly material, capturing the interest of researchers for diverse applications.<sup>2</sup> The present work focuses on developing a completely sustainable, biodegradable, and eco-friendly PLA-biocarbon composite material for 3-D printing. The synthesized additive is characterized by various techniques such as SEM, XRD, TGA-DSC, and Raman spectroscopy. The fabricated 3-D printed samples were mechanically and rheologically tested. While carrying out the performance evaluation studies, the results indicate that the interplay of extrusion and uniformly size-reduced particles significantly affect the mechanical properties of the composite by altering the framework of the polymer blends. The 3D-printed specimen containing biocarbon showed a remarkable improvement in tensile and thermal properties.

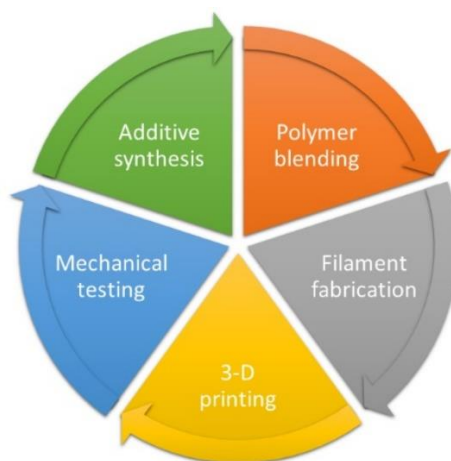


**Figure 1.** Graphical Abstract

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## Fabrication of dual-sized linearly aligned electrospun CA/PVP core-shell fiber membranes

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### Abstract

Scalable synthesis of fibers with good mechanical and barrier properties from nature derived biopolymers suitable for food packaging. Cellulose acetate (CA) is a cellulose derivative that can be easily dissolved in most organic solvents and can produce nanofibers using electrospinning.<sup>1</sup> To meet further needs, the performance of electrospun CA fibers can be improved by blending it with suitable additives, however their lack of chemical affinity and low oxidizability hinder their broad usage.<sup>2</sup> Herein, a homogenous blend solution of CA and PVP was electrospun to successfully fabricate linearly aligned core-shell nanofibers membranes. On varying the CA/PVP ratio, a consistent and normal nanofiber were formed with a lower PVP concentration, whereas a linear arrangement with branching of fibers having dual-width were formed with a higher PVP concentration. In order to optimise the size and morphology of the CA/PVP nanofiber composites, we systematically altered the polymer solution concentrations and electrospinning parameters such as needle-collector distance, applied voltage, fluid flow rate etc. The linear and branched as well as the core-shell morphology of the fibers were well characterized using SEM, polarized optical microscopy, SEM-EDS, TEM-EDS, XPS, etc.

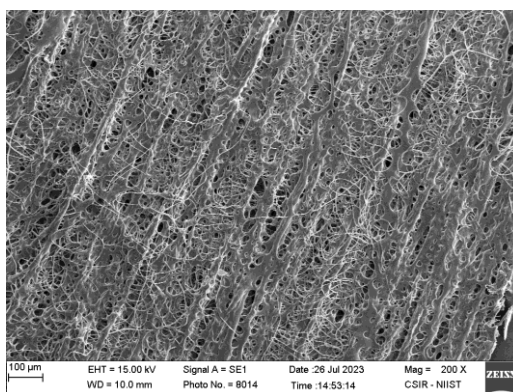


Figure: SEM micrograph showing linear and branched morphologies of electrospun CA/PVP composite.

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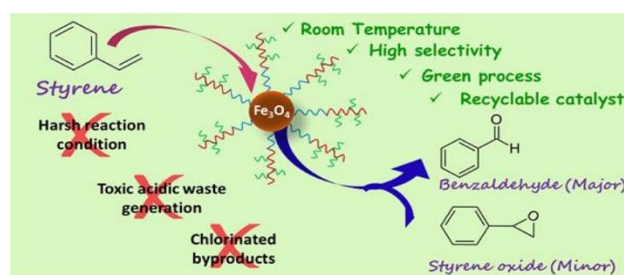
## Green Catalyst for Styrene Oxidation Reaction Using Stimuli-Responsive Polymer Stabilized Iron Oxide Nanoparticle

Sharmita Bera, Jitu Padhee, Juthi Pal, Satyagopal sahu and Dibakar Dhara\*  
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### Abstract

The traditional toluene chlorination method must be replaced with a more environmentally friendly method to produce benzaldehyde for environmental benefits<sup>1</sup>. We have created polymer-conjugated magnetic nanoparticles as "green catalysts" in that direction<sup>2,3</sup>. We have created polymer-conjugated magnetic nanoparticles as "green catalysts" in that direction. Poly[(*N*-isopropylacrylamide-*b*-acrylic acid)] and poly- [(*N*-isopropylacrylamide-*r*-*N*-vinylpyrrolidone)-*b*-(acrylic acid)] coated magnetic nanoparticles showed high catalytic activity in the synthesis of benzaldehyde by styrene oxidation reaction at room temperature in water using hydrogen peroxide as an oxidizer. Due to the presence of hydrophilic polymer on the surface of nanoparticle the catalysts allowed aqueous dispersibility and showed quasi-homogeneous behaviour in water at room temperature. Varying the temperature, the conversion of styrene to benzaldehyde and styrene oxide can be regulated, owing to the temperature responsiveness of the block copolymers. The optimal reaction condition is achieved by optimising parameters like catalyst concentration, temperature, and time. The catalysts can be quickly recovered using their magnetic property and reused without any significant loss in catalytic activity. As a result, these two nanoparticle systems shown tremendous promise for green nanocatalysts in industrial applications.



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## **Ionic liquid dispersed PDMS/SWCNT/Ag@Ni hybrid composite for temperature and pressure sensitive smart electromagnetic shielding application**

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### **Abstract**

The development of highly sophisticated self-adapting intelligent electronic and communication systems in military, aerospace, robotics, etc., prompted the requirement of externally stimulated green shielding material to protect them from electromagnetic interference (EMI). However, it remains a big challenge to develop such environmentally sensitive EMI shielding materials with extremely high green shielding performance. Herein, an ionic fluid (IL) impregnated polydimethylsiloxane (PDMS)/single-wall carbon nanotubes (SWCNT)/silver-coated nickel (Ag@Ni) nanoparticles (NP) hybrid composite was devised for thermally adjustable smart green shielding capability. In this composite system, 1M and 3M of aqueous NaCl, CaCl<sub>2</sub>, and KI ILs were mixed along with electromagnetic fillers (SWCNT/Ag@Ni) in PDMS matrix that revealed a distinct ion concentration-dependent shielding performance. The composite with 3M KI IL at 100 °C demonstrates the reversible thermally modulated smart green radiation shielding performance of 68.9 dB in 14.5-20 GHz spectrum. Moreover, the composite shows exceptionally high green index of ~101 at 100 °C, confirms an excellent thermally modified absorption shielding capability. Additionally, the IL-generated foamed composite architecture exhibits pressure-sensitive on-off switchable shielding capability, making it ideal for advanced RF switches in satellite communications.

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## Lightweight and Flexible Electrospun Polyurethane Fiber Coated with Carbon Black/Polyvinyl Alcohol for Electromagnetic Interference Shielding

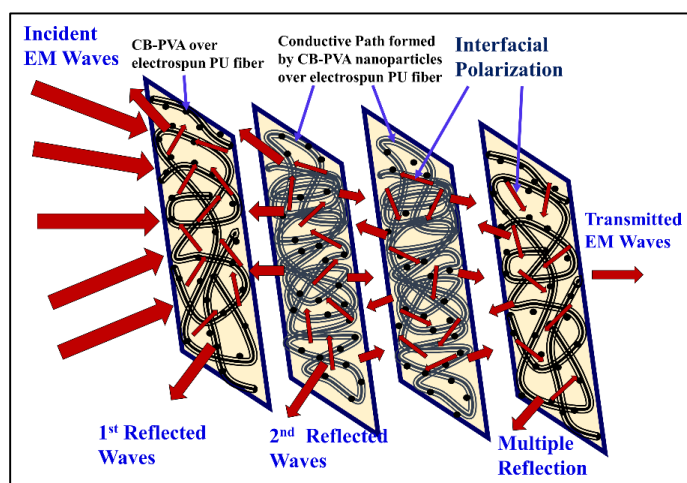
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### Abstract

The rapid proliferation of wireless technologies and miniaturization of electronic devices have led to the emergence of electromagnetic interference (EMI) which has become a serious issue in modern electronics devices. To solve this problem, there has been a lot of focus on fabricating lightweight and flexible EMI shielding materials. Electrospun polymer nanofibers assume great importance in designing efficient EMI shielding materials. The properties of nanofibers such as large specific surface area, porosity and significant interconnectivity assist in absorption and multireflection of EM waves. Herein, carbon black (CB) dispersed in polyvinyl alcohol solution was coated over electrospun polyurethane (PU) nano fiber [CB-PVA/EPUF] mat. The resultant nanofiber mat exhibited 99% attenuation of EM waves in X-band, Ku-band, and K-band. The composite nanofiber mat showed absorption dominant shielding mechanism due to the layer by layer structure, uniform coating of CB over one-dimensional electrospun PU fiber and formation of electrical conductive network. The synergistic effect of EPUF microstructure and carbon fillers along with PVA make it suitable for fabricating light weight and flexible EMI shielding material. This shielding material may be explored in wearable and flexible electronic devices.



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## Silver-loaded triazole based porous organic polymer for rapid cyclization of propargylic amines with CO<sub>2</sub> to oxazolidinone derivatives

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### Abstract

CO<sub>2</sub> footprint has been increasing rapidly in the last two decades and it is one of the significant contributors to global warming. Several strategies have been employed where CO<sub>2</sub> has been used as a C1 carbon source for the synthesis of a diverse range of value-added chemicals.<sup>1</sup> In this context, the catalytic conversion of propargylic amines to 2-oxazolidinone derivatives is highly significant due to its importance as a heterocyclic backbone in various natural products.<sup>2</sup> However, the high thermodynamic stability of CO<sub>2</sub> and sluggish reaction kinetics limit the role of CO<sub>2</sub> as an effective reagent. To circumvent the above issues, various heterogenous catalysts have been designed consisting of a CO<sub>2</sub>-philic matrix and metal centers. Porous organic polymers due to their tunable pore size and functionalities provide a suitable platform for catalytic CO<sub>2</sub> fixation.<sup>3</sup> Also, the presence of heteroatom-rich moieties further assists in anchoring the metal nanoparticles, which catalyze the CO<sub>2</sub> insertion in the propargylic amines.<sup>1</sup> Herein, we have fabricated an N-rich triazole-based porous organic polymer through click polymerization followed by *in situ* loading of silver nanoparticles. Due to its high surface area and homogeneously distributed silver nanoparticles, the heterogenous porous catalyst showed rapid conversion of propargylic amines to oxazolidinone derivatives under mild conditions of 1 atm pressure and 50 °C within 15 mins. Thus, the metal nanoparticle-loaded porous organic polymer could be a promising heterogeneous catalyst for the facile fixation of CO<sub>2</sub> to various value-added chemicals under milder conditions.

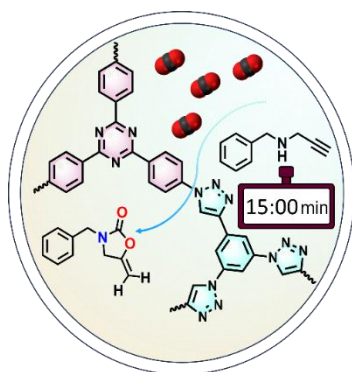


**Figure 1.** Schematic representation of the triazole-based porous organic polymer for rapid catalytic conversion of CO<sub>2</sub> with propargylic amines to its respective oxazolidinone derivative.

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## Phytic Acid Modified Boron Nitride Nanosheets as Sustainable Multifunctional Nanofiller for Poly(3-Hydroxybutyrate)

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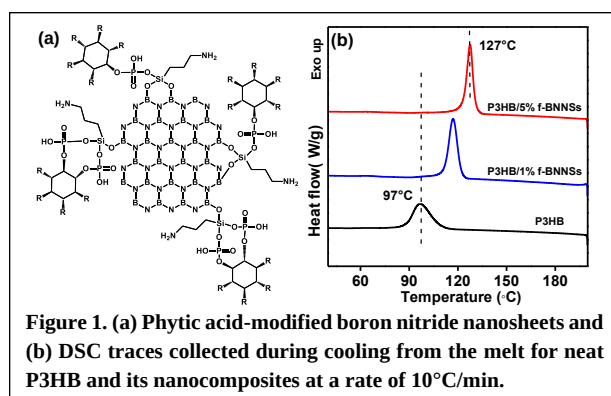
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### Abstract

The significant growing demand for sustainable materials is to minimize the dependency on petroleum-based plastics. However, most of the biobased and biodegradable polymers have inferior properties compared to those of the commodity polymers. These properties can be improved by using biodegradable and biocompatible nanofillers. Poly(3-hydroxybutyrate) (P3HB) is a semicrystalline, biodegradable bacterial polyester that belongs to polyhydroxyalkanoates family. However, P3HB suffers from inherent flammability, slow crystallization rate and thermal processability. In this work, we have developed a sustainable multifunctional nanofiller for P3HB based on boron nitride nanosheets and biobased phytic acid (Fig 1(a)). The effect of nanofillers on crystallinity, crystallization kinetics, thermal stability, and flame-retardant properties of P3HB was systematically investigated. The results showed that the melt crystallization temperature of P3HB was remarkably enhanced with the increase in filler content (Fig 1(b)). With 1 wt % addition of filler, the crystallization half-time of the nanocomposite decreases from 14.0 to 1.0 min at 120 °C compared to pristine P3HB. It is observed that the incorporation of filler favors the increase in the  $\beta$  fraction of P3HB. The presence of phytic acid-modified boron nitride nanosheets improves the char-forming capability of P3HB nanocomposites and as a result, the flame retardancy of P3HB was enhanced.



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## Role of Zeolite Nanocontainers as a Corrosion Resistant Filler in Bio-based Hybrid Coatings.

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### Abstract

The issue of “corrosion” is a critical global challenge and the economic losses contributed by corrosion accounts for up to 5% of the gross national product<sup>1</sup>. In order to abate these colossal losses, polymeric coatings came into limelight. These polymeric coatings were loaded with various agents (fillers, fibres and nanomaterials) to enhance their property and induce more efficacy. However, these materials are merely carcinogenic and are not environmentally benign. Another significant disadvantage of polymeric coatings is that the majority of the polymers we use in our everyday lives are generated mostly from fossil fuel-based feedstock, which are also depleting at an alarming rate<sup>2</sup>. In order to avoid these shortcoming's and to work for a better sustainable future, herein we report the development of a novel zeolite based nanocontainer system in which the system channels were loaded with a corrosion inhibitor. The prepared nanocontainer is characterized by various analytical and spectroscopic techniques including P-XRD, FTIR, UV-DRS and N<sub>2</sub> sorption. Subsequently, the inhibitor loaded zeolite nanocontainer was incorporated into a biobased polyurethane matrix as a filler with variable weight ratios (0 to 2%). The physicochemical, mechanical and the thermal properties of the free-standing PU-composite films are examined through ATR, TGA and DMTA respectively. Finally, the PU-composite was casted on a mild steel substrate and was subjected to corrosion inhibition study by PDP and EIS techniques. The studies revealed that the PU films exhibited a promising anticorrosive property with highest corrosion rate ( $C_R \sim 5.76 \times 10^{-6}$  mm/year), charge transfer resistance ( $R_{ct} \sim 1.51 \times 10^7 \Omega$ ) and phase angle ( $\theta > 80^\circ$ ).

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## Protonation and self-assembly behaviour of fluorophore labelled like-charged polyethylenimine chains in water

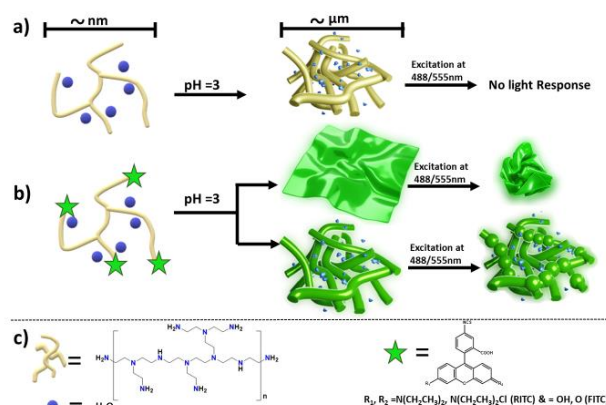
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### Abstract

Polyelectrolyte-based self-assembled structures hold significant importance in enhancing the performance of various materials employed in tasks such as drug delivery, barrier functions, separation, and catalysis. In this context, we present a new type of light-responsive hybrid soft materials crafted by covalently attaching small dye fluorophores to polyethylenimine (PEI), the gold standard non-viral vector for gene transfection. Depending on the density of dye grafting, branched PEI chains in a dilute aqueous solution within the pH range of 2.5 to 4 exhibit unprecedented self-organization, resulting in the formation of either micron-sized hollow fibrils or sheets. The interaction between PEI and the dye within this hierarchical network triggered by using the light of excitation wavelength of the dye, induces the creation of bead-necklace-type structures in the fibres and a macroscopic volume collapse of the sheets. This unique mechanism is attributed to the excited state proton transfer from the dye to the PEI chains, with the latter acting as a proton sponge at in the pH range of 2.5 to 4. Our research underscores the potential of hybrid polyelectrolyte-dye complexes, which seamlessly incorporate pH-dependent higher-order assemblies formed by PEI and light responsiveness of the fluorophores. These materials offer promising avenues for the development of soft matter for actuation-based applications and hold relevance for fluorescent PEI-DNA polyplexes utilized in gene transfection at low pH conditions.



Schematics showing the self assemblies formed by PEI at pH=3 which do not show any light response in the absence of fluorophore (a) and show light responsive behaviour after tagging PEI chains with the fluorophores (b).

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## Combination of screen printable fluorescent polymer ink with angle-dependent structurally colored colloidal photonic crystals

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### Abstract

Photonic crystals are polymeric material that exhibits a periodic optical nanostructure and has a photonic band gap in the visible region. It prevents the propagation of light through the system and reflects the same. These reflected light appear as bright, iridescent colors called structural colors and they bio-mimics the colors seen in nature like in the wings of butterflies, peacock feathers, etc. Chemical colors, on the other hand, mainly fluorescence and phosphorescence are due to the electronic transitions in molecules that absorb specific wavelengths of light. The main disadvantage of an organic dye is its photo-degrading property which can be avoided by incorporating these dyes inside the polymer matrix. Thus developed dye-incorporated polymer emulsions can tune the emission wavelength as well as the intensity because of the overlap of the photonic band gap with the emission wavelength and it can be converted into fluorescent screen printable inks by adding suitable stabilizers and solvents. Thus the importance of polymer emulsions for producing both structural colors and tuning the emission wavelengths of organic dyes are well discussed.

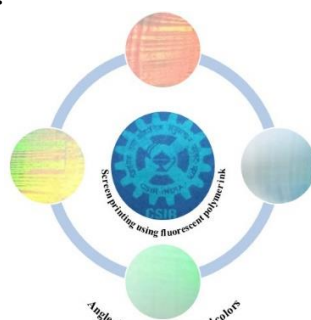


Fig. 1: Screen-printed CSIR logo (under 365nm UV light) and angle-dependent structural colors shown by colloidal photonic crystals.

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## Studies on Amphiphilic GO@CeO<sub>2</sub> - Polyurethane Hybrid Nanocomposites as Corrosion Protective Coatings

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### Abstract

Corrosion has been one of the major societal problems hampering economic growth and human life. The destruction of metallic structures impacts negatively on various industries such as automobiles, marine, construction, and aerospace. The use of protective coatings to reduce metallic corrosion by preventing the transportation of corrosive media is widely studied. Graphene and its derivatives have shown significant promise in the prevention of metallic corrosion as an additive in protective coatings. Waterborne polyurethanes (WPU) are environment-friendly organic binders in anti-corrosion coatings due to their excellent flexibility, toughness, strong adhesion to substrates, and environmental safety. Herein, we report a bioderived WPU, amphiphilic modified GO (AGO) towards the development of anti-corrosive WPU-GO composite coatings with varying compositions. Cerium-decorated AGO was also studied to improve the anti-corrosion performance of the coatings. The chemical structures and morphology of composites were studied by FT-IR and SEM along with the surface wettability and thermal properties. The optical properties of the nanocomposites were studied by UV-visible spectroscopy and photoluminescence spectroscopy. The corrosion protection efficiency was evaluated on mild steel substrates using Electrochemical Impedance Spectroscopy (EIS) and Tafel curves. The results show improved inhibition efficiency of AGO composite coatings, (up to 84%) as compared to mild steel.

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## Synthesis and Characterizations of Poly (Butyl Acrylate-co-Vinyl Acetate-co-Acrylic Acid) polymer with Kaolin Clay Composites

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### Abstract

This investigation reports the synthesis of emulsion poly (vinyl acetate) based terpolymer with kaolin clay composites and their successive characterization. The terpolymer of vinyl acetate, butyl acrylate and acrylic acid was prepared via emulsion polymerization methods. The emulsion polymerization was carried out at 70 °C using potassium persulfate (KPS) as initiator and sodium lauryl sulfate as a surfactant. Conversion of the monomers was calculated gravimetrically and found to be 90 % after 1 hour of polymerization. The successful preparation of the terpolymer was confirmed by proton nuclear magnetic resonance analysis. The polymer-Kaolin clay composites were prepared by adding different amount of Kaolin clay to the terpolymer latex. Thereafter, the prepared polymer -clay composites were characterized by nuclear magnetic resonance spectroscopy (NMR), Fourier transform infrared spectroscopy (FTIR), Differential scanning calorimetry (DSC) and Thermogravimetric Analysis (TGA) analyses. Mechanical properties like tensile strength, modulus, and elongation at break etc. were also evaluated for the prepared polymer-clay composites. Rheological nature of the polymer composites were evaluated using the rubber process analyzer.

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## Interfacial Layer Grafting of Janus-Type Covalent Organic Framework Thin Films

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Empowered by crystalline ordered structures and homogeneous fabrication techniques, covalent organic frameworks (COFs) have been realized with uniform morphologies and isotropic properties.<sup>1</sup> However, such homogeneity often hinders various surface-dependent properties observed in asymmetric nanostructures. The challenge remains to induce heterogeneity in COFs by creating an asymmetric superstructure such as a Janus thin film. In this regard, we propose a versatile yet straightforward interfacial layer-grafting strategy to fabricate free-standing Janus-type COF-graphene thin films.

Herein, two-dimensional graphene sheets were utilized as suitable grafter due to the possibility of noncovalent interactions between the layers.<sup>2</sup> The versatility of the approach was demonstrated by fabricating two distinct Janus-type films, with the COF surface interwoven with nanofibers and nanospheres. The Janus-type films showcase opposing surface morphologies originating from graphene sheets and COF nanofibers or nanospheres, preserving the porosity ( $552\text{--}600\text{ m}^2\text{ g}^{-1}$ ). The unique surface chemistries of the constituent layers further endow the films with orthogonal mechanical properties, as confirmed by the nanoindentation technique.

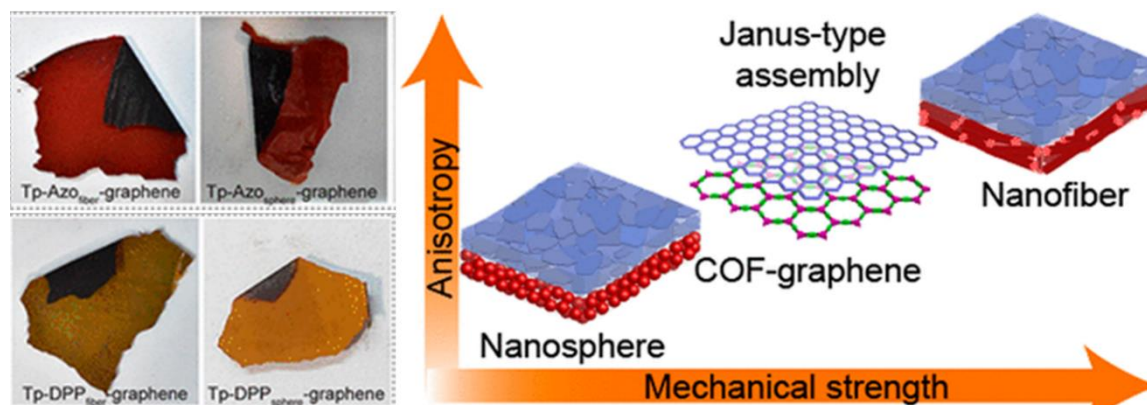


**Fig. 1** Schematic overview of the work

Findings confirm the superior mechanical properties of heterogeneous Janus-type COF films compared to homogeneous composites and highlight shape-dependent variations. Synthesis routes can be chosen to design COF Janus films with specific mechanical properties based on the application demand.

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## Mechanism of Solvent-Mediated Metal Infiltration into Block Copolymer Nanopatterns and Formation of metal-oxide arrays

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### Abstract

The nanopatterning of materials on surfaces has attracted a significant attention from interdisciplinary scientist as it has applications in the field of electronics, electrochemistry, optics, photonics, catalysis, and biology. Here, we thoroughly analyzed the effect of solvent annealing time on the ordering of highly asymmetric poly(4-vinylpyridine)-b-polystyrene (PS-b-P4VP) block copolymer. Phase separation of PS-b-P4VP was achieved by the solvent vapour annealing (SVA) in a non-selective solvent atmosphere to create cylindrical arrays. Interestingly, transition in morphology from P4VP hexagonally packed cylinders to an 'inverse' structure with PS cylinders embedded in a P4VP matrix was observed. Furthermore, we also systematically studied the effect of oxidation state and type of cation in the infiltration process, which were selectively inserted into the P4VP arrays from PS-b-P4VP BCP templated thin films. The findings showed that the stability of the as-obtained metal-pyridine complex is highly influenced by the oxidation state and type of cation, and hence, the formation of metal oxide patterns. Various metals ( $\text{Ag}^+$ ,  $\text{Ni}^{2+}$ ,  $\text{In}^{3+}$  and  $\text{Ga}^{3+}$ ) cations were inserted into P4VP arrays by solution mediated infiltration approach followed by an ultraviolet-ozone (UVO) treatment to remove the polymer and oxidize the metallic ions to their oxides. It was found that P4VP/ $\text{Ag}^+$  pattern was not intact after UVO treatment due to the weak interaction between them, however,  $\text{Ni}^{2+}$  and  $\text{In}^{3+}$  were able to reproduce the pattern of BCP. These obtained results were characterized by a variety of methods, including atomic force microscopy, scanning electron microscopy, Raman spectroscopy and X-ray photoelectron spectroscopy.

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## Photocatalytic degradation of Eosin Y dye in aqueous solution by using SnO<sub>2</sub> Nanoparticles

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### Abstract

The release of synthetic dye into water is a serious pollution problem and also contaminates the ground water. Due to improper discharge and processing, approximately 50,000 tons of dye are discharged to ground water. Most dyes have complex structures and contain aromatic rings which makes them carcinogenic and decolorization is also complicated. Eosin Y is an anionic dye used in the textile industry, dermatological agent, biological stain, and paper printing but overexposure causes skin irritation and painful sensitization to light. Over the years, various removal methods are extensively used for the removal of dyes but the photocatalytic process is the most prominent technique as it is an efficient and economical technique that converts highly toxic organic pollutants to comparatively fewer toxic fragments without producing its secondary pollutants. SnO<sub>2</sub> nanoparticles synthesized via a one-pot polymer-assisted route were used to investigate the degradation of Eosin Y in the presence of sunlight. It was observed that SnO<sub>2</sub> nanoparticles show better degradation in the sunlight when compared with dark conditions. The removal efficiency of 96.8 % for Eosin Y was observed within 30 minutes of sunlight exposure. The effect of nanoparticle dose, pH, and contact time on the removal efficiency of methylene blue was investigated. The experimental results suggested that the SnO<sub>2</sub> nanoparticles have excellent removal efficiency and have the ability to remove the Eosin Y dye at a faster rate.

**Keywords:** Photocatalysis, Water Treatment, SnO<sub>2</sub> nanoparticles, Eosin Y dye.

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## Guar gum--based gel polymer electrolytes dispersed with SiO<sub>2</sub> nanofibers

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### Abstract

The development of sustainable materials is crucial for creating more environment-friendly energy storage applications, the demand for which is upsurging [1-3]. In this context, we prepared nanocomposite gel polymer electrolytes (NCGPEs) using Guar gum (GG) complexed with silicon dioxide (SiO<sub>2</sub>) nanofiber with lithium perchlorate (LiClO<sub>4</sub>) salt. The sample containing 5 wt% nanofibers exhibits the highest electrolyte uptake of 114% and the highest ionic conductivity of  $6.2 \times 10^{-3}$  S/cm at room temperature. The advancement in enhancing the conductivity and energy transfer efficiency of nanocomposite gel polymer electrolytes by increasing the concentration of nanofibers holds significant promise for a range of applications, including batteries and fuel cells. The electrical and electrochemical properties of the produced nanocomposite gel polymer electrolytes and their structure-property correlations were investigated using SEM, FTIR, DSC, TGA, TEM, XRD, and XPS.

Keywords: Polymer electrolytes; Energy storage devices; Nanocomposites;

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## Amyloid targeting ‘artificial chaperone’ impairs oligomer-mediated neuronal damage and mitochondrial dysfunction associated with Alzheimer's disease

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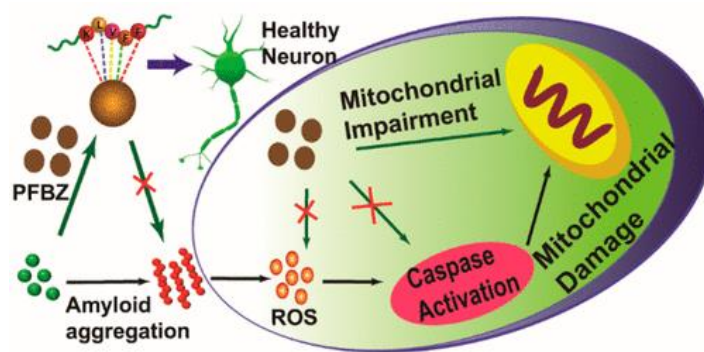
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### Abstract

Alzheimer's disease (AD) is an irreversible memory loss caused by amyloid accumulation, oxidative damage, and mitochondrial dysfunction. Benzimidazole functionalized polyfluorene (PFBZ), a novel artificial chaperone, selectively sequesters toxic amyloid beta ( $A\beta$ ) by binding at its ‘amyloidogenic domain’ ( $A\beta$ 16–21) and prevents neuronal damage in a wild-type (WT) mouse model. A correct dose of PFBZ chaperone reduced amyloid-induced cerebral cortical hemorrhage and pyknosis in WT mice. The polymer's structure allows efficient Cu(II) chelation to block a redox cycle and shield mitochondria from ROS damage. Caspase activation, mitochondrial membrane potential (MMP) biomarkers, brain histology, and electron microscopy showed that the PFBZ chaperone coated the amyloid surface, prevented cell membrane interaction, and prevented toxicity.



The conjugated polymer artificial chaperone-based nanodrug exhibits unique properties, including multipotency, biocompatibility, specific amyloid ( $A\beta$ 16–21) targeting, bioimaging, and BBB permeability. It may suppress amyloid-triggered neurotoxicity responsible for various human disorders through a synergistic mechanism.

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## Effect of dispersion on the gas barrier property of hybrid 3D nanofillers incorporated segmented polyurethane nanocomposites

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### Abstract

The hybrid 3D carbonaceous nanofillers i.e. functionalized carbon nanotube (f-MWCNT) immobilized into edge functionalized few layer graphene (f-FLG) were incorporated into segmented thermoplastic polyurethane (STPU) by twin screw extrusion (TSE) technique. The nanofillers was loaded in different weight percentages (0.25, 0.5, 1.0, 2.0 and 5 wt%). The supramolecular self-assembly route (SSAR) was espoused to enhance the level of dispersion of nanofillers at higher percentages into STPU followed by TSE. The phase morphology of prepared nanocomposites was studied and analysed by scanning electron microscope (SEM). The phase morphology unveiled uniform dispersion at higher nanofillers loading of 2 wt% through SSAR followed by TSE. The permeability of the film prepared using 2 wt% hybrid 3D nanofillers strengthened STPU nanocomposite exhibited significant improvement of gas barrier property with reduction of He (helium) gas permeability from 1287 (for neat polyurethane film) to 472 cm<sup>3</sup>/m<sup>2</sup>/day. The developed nanocomposites were also evaluated by X-ray Diffraction (XRD), Attenuated Total Reflection Fourier Transform IR (ATR-FTIR) spectra and Thermogravimetric Analysis (TGA).

**Key words:** Polyurethane; 3D nanofillers; extrusion; supramolecular self-assembly route; gas barrier property, permeability.

## Fabrication of dopamine sensor based on a carbon paste electrode modified with tetracyanoquinodimethane and cobalt tungstate nanoparticles

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### Abstract

In this study, we have fabricated TCNQ@CoWO<sub>4</sub>/CPE for precise, reliable, and sensitive electrochemical sensing of dopamine. The modified electrode was characterized by cyclic voltammetry (CV), differential pulse voltammetry (DPV), amperometry, and electrochemical impedance spectroscopy (EIS). The findings demonstrate significant electrocatalytic capability for supporting dopamine sensing. The CV studies demonstrate that TCNQ@CoWO<sub>4</sub>/CPE had intensified electrocatalytic activity for dopamine oxidation due to a synergistic interaction between TCNQ and CoWO<sub>4</sub> nanoparticles. Amperometric analysis shows a wide linear range of 2  $\mu$ M to 80  $\mu$ M for dopamine monitoring, and sensitivity was found to be 0.2028  $\mu$ A/ $\mu$ M. EIS analysis provides the low  $R_{ct}$  value (11500  $\Omega$  cm<sup>2</sup>) for TCNQ@CoWO<sub>4</sub>/CPE compared to TCNQ/CPE, illustrating high electron transfer capability. Besides this, the TCNQ@CoWO<sub>4</sub> carbon paste electrode exhibits excellent stability, selectivity, and reproducibility. The modified sensor also applies for real sample analysis in commercially available dopamine injection, and a good recovery result was found.

## Transient self-assembly of nanoparticle via cucurbit[7]uril host-guest interaction

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### Abstract

Numerous biological processes require energy and involve dissipative self-assembly. Nature employs this for temporal function control, offering enhanced catalytic efficiency and selectivity compared to typical catalysis. However, explorations into nanoparticle-based transient assemblies are rare. Here, we present a transient catalytic approach employing host-guest chemistry. A dissipative self-assembly approach is established by temporal transitioning from a high-affinity to a low-affinity guest for the host, here macrocycle CB, which exhibits varied binding affinities. The modulation of the host-guest interactions was achieved by tuning the ion-dipole repulsion between the host-guest, where an unfavorable ion-dipole repulsion hinders the binding of negatively charged guests with the electronegative carbonyl-lined portal of CB[7]. Further, a temporal change in affinity was established by hydrolysis of the guest molecule where the high-affinity guest hydrolyzes to low-affinity guest at physiological pH. Interestingly, reintroducing the guest allows for cycle repetition. Finally, transient catalysis was attained by employing the aforementioned approach. Also, a precise spatiotemporal regulation of therapeutic release can be possible by the transient control of assembly-disassembly of catalyst-bound nanoparticle-CB complexes. By extending this research, we can address key challenges associated with conventional drug delivery systems, such as poor bioavailability, non-specific distribution, and off-target effects.

## Polymeric 3D scaffolds for cell capture and evaluating drug efficacy

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### Abstract

Polymeric materials are being used for creating 3D scaffolds for culturing cells.<sup>1,2</sup> We hypothesized that 3D scaffolds fabricated using blends of poly(lactic acid) (PLA) and poly(lactic-co-glycolic acid) (PLGA) would impart spatial constraints mimicking extracellular matrix (ECM) by enabling cellular interactions and proliferation. Furthermore, covalent conjugation of proteins including transferrin, collagen and bovine serum albumin (BSA) would alter the cellular growth patterns and proliferation potential. Further, incorporation of anticancer drug agents such as doxorubicin in these 3D scaffolds would enable the evaluation of 3D cellular localization via cell volume and nuclear volume alterations. We characterized 3D polymeric scaffolds using scanning electron microscopy (SEM), optical microscopy, Fourier-transform infrared (FTIR) spectroscopy and contact angle ( $\theta$ ). Viability of breast cancer cells (MCF-7) was determined using 3-[4,5-dimethylthiazol-2-yl]-2,5 diphenyl tetrazolium bromide (MTT) and cellular growth patterns were studied using confocal laser scanning electron microscopy (CLSM) and the anti-cancer drug activity was also evaluated. The designed polymeric 3D scaffolds mimic *in vivo* microenvironment with aggressive cell proliferation and tissue regeneration.

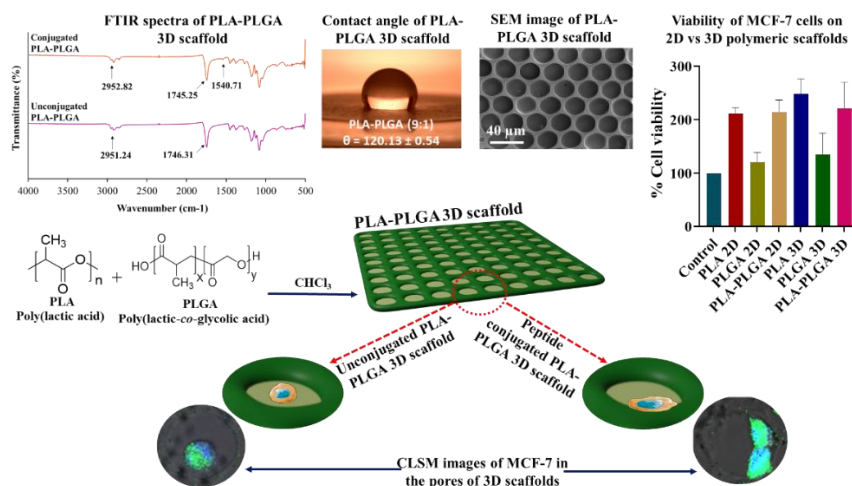


**Figure 1.** Graphical representation of fabrication of polymeric 3D scaffolds, characterization and cellular growth patterns.

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## Aesthetic Transparent Wood: Preparation and Characterizations

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### Abstract

Wood has been in use from time immemorial as a building material. Wood's complex hierarchical structure continues to intrigue scientists. The most salient feature is the structural anisotropy, where many aligned vertical channels are present.<sup>1</sup> It is through these vertically aligned channels, that ions, water, and other ingredients are pumped. Wood displays great diversity in porosity and density due to the high anisotropy, high transparency, high haze, excellent thermal insulation, and high impact absorption capability. Manipulation of its structure could lead to aesthetic transparent wood (ATW), elastic behaviour, and provide great potential for multifunctionalization.<sup>2</sup> Transparent wood is obtained when lignin is removed and the vertical channels are filled with a polymer of tailored refractive index. The hierarchical structure of the wood is also preserved.<sup>1-3</sup>

Here we present our preliminary work on the preparation of aesthetic transparent wood. Ice-cream sticks and jack-plane shavings of veneer and other wood were selected for this study. A careful removal of opacity-causing lignin would result in empty channels. These could be strengthened with an epoxy or other fillings. Thus we obtained delignified wood pieces that possess about 75% transparency. ATW is a potential candidate for lightweight low-cost, light-transmitting buildings and transparent solar cell windows. Various methods for the preparation of ATW and optical and mechanical properties will be presented. It is our dream to make this an exercise in sustainability thereby reducing the carbon footprint.



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## Napthalimide-Based Fluorescent Polymeric Probe for Ultrafast Sensing of Formaldehyde: In Both Gaseous and Aquous Phase

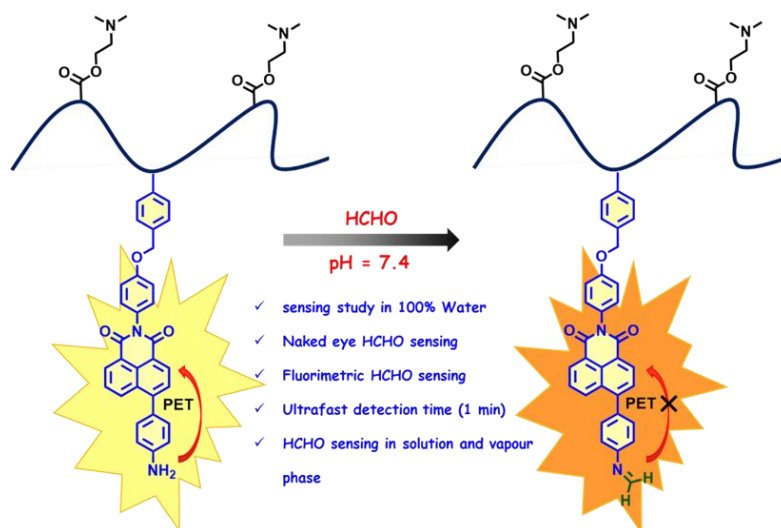
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### Abstract

Formaldehyde, a colorless and pungent-smelling gas, is a common volatile organic compound (VOC) and simplest aldehyde found in various indoor and outdoor environments. The International Agency for Research on Cancer (IARC) and the World Health Organisation (WHO) have classified formaldehyde as a Grade-I carcinogen, emphasising its potential to cause significant health concerns when it is present above established safety thresholds.<sup>[1]</sup> In humans, formaldehyde exposure has been associated with respiratory discomfort, allergies, cancer, etc. As a result, developing effective formaldehyde detection technologies becomes essential for ensuring occupational safety, maintaining healthy indoor air quality, and monitoring environmental pollution. In this research area, water-soluble polymeric systems show promise in addressing the limitations of small molecule-based systems.<sup>[2]</sup> In this work, a naphthalimide-based water-soluble polymeric fluorescent probe was developed for formaldehyde sensing in both aqueous and vapours phase, by colorimetric and fluorimetric ways. The aromatic amine group present in the side chain of the polymer reacts with formaldehyde via FA-induced Schiff-base reaction. Due to the formation of imine via addition-elimination reaction of aromatic amine (electron donar) and formaldehyde, photoinduced electron transfer (PET) off and fluorescent “turn on” phenomenon is observed.<sup>[3]</sup>



**Scheme 1.** Schematic illustration of formaldehyde sensing mechanism.

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## Electrochemical determination of NADH using Pd-Co nanocomposite-modified carbon paste electrode

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### Abstract

Here we have synthesized a nanocomposite Pd-Co endoped on carbon using the hydrothermal method. The obtained material was confirmed by using PXRD, XPS, HR TEM, and SEM EDX characterization. The nanocomposite was used to modify the carbon paste electrode. The cofactor NADH is required by several different dehydrogenases. It is common practice to quantify enzyme activity by monitoring NADH levels. An electrochemical sensor that can detect NADH without the need of enzymes has been developed. Several illnesses are directly influenced by NADH concentration abnormalities. To confirm the activity of the modified electrode, electroanalytical techniques such as cyclic voltammetry, amperometry titration, and electrochemical impedance spectroscopy have been used. A lot of work has gone into creating electrochemical sensors for NADH measurement at low overpotentials, where interferences are less likely to occur. The Co-NC/Pd-modified electrode displayed a low detection limit of 2 $\mu$ M and a broad linear response range(5-1250 $\mu$ M) for the electrochemical sensing of DA.



## Designing Balanced Janus Nanocatalysts for Biocatalytic Applications

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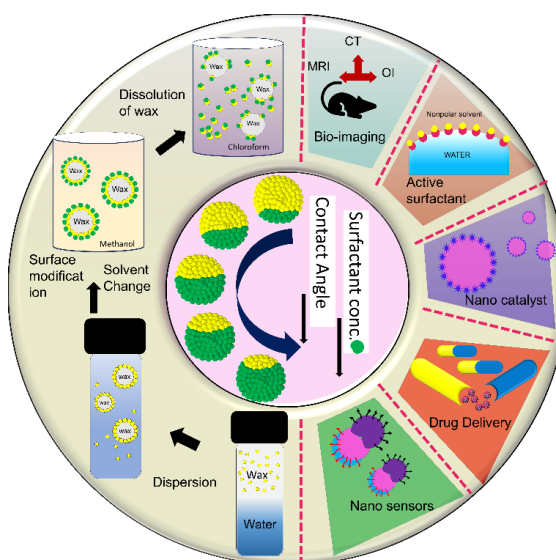
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### Abstract

Janus particles are colloidal particles with multiple surface chemistry, allowing controlled molecular recognition and self-assembly, offering versatility in designing and tailoring functional materials with diverse applications, including sensing, bioimaging, microprobes, drug delivery, and catalysis. Their significance lies in their ability to incorporate various properties within a single particle, such as amphiphilicity, di-functionality, or dipolarity. Polymeric Janus particles have attracted much attention from industrial and academic areas as hemispheres coated with different chemical groups could be topo-selectively functionalized using the right antagonist reagents. However, control over their Janus balance to achieve particles with relative portions of different functional groups would be a very emerging field. Herein, we provide a rational approach to synthesizing micron-sized silica particles and designing silica-based Janus particles of different Janus balances by utilizing the simple water-wax system, varying the surfactant concentration, followed by di-functionalizing surfaces of the particles. Due to their versatility, our next strategy will be to demonstrate a new type of nano-catalyst by incorporating different enzymes with the particle surfaces.



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## **Interaction of Doxorubicin drug and LDHs nanocarriers: Potential Innovation in Nanotechnology as Inorganic Drug Delivery Nanovehicle for Cancer treatment**

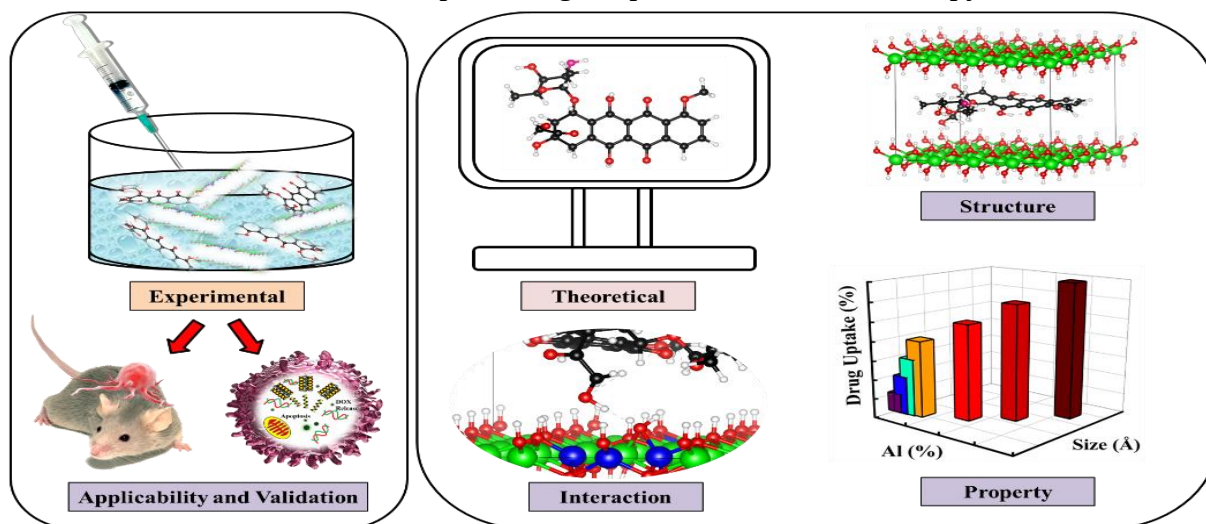
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### **Abstract**

Cancer has become one of the greatest causes of death around the world. The treatment of cancer still remains a great problem. The use of cationic polymer based drug delivery vectors has several limitations such as low transfection efficiency, high toxicity, and inactivation by serum. With recent advances made in the field of nanotechnology, inorganic layered double hydroxide based nanosystems have drawn special attention because of their good biocompatibility, pH-dependent biodegradability, anion exchange capacity, easy surface modification and high chemical stability, giving rise to great potential for cancer therapy. Although inorganic layered double hydroxide provides protection against thermal damage, target delivery of drugs and genes to the desired tumor sites is a major challenge in cancer therapy. In this work, compositional variable inorganic Li-Al based layered double hydroxide based nanoparticles are developed for target delivery of drug to cancer cells. The designed layered double hydroxide is capable of target-delivering of drugs to tumor cells for more effective cancer treatment, which provides great potentials in cancer therapy.



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## Azo-Bridging of Poly(2-oxazoline) with Phenolic Polymers: Multi-Stimuli Responsiveness and Micellization for Guest Encapsulation

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### Abstract

The bridging of hydrophobic polymer with hydrophilic polymer via azobenzene chromophore is an interesting approach to introduce amphiphilicity and sometimes stimuli-responsiveness in the conjugate materials, potential for optical data storage, fabrication of liquid crystal displays, and optical switching. Herein, we report the bridging of phenolic polymers with poly(2-ethyl-2-oxazoline) (PEtOx) segments via azobenzene moiety. Cationic ring-opening polymerization of 2-ethyl-2-oxazoline (EtOx) followed by termination reaction produces phenyl amine end-functionalized PEtOx, which is attached with phenolic groups of chosen polytyrosine (PTyr) and poly(vinyl phenol) (PVP) coupled through azo coupling to produce PTyr-N<sub>2</sub>-PEtOx and PVP-N<sub>2</sub>-PEtOx conjugates. Interestingly, owing to the grafting of hydrophilic PEtOx block, these conjugates exhibit reversible LCST-type thermoresponsive behavior in aqueous solutions, even though PEtOx block itself does not show such properties. An attempt is also made to attach functionalized PEtOx with Bovine serum albumin (BSA) to prepare thermoresponsive protein. These conjugates also show pH- and photo-responsive behaviors in water that allow the tuning of their cloud points. The proper balance between the hydrophilic PEtOx and hydrophobic PTyr or PVP segments imparts amphiphilic properties into these conjugates, leading to the formation of micelles in water. In addition, a model hydrophobic dye (Nile red) can readily be captured within the hydrophobic PTyr or PVP domains of conjugates' micelles in water. The cleavage of the azo bond upon treatment with Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>, as confirmed from absorption spectroscopy, further indicated the potential utility of PTyr-N<sub>2</sub>-PEtOx/PVP-N<sub>2</sub>-PEtOx conjugates' micelles as sustainable drug delivery vehicles under hypoxia environment.

## Versatile Applications of Polyacrylates and their Derivatives: A review

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### Abstract

Polyacrylates are basically derived through polymerization of acrylate monomers of varied types. These polymers have various applications in different industries that engaged in textile, medical, packaging, paint, and printing. This paper will explore some of the aforementioned applications made possible through different modifications instance acrylate-based PSAs have gained popularity due to their excellent balance of tack, peel strength, shear resistance, and flexibility<sup>1</sup>. Another interesting application is their use as demulsifying agents in the oil and gas industry to break down and separate emulsions by reducing the stability of emulsions, and thereby, separate oil from water, etc<sup>2</sup>.

Further acrylates is find potential applications as binders in formulating various types of inks, including water-based, solvent-based, and UV-curable inks<sup>3</sup>. Acrylate monomers are also used as reactive diluents, which help to control the ink's viscosity and enable rapid curing upon exposure to UV light.

Applications are based on the unique qualities of acrylates, including their fast UV-induced polymerization ability, flexibility, and adhesion traits, to deliver the needed performance results. This paper reviews how acrylates can be carefully formulated and potentially used to fulfil the unique requirements of each application.

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## A copolymerization approach to stabilize PPI and PPII structures of polyproline

P. Maity, A.S. Bisht and Dr. Raj Kumar Roy\*

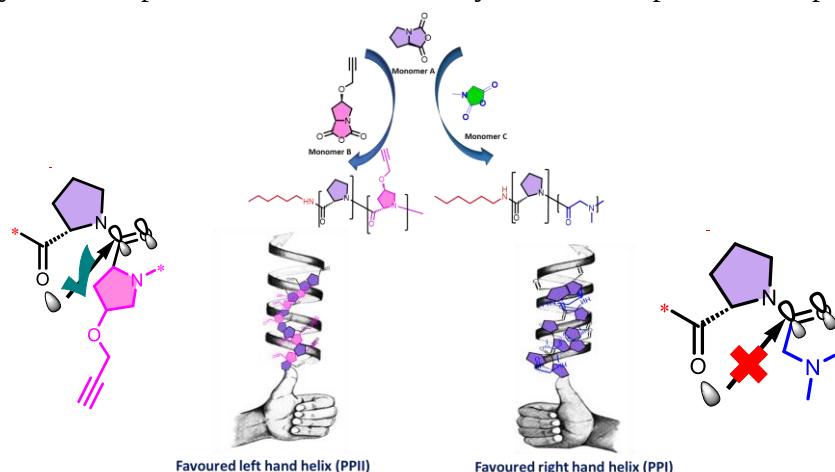
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### Abstract

Among other amino acids, proline is the only one whose side chain is covalently attached to a pyrrolidine ring. Polyproline (PLP) is unique with its cyclic side chain and absence of hydrogen bond-donating amide backbone. A polypeptide's amide backbone is typically in trans conformation, while for PLP, it can be both a -cis or -trans conformation. In polyproline, tertiary amide bonds are essential in forming their secondary structure. Polyproline assumes a PPI (right-handed helix) or PPII (left-handed helix) type secondary structure when the backbone amides are exclusively cis or trans conformations, respectively. A substantial 20 kcal/mol energy barrier for cis-to-trans isomerization independently secures the stability of both secondary structures<sup>[1]</sup>. The secondary structure of PLP is crucial for various biological functions like transcription and immune response<sup>[2]</sup>. Although in nature, PPII is more common and stabilized by n- $\pi^*$  interactions (collagen). Tuning of PPII to PPI was influenced by factors like solvents, aromatic groups<sup>[3]</sup>, terminal charges, and electronegative groups at the fourth position<sup>[4]</sup>.

Understanding model peptide, we prepared complex polypeptide with two sets of copolymers wherein proline was copolymerized with either hydroxy proline or sarcosine using ring-opening polymerization.<sup>[5]</sup> All the polymers were characterized using <sup>1</sup>H NMR and SEC analysis. The secondary structure of the polymers was characterized using CD spectroscopy. Despite having a random sequence of monomers in the copolymer chain, we can make a good correlation between the choice of a comonomer to stabilize a particular secondary structure of polyprolines. Therefore, this study could help understand the secondary structure of proline-rich peptides.



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## Design and synthesis of periodically grafted TEG-polypyrrolone via click chemistry:

### A comparison of its thermo-responsive behavior with native polypyrrolone

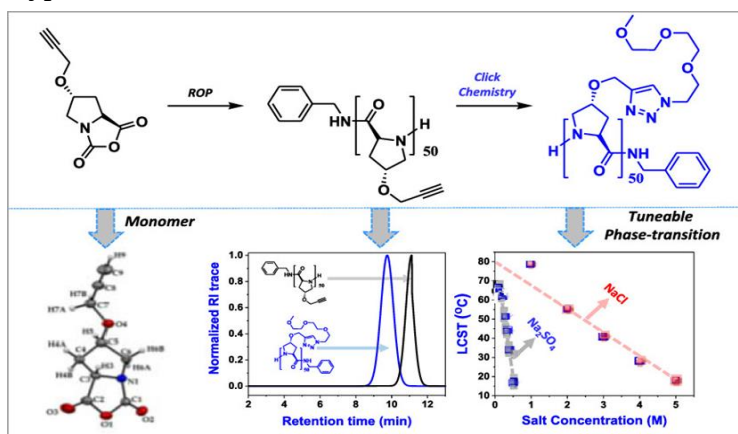
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#### Abstract

Among homopolypeptides, polypyrrolone is unique due to its conformational flexibility between right-handed PPI and left-handed PPII helices. Herein, we designed a propargyloxy functionalized pyrrolone-NCA monomer so that the former's ring-opening polymerization (ROP) provides a reactive propargyl group in each repeating unit to enable post-polymerization modifications. A close match between the feed ratio and degree of polymerization estimated using <sup>1</sup>H NMR along with a low dispersity (*Đ*) suggests that the ROP was controlled. We then used azide-yne click chemistry to prepare polypyrrolone chains that had been triethyleneoxy (TEG) functionalized (periodically grafted). Later, functionalized polypyrrolones were compared with native polypyrrolones in terms of thermoresponsive behavior using turbidimetric analysis, circular dichroism, and variable temperature NMR (VT NMR) spectroscopy. Compared with native polypyrrolone, the TEG-functionalized polypyrrolone chain exhibits better tuneability and reversible thermoresponsive properties in salt solution. VT NMR experiments found that polar amide groups' solvation is the sole cause of thermoresponsive behavior in functionalized polypyrrolones, while grafted TEG segments enhanced polymer chain solubility. The enhanced conformational stability and the water-soluble TEG segment in functionalized polypyrrolones were attributed to the difference in thermoresponsive behavior between native and functionalized polypyrrolones.



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## Polyprolines with periodically placed clickable units: An investigation of structural dynamics and thermoresponsive behavior

Sneha , P.Maity, A.S. Bisht and Raj Kumar Roy\*

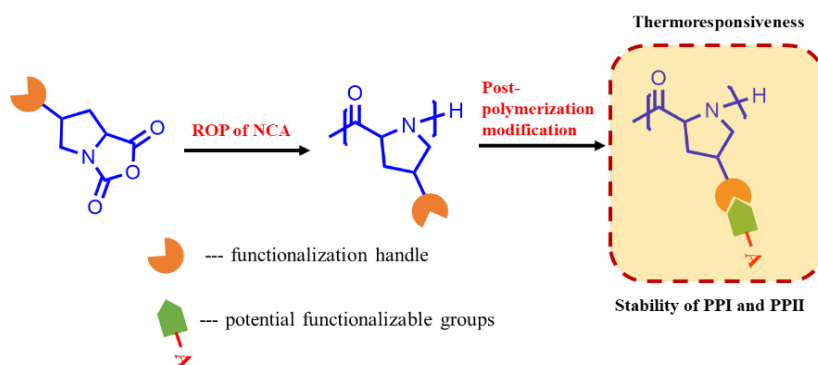
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### Abstract

Functionalizable polymers pave the path for accessing leading-edge and multifaceted synthetic materials. While advancement continues in this field, polymers with polyproline backbone are also growing as a favorable choice for the design of biomaterials<sup>[1]</sup>. Proline's unique structure arises due to the five-membered pyrrolidine ring side chain and secondary amine. Thus, unlike other polypeptides, the amide backbone of polyproline can induce both cis and trans conformations. The high energy barrier (~20 kcal/mole)<sup>[2]</sup> for cis-to-trans isomerization ensures stability of both conformations and prevents isomerization under normal physiological conditions. However, altering factors like solvent environment, temperature can make isomerization feasible. Recent studies have already demonstrated the connection of polyproline structure with isomerization and thermoresponsive behavior.<sup>[3,4]</sup> Thus, synthesizing a functionalizable polymer will serve the purpose of delivering polymers bearing tailor-made properties that can be fine-tuned for specific applications in the future.

In this work, we synthesized clickable polyproline having propargyl moiety as reactive handle for post-polymerization modifications. Our primary objective is to study the effect of periodically-grafted functional groups on the secondary structure of polyproline (PPI and PPII). Additionally, we examine how thermoresponsive property gets affected by periodic functionalizations. All the polymers were characterized using <sup>1</sup>H NMR and SEC analysis. The secondary structure of the polymers was characterized using CD spectroscopy. The thermoresponsive properties of the functionalized polyprolines were evaluated using turbidimetry and variable-temperature CD measurements. The post-polymerization modification of these polymers makes them a prospective choice for more exquisite applications in different fields and can be tailored meticulously by changing the functionality.



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## Synthesis of stimuli responsive fluorescent microgels and application in temperature, pH and metal ion sensing.

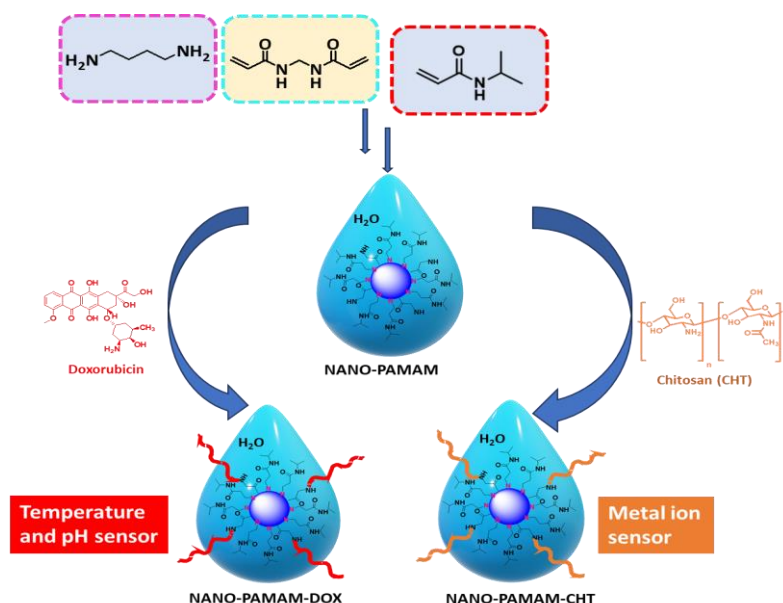
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### Abstract

Stimuli responsive materials are reported as a sensor for temperature, pH and metal ions.<sup>[1,2]</sup> Herein, we have demonstrated a new strategy to prepare stimuli responsive fluorescent microgels as a fluorescent probe for temperature,<sup>[3]</sup> pH<sup>[3]</sup> and metal ion sensing via functionalization of NANO-PAMAM with doxorubicin and chitosan. NANO-PAMAM is a reactive, biocompatible, dual stimuli responsive microgel and was successfully synthesized via Aza-Michael addition reaction between 1,4-diaminobutane and N,N'-Methylenebisacrylamide at room temperature in water followed by the addition of NIPAM (N-isopropyl acryl amide). Functionalization of NANO-PAMAM with doxorubicin leads to the formation of ratiometric fluorescent probe, (NANO-PAMAM-DOX) for temperature as well as pH sensing. On the other hand, functionalization of NANO-PAMAM with chitosan leads to the formation of fluorescent probe, (NANO-PAMAM-CHT) for metal ion sensing.



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## Solvent responsive polymer gel with inherent antimicrobial properties

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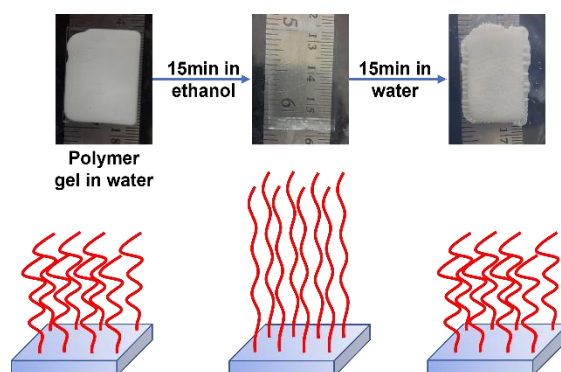
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### Abstract

Solvent responsive polymer gels are a class of materials that can undergo reversible changes in their physical properties in response to changes in the solvent environment. Recently, solvent responsive polymer gels with inherent antimicrobial properties have been developed, which can be used to create materials with enhanced antimicrobial activity. These materials can be used to create surfaces with improved antimicrobial properties, which can be used in a variety of applications, such as medical devices, food packaging, and water treatment.

Polymeric gels functionalized with active quaternary ammonium cation attached to hydrocarbon chain have been fabricated. The prepared gels were characterized using field emission scanning electron microscopy (FE-SEM) and water uptake studies to determine the swelling behaviour in water as well as in ethanol. In addition, antimicrobial activity of the gels has been determined for both gram negative and gram-positive bacteria E. Coli and S. Aureus respectively.



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## An Intelligent Nanobot Resonance Drug for Anti-Cancer Activity

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### Abstract

In past decades of research, various advantages of molecular machines were explained in numerous reported literature. Molecular machines are remarkable for their ability to autonomously carry out significant work, as evidenced by the functions of natural motor proteins. Researchers have described several designs of different artificial and biomimetic molecular machines, and the study of their basic properties and mechanical and technological features were investigated for advancement and usability. Here, we present the building of subnanometer-size supramolecular nanorobots holding significant potential in bionanotechnology for treating genetic diseases and other health challenges. Nanobots are designed with multiple components such as controllers, machines, sensors, etc. A new compatible multipurpose double ratchet motor (DRM) was developed for building our programmable nanobots. Nanorobots, operating at the molecular level, offer precise targeting and reduced side effects, making them advantageous in combating diseases like cancer, inflammatory/infectious diseases, etc. The application of nanomedicines in critical disease treatment has paved the way for implementing nanorobotics in medical sciences. Herein, we present PCMS supramolecular nanorobotic architecture bearing novel molecular machines and exploit the nanomechanical physical drug properties towards anti-cancer activity. The acronym PCMS is extracted from the components PAMAM dendrimer (P), controller (C) [e.g., Nile red], molecular motor (M) [e.g., DRM] and sensor (S) [e.g., NIR797 isothiocyanate). A triangular energy transmission pathway is tracked among the three components, S, C, and M, for its characteristic operational mode. Studies revealed that PCMS can distinctly interact with VEGF and cancer-related DNA by resonance frequency communications, thus emerging as an anti-cancer agent for the future.

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## **Innovation of shola (*Aeschynomene Aspera*) as a natural 3D porous hydrophobic–oleophilic sorbent for oil spill cleanup**

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### **Abstract**

*Aeschynomene Aspera*, commonly known as shola, was innovated as an oil-absorbing material for the removal of oil from water. The inner white stem of the shola is rich in cellulose (< 70 wt%) and has a naturally made three-dimensional porous architecture. Preliminary experiments show that water droplets have a high contact angle (135°) on the shola stem, while oil droplets can instantly spread over the surface completely, indicating its excellent hydrophobic–oleophilic properties. Further studies reveal that this material exhibits a fast and high absorption capacity of about 40–55 g/g for various oils and organic liquids. When applied to oil-over-water baths, the shola exhibited high selectivity for the oil over the water; almost all oil spilled could be removed with the material, leaving an invisible oil slick on the water surface. Shola can efficiently recover oil from an oil-water emulsion. After the 6–7th cycle of reuse, the reused material still absorbed a considerable volume of the oil. Moreover, shola can be a recyclable absorbent, and about 95% of absorbed oil was recovered from the material. In this study, for the first time, we have innovated the shola as an eco-friendly and cheap natural sorbent with excellent absorption capacity for oil spill cleanup.



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## Synthesis of Polymer Brush Modified Multicompartment Particles and their Application as Pickering Emulsion Stabilizer

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### Abstract

Microparticles that exhibit anisotropy have gained significant attention due to their various advantages<sup>1</sup>. This anisotropy can stem from surface, shape, or composition factors<sup>2</sup>. Janus particles, for example, provide composition anisotropy because of their dual compartment<sup>3</sup>. Tri-compartment particles offer even more possibilities for variation in composition across compartments<sup>4</sup>. In this work, we synthesized tri-compartment microparticles using an Electrohydrodynamic co-jetting machine. The particles were made up of polymer phases consisting of Poly Lactic Acid (PLA) and a random copolymer of Methyl Methacrylate and 2(2-bromopropionyloxy)ethyl methacrylate (BEMA), known as poly(MMA-co-BEMA). We selectively modified the particles using a hydrophilic polymer brush called poly(2-dimethyl amino ethyl methacrylate) poly(DMAEMA). We then explored the amphiphilicity produced in the particles to determine their potential for use in stabilizing Pickering emulsions.

Key words: Electrohydrodynamic co-jetting, Polymer brush, Janus Particles, ATRP, Interfacial Catalysis.

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## Biopolymer membranes for carbon capture

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### Abstract

Bio-based sorbents are potential sources for carbon-negative CO<sub>2</sub> capture process. Although the use of biochar as an adsorbent has been reported as a promising adsorbent, it requires CO<sub>2</sub> to be spent while carbonising the biomass. Direct use of biopolymer-based membranes that can be easily synthesised using methods which require less energy emerges as an attractive option for carbon capture. In this work, we investigate the use of selected biopolymers – pectin and bacterial cellulose systems as sorbents for CO<sub>2</sub> capture through chemisorption. Amine groups are introduced into the polymer backbone by amine grafting in order to enhance the CO<sub>2</sub> uptake. The CO<sub>2</sub> uptake by the sorbent was measured using the gravimetric technique. When biopolymers containing amine groups are exposed to CO<sub>2</sub>, the reaction between the gas and the amine group on the polymer causes the dielectric properties to change. Electrochemical impedance spectroscopy (EIS) was also used in order to understand the mechanisms involved. Permittivity and dielectric loss of biopolymers before and after CO<sub>2</sub> exposure was measured to understand the influence of CO<sub>2</sub> capture.

**Keywords:** Biopolymers, CO<sub>2</sub> capture, Electrochemical Impedance Spectroscopy



## Coherent fabrication of bio-based ion conductive interpenetrating polymer network flexible organohydrogel for physiological temperature sensing

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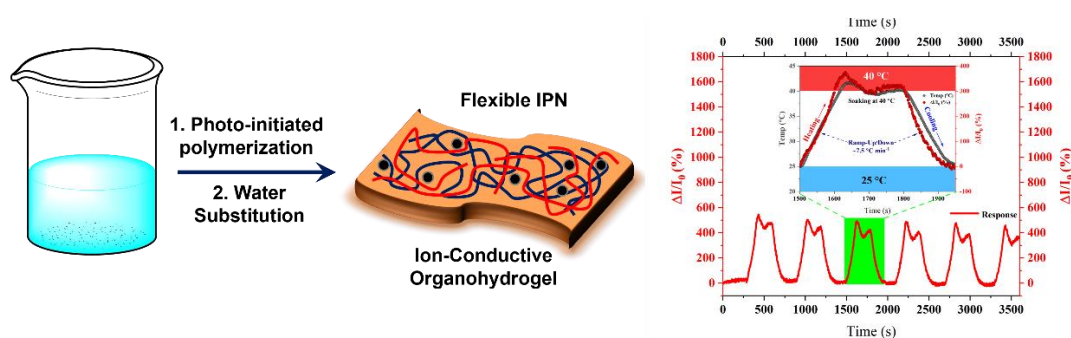
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### Abstract

Recently, ionic flexible sensors (IFSs) have come up as advanced sensors based on conducting soft materials which work on the concept of ion migration in the devices. Conductive hydrogels, a class of soft materials like human tissue, have been reported as IFSs for thermal sensing applications but have shown less sensitivity due to high-water content, heat capacity, and free volume in the polymer network. Dehydration leads to a highly thermal sensitive polymer network but develops a rigid network structure, which limits their applications in wearable and flexible electronics. This study aims to establish a facile and versatile method to fabricate a bio-based interpenetrating polymer network (IPN) as a flexible organohydrogel by partly substituting water molecules within the pre-prepared hydrogels with organic molecules. The flexible organohydrogel as a single ion conductor has demonstrated excellent and enhanced temperature sensing of physiological state, exhibiting a monotonic linear thermal response, a high sensitivity in the temperature window of 35–40 °C with a fast response time, high resolution, and an oriented behaviour with thermal flux at different rates. This high-temperature sensitivity is observed due to the mechanism of inward ionic flux under thermal and electric perturbation. The research opens a platform for the development of bio-based sensing materials for wearable and flexible electronics.



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## Phenoxazine-based Self-assembled Luminescent Liquid Crystals

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### Abstract

Luminescent liquid crystals (LLCs) have drawn growing attention because of their primary phenomenological interest and attractive technological applications such as anisotropic light emitting diode [1], polarized organic lasers, light-emitting liquid-crystal displays (LCDs), information storage, sensors and one-dimensional semiconductors [2,3,4]. Combining intrinsic light-emitting properties with unique self-organizing features endows LLCs with numerous novel advantages. For example, LLCs can manufacture stimuli-responsive luminescent materials owing to the sensitive response of LCs to external force stimuli, such as grinding, smearing, and pressing. Among the various LLC applications, linearly or circularly polarized luminescence is especially important in constructing highly efficient emissive LCDs. As an emissive display, the fabricant LCD fabricated from LLCs may enjoy several advantages. For instance, the power-consuming extra backlight, polarizers, and color filters would be obviated and thus enhance the power efficiency remarkably. Moreover, the LLCs allow simpler devices; hence, the brightness, efficiency, contrast ratio, and viewing angle of LCDs would be substantially increased [5].

In this work, we have synthesized new novel luminescent-based molecules using di aldehyde phenoxazine and cyano vinyl derivatives. Phenoxazine molecule is a non-planar butterfly-like structure, which regulates  $\pi$ - $\pi$  stacking and, as a result, reduces non-radiative decay channels, leading to enhanced emission in the aggregated/solid state. The thermal behavior of PHNX-CN was probed by polarizing optical microscope (POM), differential scanning calorimeter (DSC), and thermogravimetric analysis (TGA) studies. The photophysical properties of these compounds in solution and solid films were studied. Density functional theory (DFT) calculations were compared with the experimental data, which provided information on the geometry and electronic structure of PHNX-CN.

**Keywords:** Polarised Optical Microscope (POM), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Density functional theory (DFT).

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## Polycationic nanoparticles for microbial inhibition and killing

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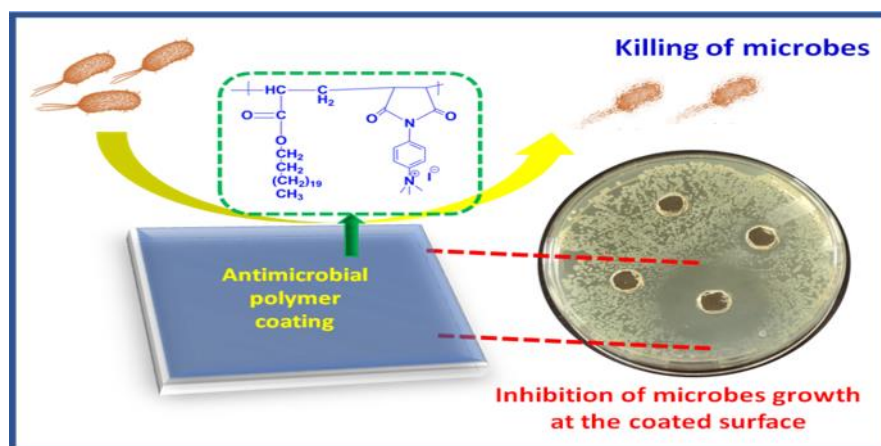
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### Abstract

Antimicrobial polymers (AMP) appear to be a promising candidate to deal with the current scenario of bacterial resistance against conventional drugs and antibiotics as they mainly depend on disrupting the bacterial membrane. This work investigates the effect of polycations bearing aromatic and aliphatic pendant cationic groups on the antimicrobial performance of AMP. A radical polymerization strategy was adopted to synthesize two different copolymers and convert them into polycations upon post-modification. Polyelectrolytes were converted into nanoparticles by nanoprecipitation and named PE1 and PE2. Polymers were analyzed by NMR, FT-IR, and gel permeation chromatography (GPC). PE1 and PE2 nanoparticles were uniform, spherical particles as confirmed by FESEM, size, and zeta potential measurements. The antimicrobial properties of polyelectrolytes were determined against pathogenic *Escherichia coli* (*E. coli*), *Bacillus Subtilis* (*B. Subtilis*), *Bacillus Amylolyquefaciens* (*B. Amylolyquefaciens*) and *Citrobacter Freundii* (*C. Freundii*) bacteria. The biocidal activity determination studies showed that polyelectrolyte PE2 with aromatic pendant units outperformed PE1 with the aliphatic pendant group. This work highlights the remarkable effect of aromatic segmentation, which provides microbial inhibition, and killing is demonstrated as an antibacterial surface coating.

**Keywords:** Polyelectrolytes, nanoparticles, biocidal activity, antimicrobial coatings



## **Ca<sup>2+</sup> and Fe<sup>3+</sup> Ion Doped Low Methoxy Pectin (LMP) and Sodium Carboxymethyl Cellulose (NaCMC) based Conductive Hydrogels: Rheological and Broadband Dielectric Spectroscopy Investigations**

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### **Abstract**

Development of conductive hydrogels is of great importance for preparation of multifunctional soft materials for tissue engineering, drug delivery, soft robotics, and electronic devices etc. We chose Low Methoxy Pectin (LMP) and Sodium Carboxymethyl Cellulose (NaCMC), both are anionic and water-soluble polymers and have ability to interact with divalent and trivalent cations. We added Ca<sup>2+</sup> and Fe<sup>3+</sup> ions in both NaCMC and LMP to form conductive hydrogels due to electrostatic interaction ions with carboxylic acid (COOH) groups. Rheology (Frequency Sweep test) and Electrochemical Impedance Studies (EIS) were performed to understand the structure property relationship. It was found that both NaCMC and LMP showed enhanced storage modulus (G') and loss modulus (G'') on interaction with Ca<sup>2+</sup> and Fe<sup>3+</sup> ions, However, magnitudes of G' and G'' were an order higher for LMP based conductive hydrogels at a stoichiometric ratio of 1. It was found that dc conductivity for LMP based conductive hydrogels were in the range of 0.9 S/cm - 3 S/cm, whereas, NaCMC showed dc conductivity in the range of 0.2 S/cm - 0.4 S/cm. Electrode polarization was an order higher for LMP based conductive hydrogels than NaCMC based conductive hydrogels. Dielectric relaxation spectrum revealed an increase in dielectric relaxation times with increasing Ca<sup>2+</sup> and Fe<sup>3+</sup> in both LMP and NaCMC at lower concentrations.

**Keywords:** Ionically Crosslinked Hydrogels, Rheology, Broadband Dielectric Spectroscopy

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## Building Soft and Responsive Colloidosomes using Pickering Emulsion

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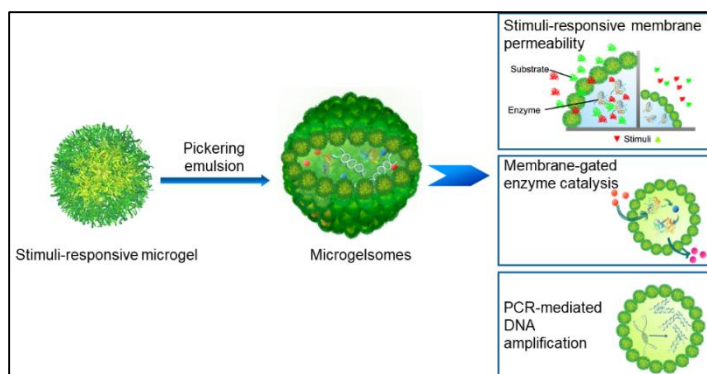
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### Abstract

**Keywords:** Colloidosome, enzyme, biocatalysis, microgel, biomimetic, microreactor, protocell

Microgel colloidosomes with hierarchical framework and advanced function may act as biomimetic microreactors to perform catalytic reactions by housing biological molecules/species within selectively permeable membranes. Contrary to Pickering emulsions stabilized by rigid particles, microgels as soft colloidal particles are considered an interesting alternative because they exhibit better elasticity at liquid interfaces. The soft, porous, and stable crosslinked structure allows to design microgels with different chemical functionalities and morphologies like core-shell, or hollow microgels which exhibit distinct properties. The open framework of microgel is favorable for the efficient transport of active molecules and post-modification processes. The unique ability to retain colloidal stability and swelling degree both in water and in various organic solvents endows them with unique interfacial and adsorption behaviors. Herein, we present a rational design of colloidosomes by the Pickering emulsion process. The microreactor consists of crosslinked microgel particles as the semipermeable shell and an enzyme-incorporated catalytic lumen. The microgel colloidosomes provide a robust platform to integrate stimuli-responsive building blocks into a compartmentalized microreactor with spatially controlled organization and biological functions. Integration of biomimetic functions within colloidosomes was successfully achieved for applications like membrane-gated enzyme cascade reactions, DNA amplification, and guest molecule encapsulation. Our work demonstrates a facile approach to constructing compartments with optimized functions, which can find potential applications in areas like microreactors, synthetic biology, biomimetics, and nanomedicine.



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## Hydrophilic modification of electrospun Poly ethylene co-vinyl alcohol for WBC syringe filter membrane

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### Abstract

WBC syringe filter is an efficient tool to remove WBC's from blood. Less than 15 mL of blood can be filtered by this method. The trapped WBC's can be cultured and used for various research applications including cell receptor analysis, lymphocyte recovery for cell therapy, antigen modulation studies. In this study the effect of hydrophilic modification of poly ethylene co-vinyl alcohol (EVAL) on the leukodepletion efficiency was investigated by blood filtration studies. EVAL is a versatile polymer used in various biomedical application but its hydrophobic character limits its use, so by incorporating hydrophilic polymer such as poly ethylene oxide (PEO), the surface wettability can be improved. The contact angle measurement of unmodified EVAL membranes was  $93 \pm 2^\circ$  and after incorporating PEO it significantly reduced to  $75 \pm 3^\circ$ . The percentage of WBC adhesion, platelet adhesion and RBC recovery were studied by conducting blood filtration. The percentage of WBC adhesion of EVAL and EVAL/PEO were  $97 \pm 0.3\%$  and  $100\%$  respectively. PEO incorporation to EVAL has also resulted in enhancement in tensile strength of the membrane which was obtained from UTM (Universal Testing Machine) results. *In vitro* cytotoxicity evaluation done using L929 cell lines concluded that the fabricated membranes were non-cytotoxic. The modified EVAL/PEO membranes showed improved blood filtration properties on comparing with unmodified EVAL membranes based on their enhanced surface wettability, reduced filtration time and increased WBC adhesion.

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## Biotin Tagged Theranostic Polymer Prodrug Nanoparticle for Dual Drug Delivery

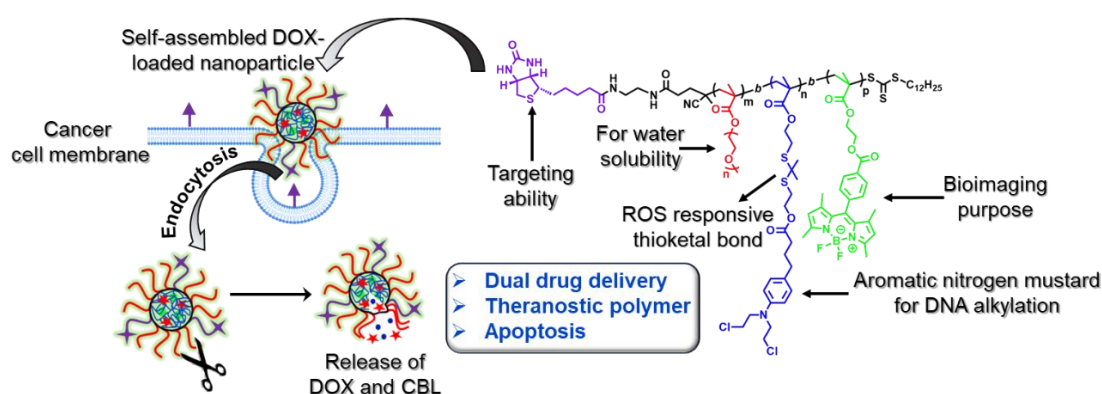
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### Abstract

Co-delivery of two drugs from one nanoparticle is increasingly used to overcome multi-drug resistance in cancer therapy. In recent decades, drug delivery systems (DDSs) based on polymer nanoparticles have been explored due to their potential to deliver poorly water-soluble drugs.<sup>1</sup> Some of the limitations of nanoparticle-based DDSs can be overcome by developing an appropriate polymer prodrug. Here, we have synthesized amphiphilic triblock copolymers consisting of segments from hydrophilic poly(ethylene glycol) methacrylate (PEGMA) monomer, pendent thioketal-labeled chlorambucil (CBL) prodrug monomer, and difluoroboron dipyrromethene (BODIPY) based methacrylate monomer *via* reversible addition–fragmentation chain transfer (RAFT) polymerization. Using nitrogen mustards, CBL as anticancer drugs opened the way for precise cancer chemotherapy owing to their ability to cross-link with deoxyribonucleic acid (DNA). The biotin unit in the chain end brings potential targeting capability to the block copolymer.<sup>2</sup> The prodrug micellar nanoparticles were capable of encapsulating a second drug doxorubicin (DOX) in their hydrophobic core. ROS-induced<sup>3</sup> breaking of the thioketal bond releases attached CBL and also causes disruption of the nanoparticles which facilitates the release of DOX. Incorporation of BODIPY unit into the polymeric architectures enables tracking the cellular internalization process. As a whole, the present self-assembled polymeric scaffold can effectively serve as a dual drug delivery vehicle.



**Scheme 1.** Schematic illustration of self-assembled polymer prodrug for dual drug delivery.

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## Photo and pH dual stimuli-responsive polymer assemblies for drug delivery application

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### Abstract

A dual stimuli-responsive amphiphilic diblock copolymer with pH-cleavable linkage at the junction between hydrophilic and hydrophobic linear blocks and photo-cleavable linkages as pendent groups was synthesized. The hydrophilic block is polyethylene glycol monomethyl ether (PEG) and the hydrophobic block is polycaprolactone (PCL) containing o-nitrobenzyl (ONB) ester as pendent groups. The blocks are connected using click chemistry. A series of polymers is synthesized by varying the content of ONB groups. The resultant block copolymers self-assemble into nanomicelles of well defined spherical morphology with average size of 150-200 nm in aqueous solution. The two stimuli are used individually as well as simultaneously to study the controlled release of encapsulated drug Camptothecin. Nanomicelles are disassembled under UV light irradiation, due to ONB ester photocleavage and acidic pH due to the cleavage of pH-sensitive acetal linkage. The photo and pH-controlled release behavior of Camptothecin is studied using fluorescence spectroscopy. The synergistic effect of two stimuli on drug release is demonstrated and the non-cytotoxic nature of the polymer is shown using MTT assay. Cell uptake and photoinduced release of Dox-loaded micelles in MDA-MB-231 anti-cancer cells is demonstrated. The newly designed copolymers with dual-stimuli-response have significant potential application as a smart nanomedicine against cancer.

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## Comparison between hyperbranched and linear polymer aggregates for intracellular drug delivery

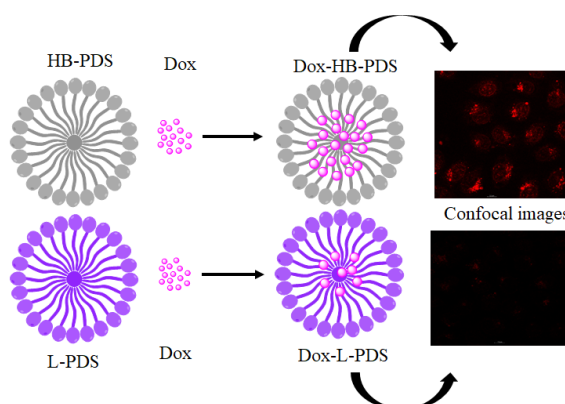
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### Abstract

In the recent past we have reported redox-responsive amphiphilic poly(disulfide)s (PDS)<sup>1</sup> with linear as well as hyperbranched (HB) structure and shown their utility in producing redox-responsive aqueous aggregates (micelle/ polymersome), capable of sequestering guest molecules and releasing them in presence of glutathione (GSH), a tri-peptide, present in excess in the intra-cellular environment compared to the extra-cellular environment and also known to be over-expressed in cancer cells. We have compared the aqueous aggregation, drug encapsulation and GSH responsive intra-cellular drug delivery of the two polymers L-PDS and HB-PDS having linear and hyperbranched structure, respectively. Both polymers produce micellar particles of comparable size in water. However, the hyperbranched polymer micelle exhibits much superior drug loading content and drug loading efficiency compared to those for the linear polymer. GSH triggered drug release rate appears to be much faster for the hyperbranched polymer aggregate. Cellular uptake is significantly better for the hyperbranched polymer compared to the linear polymer. As a result of these factors, cell killing efficiency of doxorubicin (Dox) entrapped hyperbranched polymer is significantly higher compared to the linear polymer. Based on these inspiring results, we have now synthesized covalent polymer-drug conjugate using similar hyperbranched or linear PDS derivatives.<sup>2</sup> Physical and biological studies have been done with these amphiphilic polymeric pro-drug conjugates to understand whether similar contrast exists also for these systems. Our recent results indicate indeed hyperbranched polymers perform better than linear analogous even for covalent drug conjugates. This presentation will highlight such sharp contrast between linear and hyperbranched polymer in context of intra-cellular drug delivery applications<sup>3</sup> and synthetic approach of drug conjugated amphiphilic polydisulfides.



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## Synthesis and Self-Assembly of polyurethane based ABA type Amphiphilic Polymers

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### Abstract

Small molecule-based anti-cancer drugs have severe side effects, such as nausea, vomiting, and hair loss during chemo-therapeutics treatments.[1] The non-targeted systemic distribution of the drugs causes a dramatic decrease in the life quality of cancer patients. Therefore, many attempts have been made to develop suitable drug delivery systems where drugs or therapeutic proteins are entrapped or covalently bound to polymeric carriers (10-200 nm). Polythiourethanes have some advantages, a. it has H-bonding functionality along the chain, which could direct the assembly rather collapse due to the hydrophobic effect; b. during polymerization, each addition of amines generates free thiols that could further be utilized to couple hydrophobic groups, drugs or crosslinking of the hydrophobic membrane to increase the stability of the formed nano-aggregates.[2,3] In this project, we have prepared nanoaggregate using self-assembly of amphiphilic polythiourethanes (ABA type linear block copolymer) where polyethyleneglycol act as a hydrophilic entity, and polythiourethanes used as hydrophobic block. The interior of nanoaggregates can efficiently transport hydrophobic drugs. Furthermore, stimuli-responsive groups (reactive oxygen species (ROS) and pH, etc.) was incorporated to make the nanoaggregates degradable and release the loaded cargo at the target site on demand. ROS are overproduced in cancerous tissue compared to ROS levels in normal tissues.[4]

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## Synthesis & Transport Potential Study of A<sub>2</sub>B Type Amphiphilic Architectures

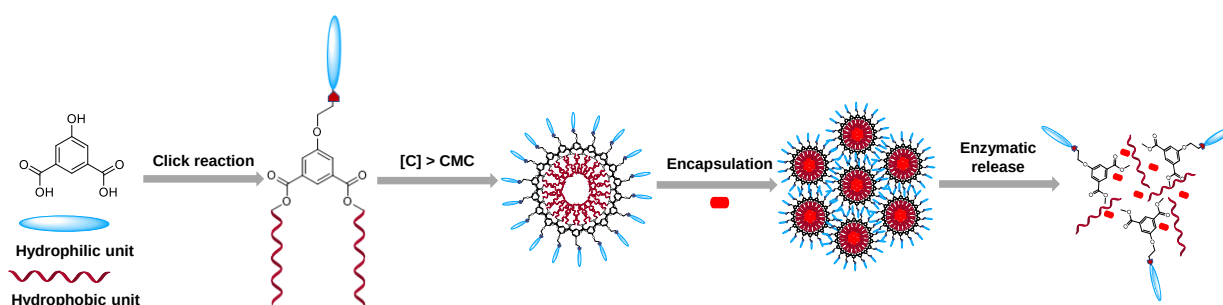
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### Abstract

Interest in nano-transporters is growing rapidly, and research in this area appeals to a broad, multidisciplinary audience. Amphiphilic nano-architectures are unique in their constitution and properties that provide excellent transport and controlled release capabilities enabling them to deliver water-insoluble drugs at target site. In this endeavour, herein we report the synthesis of a newer A<sub>2</sub>B type of non-ionic double chain amphiphilic nano-transporter by using dimethyl 5-hydroxy isophthalate which has been suitably modified using propargyl bromide followed by ester hydrolysis to develop a central core.<sup>[1]</sup> The core was then decorated with hydrophobic alkyl and perfluoroalkylated chains *via* ester coupling followed by the incorporation of hydrophilic monomethoxy polyethylene glycol units by click chemistry approach. Polyethylene glycol and its derivatives are promising candidates for polymeric drug delivery systems due to their excellent water solubility and high biocompatibility. In order to achieve this, Furthermore, we have evaluated the aggregation behavior of synthesized non-ionic amphiphiles by using dynamic light scattering and fluorescence spectroscopy. The nano-transport potential was studied by model hydrophobic guests, *i.e.* the dye Nile red and the drugs (nimodipine and curcumin) by using ultraviolet-visible and fluorescence spectroscopic techniques.<sup>[2]</sup> Evaluation of the viability of amphiphile-treated HeLa cells showed them to be well tolerated up to the concentration studied. The release profile of encapsulated Nile red dye was successfully carried out in the presence of immobilized *Candida antarctica* lipase (Novozym 435).<sup>[3]</sup> In a nutshell, the obtained results of A<sub>2</sub>B type non-ionic amphiphiles may help in the development of promising nano-transporters in the biomedical applications.



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## Phloroglucinol Based Stimuli Responsive Non-Ionic Amphiphiles for Controlled Drug Delivery

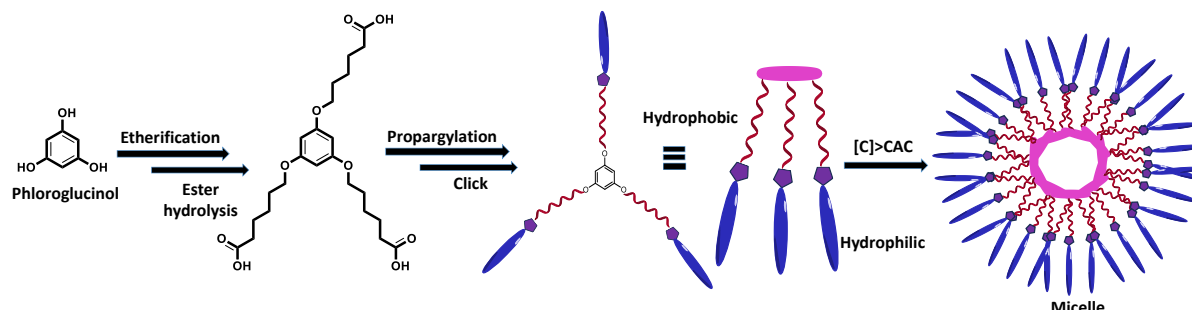
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### Abstract

Amphiphiles are a class of molecules which are known to assemble into a variety of nanostructures. The use of amphiphiles for drug encapsulation and transport has been extensively reviewed.<sup>[1-2]</sup> Herein, we have synthesized a newer type of amphiphiles using phloroglucinol moiety as a part of central core.<sup>[3]</sup> Phloroglucinol was first reacted with ethyl-6-bromohexanoate. The resulting tri-ester was subjected to ester hydrolysis to yield corresponding triacid which was reacted further with propargyl bromide to yield tri-propargylated ester as a lipophilic moiety. The hydrophilic group was incorporated on this moiety by reacting it with monomethoxy poly(ethylene glycol) azide (mPEG azide) ( $M_n$ : 350/550) or lactose azide by following click chemistry approach. Further, the aggregation behavior of synthesized amphiphiles was evaluated by using dynamic light scattering (DLS) and fluorescence spectroscopy. The encapsulation potential and controlled release of the guest were also systematically studied.<sup>[4]</sup> Since our amphiphiles consists of ester functionality they exhibit stimuli responsive behavior with hydrolases. The preliminary results from this study will be shared during poster presentation.



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## **Optimizing Sonocatalytic Degradation with Hydrogel Beads of Nanoparticles for Effective Industrial Wastewater Treatment**

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### **Abstract**

This study focuses on the treatment of Industrial wastewater using a sono-heterogeneous Fenton process with newly designed floatable hydrogel beads of chitosan nanocomposites. The nanocomposites were thoroughly characterized through various techniques, including Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), thermogravimetric analysis (TGA), magnetic properties measurements, and point of zero charge (pH pzc) analysis. Optimizing the degradation parameters using RSM, such as H<sub>2</sub>O<sub>2</sub> concentration at 10 mM, chitosan hydrogel beads at 1.5 g/L, pH set at 3.5, and a temperature of 35 °C for 60 minutes, resulted in nearly complete mineralization of wastewater solution and significant decolorization. The sono-heterogeneous catalytic Fenton process demonstrated efficient degradation rates for chemical oxygen demand (COD), with rates reaching 95.66%, respectively within 60 min of treatment at optimized conditions. Toxicity analysis was done using seed germination as a response which demonstrated that 80% toxicity is reduced after treatment of wastewater. Furthermore, the magnetic catalyst exhibited excellent stability over multiple cycles, indicating its potential for practical application. The overall findings support the effectiveness of the sono-heterogeneous catalytic Fenton process as a promising technology for treating industrial wastewater.

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## Design & Synthesis of Gemini Amphiphiles and Study of their Transport Potential

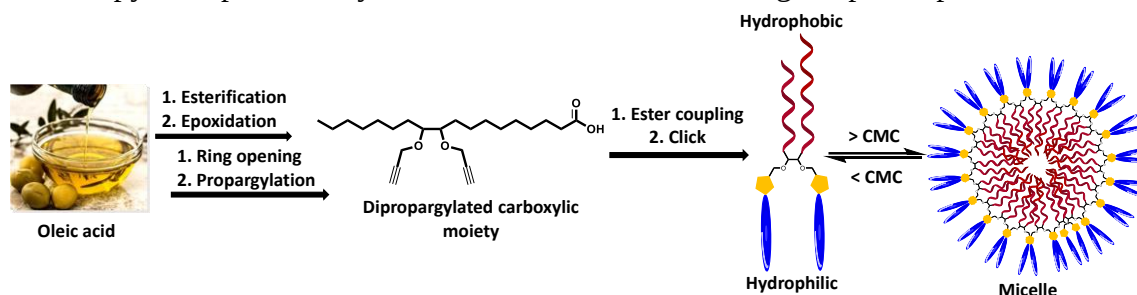
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### Abstract

The major obstacles in the area of drug delivery are the low aqueous solubility of drug, non-targeted delivery, and less duration of circulation in the blood. In the past few decades the contribution of nano-transporters have been recognized worldwide for addressing these challenges and improving the overall drug efficacy. As a part of our ongoing research program to design and develop efficient drug delivery agents,<sup>[1]</sup> herein we report the synthesis of a newer type of non-ionic Gemini amphiphilic architectures. These amphiphiles possess desirable physicochemical properties to enable them to act as promising drug transporters.<sup>[2]</sup> For this study we have used commercially available and biocompatible oleic acid as a starting material which is suitably modified at its olefinic bond using epoxidation followed by the opening of the epoxide ring to yield a diol. The diol was propargylated and the carboxylic acid group esterified with hydroxy alkyl/perfluoro chain to develop a hydrophobic core. Further, the hydrophobic core was clicked coupled with hydrophilic monomethoxy polyethylene glycol (mPEG) azide ( $M_n$ : 550/750). The decision to incorporate polyethylene glycol was made on the basis that its derivatives are highly biocompatible and are frequently used in drug delivery systems to improve the solubility, immunogenicity, toxicity, and regulated drug release of therapeutic agents.<sup>[3]</sup> The physicochemical characterization of the synthesized amphiphiles was carried using dynamic light scattering and spectroscopic tools. The encapsulation and nano-transport potential studies were carried using fluorescence spectroscopy. The preliminary results will be discussed during the poster presentation.



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## Fluorophore-derived Multi-stimuli Responsive Polymers

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### Abstract

Environmentally sensitive polymers are well-known as valuable materials in the biomaterial sciences and biomedical technologies.[1] These polymers rapidly and reversibly alter their structural and physical properties in response to external stimuli like temperature, pH, and light. For understanding complicated cellular dynamics, live cell imaging is essential. Fluorescence microscopy is a potent method that is frequently used to visualize organisms and gain a deeper understanding of how cells work and the related biomolecular processes. A fluorophore-containing substance is needed for this.[2] Fluorophores are incorporated into multi-responsive polymers, which have become effective tools for sensing various stimuli in the cellular microenvironment.[3] Since almost all materials are susceptible to degradation over time, self-healing is a desirable property to increase a material's lifespan. While self-healing occurs regularly in natural systems, applying it to materials produced by humans creates difficulties. Although the introduction of microencapsulated healing agents marked a significant advancement, a limitation lies in their inability to repair cracks multiple times. Nonetheless, the incorporation of external triggers into non-autonomous healing methods holds promise for achieving repeated restoration of materials.[4]

We have developed a facile protocol based on RAFT polymerization for the synthesis of a series of well-defined poly(*tert*-butyl methacrylate-co-coumarin methacrylate) poly(TBMA-co-CMMA) copolymers bearing photoreactive coumarin moieties as pendant functionalities. Detailed kinetics and mechanistic studies of polymerization were also carried out. Potential applications of the developed coumarin-derived poly(TBMA-co-CMMA) copolymers for live cell imaging and self-healing coating materials are being explored.[5]

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# Application of dual thermo-responsive block copolymers in size-tunable strategy toward improved retention in tumor tissues and AIE-based real-time monitoring

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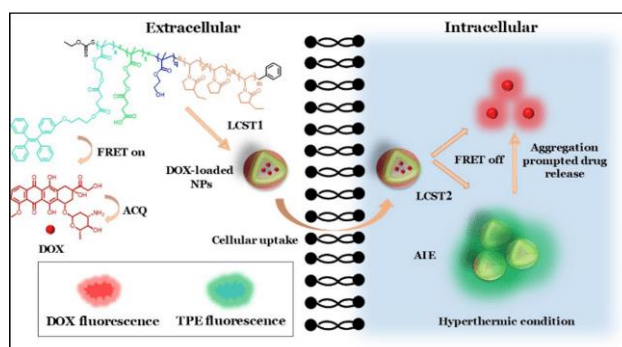
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## Abstract

Intelligent size-tunable strategies are very beneficial in eliminating the limitations associated with fixed-size nanoparticle-based drug delivery. Small-sized nanoparticles, although advantageous for accumulation in tumor tissue, suffer from poor retention, decreasing the overall therapeutic efficacy. Aggregation strategies can be beneficial in overcoming this dimensional barrier by post-accumulation size expansion.<sup>1</sup> Our work mainly explored the potential of dual thermo-responsive polymer nanoparticles for this purpose. Thus, we synthesized N-vinyl-2 pyrrolidone (NVP) and sub-NVP (ethyl, butyl) based dual temperature-responsive polymers with precisely controlled lower critical solution temperatures (LCSTs) by RAFT (reversible addition-fragmentation chain transfer) polymerization technique. The minimal compositional heterogeneity of the thermo-responsive blocks facilitated the control of LCSTs within the physiological range, which is the principal criterion for their application in drug delivery.<sup>2</sup> The LCSTs were tuned by varying the ratio of NVP and sub-NVP, where the first LCST value was kept below 37 °C to promote drug loading and the second LCST value around 41-43 °C to ensure mild hyperthermia-induced drug release. As drug loading and release highly depend on the hydrophobicity of the nanoparticle core and the hydrophilicity of the corona, the composition of the core and corona forming blocks was varied by different sub-NVP monomers and their combination. The release of the anticancer drug Doxorubicin was monitored at two different temperatures (37°C and 43 °C). Again, to incorporate aggregation-induced emission (AIE) property in our system, we covalently attached an AIEgen (TPE molecule) to the polymer, which facilitated real-time monitoring of drug release by the FRET (Fluorescence resonance energy transfer) phenomenon.



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## Design and Synthesis of Multi-stimuli Responsive Multi-arm Star Polymers

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### Abstract

The importance of multi-stimuli responsive multi-arm star polymers lies in their potential to revolutionize diverse applications. These polymers exhibit remarkable responsiveness to various stimuli, offering unprecedented control over their behavior and properties.[1-4] This has led to potential applications of such polymers. However, wider use of such polymers is still in their infancy due to stringent multi-step synthesis protocol and lack of control of the functionalities of the polymers which in turn lead to cost increase.

In This work, we will present the development of a multi-arm star fluorinated polymer via RAFT polymerization of dimethylacrylamide (DMA) and synthesis of well-defined dual-stimuli (pH/temperature) responsive poly(dimethyl acrylamide)-*block*-poly(octafluoropentyl acrylate) diblock copolymers via sequential RAFT polymerization. Detailed structure-property relationship of the polymer was carried out to have better understanding of their potential applications.[5]

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## **pH-responsive nanovesicles for effective combination therapy of drug-resistant cancer**

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### **Abstract**

Controlled and specific delivery of therapeutic drugs to the diseased site in the body in precise amounts can minimize drug toxicity to normal body parts and also improve the therapeutic activity and effectiveness of drugs. In this work, we have presented the design and preparation of a novel and smart nanovesicle for the combinational delivery of hydrophilic and hydrophobic anti-cancer drugs. Different characterization techniques such as FTIR, DLS, TEM, and UV-Vis spectroscopy were used to study different physicochemical properties of the prepared nanovesicles. After systematic characterizations, anti-cancer drug loading studies of blank, single, and co-loaded nanovesicles were carried out. The encapsulation efficiency of Curcumin (Cur) and Doxorubicin (Dox) in co-loaded nanovesicles was found to be ~ 91% and ~ 80% respectively. To evaluate the potential of prepared nanovesicles as a suitable drug carrier, in vitro drug release studies from co-loaded vesicles were performed in two different buffers of pH 7.4 and 5 at 37°C for 60 hours. Different mathematical models were employed to fit the release behavior of Cur and Dox. MD simulations were performed to further understand the structural dynamics, stability, drug interaction, and release kinetics of co-loaded nanovesicles. MTT assays on non-cancerous (3T3) and cancerous cells (Hela and MCF-7) confirmed the biocompatible nature of the prepared nanovesicles. Such a co-loaded drug delivery nanovesicle could have excellent potential for controlled drug delivery in cancer treatment.

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## Development of L- Aspartic Acid based biodegradable polyesters for drug delivery in cancer cells.

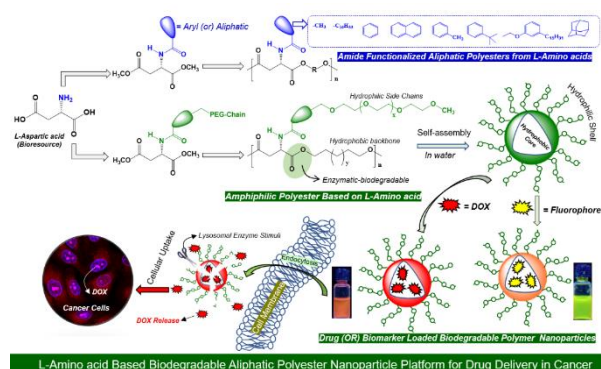
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### Abstract

Aliphatic polyesters are intrinsically enzymatic-biodegradable and they have found ever increasing demand for safe and smart next generation biomaterial application including drug delivery nano-vectors in cancer research. Bioresources based biodegradable polyesters is one of the elegant strategies to cater this requirement; here, we report L-amino acid-based amide-functionalized polyester platform and explore their lysosomal enzymatic biodegradation aspects to administrate anticancer drugs in cancer cells. L-Aspartic acid was chosen and different amide-side chain functionalized di-ester monomers were tailor-made having aromatic, aliphatic and bio-source pendant units. Under solvent-free melt polycondensation methodology developed from our laboratory; these new monomers were polymerized to yield high molecular weight polyesters with tuneable thermal properties. PEGlated L- aspartic monomer was designed and thermo-responsive amphiphilic polyester was synthesized. This amphiphilic polyester was self-assembled into  $140 \pm 10$  nm sized spherical nanoparticle (NPs) in aqueous medium which exhibited LCST at  $40-42$  °C. These nano-assemblies showed excellent encapsulation capabilities for anticancer drug and biomarkers. The polymer NPs was found to be very stable under extracellular conditions and underwent degradation upon exposure to lysosomal enzyme-horse liver esterase in PBS at  $37$  °C to release  $90$  % of the loaded cargoes. Cytotoxicity studies in MCF 7 and MEFs cell lines revealed that the amphiphilic polyester was non-toxic cell lines up to  $100$   $\mu\text{g/mL}$  while their NPs with drug were able to inhibit the cancerous cell growth. Confocal laser scanning microscopy (CSLM) assisted time-dependent cellular uptake analysis directly evident for the of DOX loaded polymer NP endocytosis and their internalization for biodegradation. In a nut shell, the present investigation opens up new avenue for the L-amino acid based biodegradable polyesters from L-aspartic acids, and the proof-of-concept is demonstrated for drug delivery in cancer cell line.



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## Transforming C-peptide through Strategic modifications into a Prospective Therapeutic Peptide Hormone for Type 2 Diabetes mellitus

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### Abstract

As diabetes and its related diseases continue to pose global concern, C-peptide (connecting peptide) is emerging as a promising candidate in ameliorating diabetes associated complications owing to its diversified biological functions [1,2]. C-peptide, a 31-residue biologically active hormone, is released from  $\beta$ -cells in equimolar amounts with insulin, exhibits therapeutic potentials against hyperglycemia, organ dysfunction, and more [3]. While C-peptide replacement therapy shows improvement in biological functions linked to Type 2 Diabetes Mellitus (T2DM), the underlying biochemical mechanisms remain unclear [4]. Herein, we are going to present calculated structural modifications at specific positions within the C-peptide chain. These modifications aim to achieve an ordered structure, consequently enhancing its biological activities. The synthetic process employed a Solid Phase Peptide Synthesis strategy (SPPS) with microwave irradiation to get the peptide with desired chain length. Notably, various biological studies unveiled significant and intriguing outcomes.

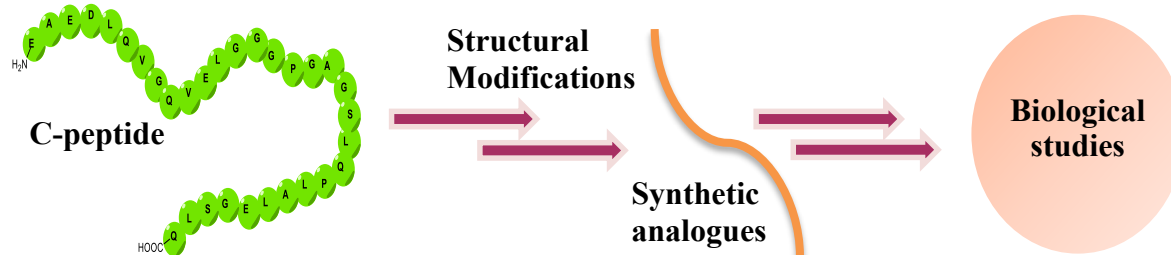


Fig: Cartoon representation of modified C-peptide synthesis against T2DM.

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## Design and Synthesis of Homo-arginine and Shikimic based Cationic block-copolypeptides for Cancer Cell Specific Gene Transfection

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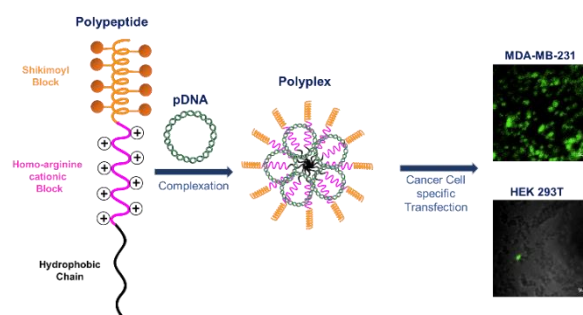
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## Abstract

A popular approach to treat genetic disorders is gene therapy. But the fundamental obstacle to gene therapy is the delivery of exogenous genetic material into cells as the genetic materials are prone to degradation by the nucleases. The creation of transport systems is critical for the implementation of nucleic acid-based gene therapies. The development of secure and efficient gene therapies using polymer-based vehicles that can precisely transport therapeutic nucleic acids to the mammalian cells needs attention of the scientific world.<sup>1,2</sup> Polyplexes are a class of complex nanoparticles made up of nucleic acid-carrying polymeric delivery systems. Genomes get translated to the proteins of interest upon successful delivery, leading to a successful transfection. It is even more challenging to design a specific delivery system which will transfect particular cells of interest.

Here, we have designed and manufactured some biodegradable delivery system that may be manoeuvred to treat genetic abnormalities and deliver genetic materials specifically to cancerous cells. Most of the cationic polymeric carriers have limited therapeutic applications as these are cytotoxic to the cells. So, we have developed some glyco-polypeptide based system having one homo-arginine based cationic block<sup>3</sup> for complexation with the nucleic acid and another shikimoyl<sup>4,5</sup> functionalized block for cell specific receptor mediated endocytosis. After successfully synthesizing and characterizing the polypeptides, we have studied their complexation with plasmid DNA and have characterized the polyplex using DLS, Zeta potential, EMSA, TEM, and AFM. Then we went onto explore their biological applicability, first by checking their cytotoxicity profile. The polyplex system was very much effective in transfecting cancerous cell line (MDA-MB-231, breast cancer cell line) and was ineffective in transfecting normal cell line (HEK 293T). With this system, we are hopeful to transfect dendritic cells (antigen presenting cells) which are very hard to transfect.



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## Sound Responsive Nanomicelles for Cancer Cell Therapy via Intracellular Reactive Oxygen Species Generation

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### Abstract

Sonodynamic therapy (SDT), as a new method of non-invasive tumor treatment developed from photodynamic therapy (PDT), can overcome the disadvantage of poor laser penetration while retaining the function of PDT. We have developed ultrasound responsive new generation nanoparticle to generate reactive oxygen species (ROS) which can be used for Sonodynamic therapy

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## Redox-Responsive Core-CrossLinked Block Copolymer Micelles to Overcome Multidrug Resistance in Cancer Cells

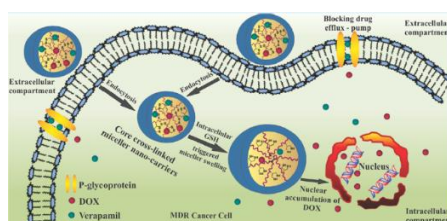
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### Abstract

Multidrug resistance (MDR) is a major challenge in cancer treatment, where cancer cells become resistant to multiple chemotherapeutic drugs. This resistance hampers the effectiveness of chemotherapy. We aimed to develop strategies to overcome MDR by designing specialized micellar nanocarriers for drug delivery to cancer cells. In this work we have developed a copolymer poly(ethylene glycol)-block-poly(2-(methacryloyloxy)ethyl 5-(1,2-dithiolan-3-yl)pentanoate) (PEG-b-PLAHEMA). This copolymer was chosen due to its ability to form micellar structures. The micelles were designed to be redox-responsive and core-crosslinked. The copolymer was synthesized using reversible addition-fragmentation chain transfer (RAFT) polymerization which allows precise control over the copolymer's composition and structure. The core of these micelles was cross-linked in response to reduction conditions. This core-crosslinking and the subsequent de-cross-linking were controlled over time, leading to tunable swelling properties of the micelles. We have used techniques such as dynamic light scattering, fluorescence spectroscopy, and transmission electron microscopy to study the self-assembly, cross-linking, and swelling behavior of the micelles. The study assessed the cytotoxicity of the developed micellar nanocarriers loaded with the chemotherapeutic drug doxorubicin (DOX) in both drug-sensitive MDA-MB-231 cancer cells and drug-resistant MDA-MB-231 (231R) cancer cells. The DOX-loaded core-cross-linked micelles (CCMs) showed promising results in reducing the IC<sub>50</sub> against drug-resistant 231R cancer cells. Co-encapsulating DOX and verapamil, a P-glycoprotein inhibitor known to counter MDR, further improved the performance of the micellar nanocarriers against drug-resistant cells. This work suggests that the redox-sensitive and core-cross-linked micellar nanocarriers have potential as a strategy to overcome multidrug resistance in cancer cells.



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## Disulfide-based micellar system for glutathione-responsive drug delivery

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### Abstract

A glutathione (GSH) responsive disulfide-based drug delivery system was developed based on a polyethylene glycol methyl ether (PEGME) and a polydisulfide (PDS) diblock copolymer. The cyclic lactone containing a disulfide link, 1,4,5-oxadithiepan-2-one, was prepared using a thiol-free method by reaction of 2-bromoethyl bromoacetate with sodium disulfide in 72% yield. Ring-opening polymerization (ROP) of 1,4,5-oxadithiepan-2-one using 1-butanol in presence of  $\text{Sn}(\text{oct})_2$  generated the homopolymer PDS whereas with PEGME as the macroinitiator, the diblock copolymer PEGME-*b*-PDS was obtained. The average particle size of the micelles formed from PEGME-*b*-PDS as measured by Field-emission Scanning Electron Microscopy (FESEM) and Dynamic Light Scattering (DLS) was found to be ~518 nm. The reduction responsiveness of the disulfide-based micelle was studied by encapsulating doxorubicin (DOX) at pH=7.4 in the presence and absence of 2 mM dithiothreitol (DTT) which is analogous to the intracellular GSH-based redox process. The cumulative percent release of DOX after 72 h was ~98.2% in presence of DTT and ~1.9% in absence of DTT clearly demonstrating the redox responsiveness of the PDS block facilitating drug release. The kinetic data showed the best fit with the Korsmeyer-Peppas model with a correlation coefficient of  $R^2=0.97$  with  $n=0.58$  suggesting a Fickian diffusion as well as chain relaxation controlled drug release mechanism from PEGME-*b*-PDS micelles. DOX loaded micelle and free DOX showed similar cytotoxicity in both 4T1 and MCF-7 cells indicating that the encapsulation of drug inside the micelle did not affect the anticancer efficacy of the drug. The drug loaded micelle showed higher cellular uptake than free DOX in both 4T1 and MCF-7 cell lines.

## Design and synthesis of piperazine based water dispersible polyurethane coatings for biomedical applications

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### Abstract

Considering the infections associated with urinary catheters as a major concern in healthcare, herein we developed environment-friendly water-dispersible polyurethane coatings with anti-bacterial properties to prevent bacterial colonization on medical catheters and enhance their durability. To accomplish this, the nitrogen-containing compound, piperazine, was chosen and a nucleophilic substitution reaction with 2-bromoethanol was performed to produce 1,4-bis(2-hydroxyethyl)piperazine (HEPZ) that was utilized as a chain extender for polyurethane synthesis. Furthermore, it possessed anti-bacterial properties upon quaternization which makes it an appropriate choice for medical purposes. Briefly, in this study, the diisocyanates (MDI/HDI), and polyether polyols (PEG<sub>600</sub>/PPG<sub>400</sub>) were varied by keeping the chain extender constant to form a series of polyurethanes using the prepolymer method. The structures were confirmed using <sup>1</sup>H NMR, <sup>13</sup>C NMR, and FTIR. The molecular weights of the synthesized polyurethanes were determined using GPC. Furthermore, the water dispersibility and anti-bacterial properties were achieved with the controlled treatment of methyl iodide (5-10 mol%). The methylation was confirmed by <sup>1</sup>H NMR and FTIR. The additional signal was observed in <sup>1</sup>H NMR from ~3.3-3.4 ppm due to the methyl protons bonded with positively charged nitrogen atoms (-CH<sub>3</sub>-N<sup>+</sup>). The contact angles were also measured before and after the quaternization and observed that post-methylation, the water contact angles were decreased owing to an increase in the hydrophilicity. Thereafter, the water-dispersible polyurethanes were formulated into coatings and further coated over urinary catheters. The anti-bacterial studies were also analyzed for the coated catheters and obtained good anti-bacterial activity against *E. coli* and *S. aureus*. Thus, the water-dispersible polyurethane coating for urinary catheters is an effective approach to reduce bacterial growth and extend their shelf life, promoting a healthy and safe treatment for patients.

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## Development of biobased conductive self-healing polymer blends based on natural rubber latex/ dextrin as flexible wearable sensors for biomedical applications

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### Abstract

Biodegradable, biocompatible elastomeric polymers with enhanced mechanical properties and self-healing capabilities for developing flexible stretchable sensors for motion detection and health care monitoring have gained immense attention in the present era<sup>[1,2]</sup>. In this work, bio-based crosslinked polymer blends of natural rubber latex and dextrin with robust mechanical properties, self-healing ability, printability and conductivity have been developed. Preliminary characterization of the crosslinked polymer blends has been carried out employing infrared spectroscopy, thermogravimetric analysis and X-ray diffraction techniques. The phase morphology evaluation and soil degradation studies have been done using scanning electron microscopy (SEM). Cytotoxicity evaluation by MTT assay confirmed the biocompatibility. The self-healing ability effect of crosslinked polymer blends have been confirmed through the dissolution and equilibrium swelling experiments along with the aid of mechanical properties' evaluation before and after healing at different time periods with the validation from SEM images. A conductive polymer blend based on natural rubber latex and dextrin have been developed which offers a new route for the fabrication of high performance complex wearable sensors to monitor human motions.

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## Naphthalene Derived Hyper-Branched Polymeric Self-assembly for Monitoring Azoreductase Activity under Hypoxic Environment

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### Abstract

The design and synthesis of macromolecules through the introduction of controlled branching via hyperbranch polymerization gained recent attention of the scientific community due to its diverse application in the biomedical field starting from diagnosis to drug delivery.<sup>1</sup> This article emphasizes the development of naphthalene-derived, self-assemble hyperbranch polymer (PNAZO) in an aqueous medium where the azo bond works as a stimuli-responsive function in the presence of an overexpressed enzyme in hypoxic microenvironment. Here the monomer is completely water-insoluble. On the other hand, our polymer is completely soluble in an aqueous medium due to the presence of rich hydrophobicity on both sides of the monomer. Due to the amphiphilic nature of the compound and the presence of extensive hydrogen bonding, it is showing excellent twisted-rod-like morphological architecture with increasing the concentration of the polymer from below CAC to above CAC. It is well documented that the azo bond reduced very easily in the presence of azoreductase enzyme which is beautifully explained by our polymer.<sup>2</sup> Initially, our polymer remain nonfluorescent in the absence of azoreductase. On the other hand in the presence of azoreductase extracted from E. coli bacterial cells, our polymer shows intense green fluorescence at 550 nm in a hypoxic microenvironment. The same phenomenon was also proved by sodium dithionite (mimic of azoreductase) for both monomer and polymer with the help of mass spectrometry and gel permeable chromatography. It is also established that our polymer can able to monitor the level of azoreductase selectively in hypoxic cell lines over normoxic cell lines.

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## Hierarchical Self-Assembled Structure of Norbornene-based Amphiphilic Polymers

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### Abstract

The self-assembly process, which is inspired by biosystems and also for mimicking the biological systems, incorporates amphiphilic macromolecules to provide unique and new openings to yield advanced materials in biotechnology or in nanoscience.<sup>1</sup> The extension of simple methods of amphiphilic assembly to the innovative concept of supramolecular self-assembly for the production of more complex and hierarchical nanostructures with precise control has become an important challenge in recent eras.<sup>2</sup> Therefore, norbornene-based amphiphilic polymers are developed to evaluate their supramolecular self-assembly nature in aqueous media.<sup>3</sup> Initially, NORCN was synthesized to copolymerize with NORPEG by various feed ratios to produce block copolymers and random copolymers via ring-opening metathesis polymerization (ROMP). The monomers and polymers are thoroughly characterized by using instruments like NMR, mass spectra, APC, and so on. After that, these synthesized polymers are allowed to undergo self-assembly into nanostructures. The random copolymers are found to execute twisted rod morphologies which eventually transform into their hierarchical structures, whereas, block copolymers are envisioned to form toroidal structures. These morphological changes are found to be pH-dependent. Finally, the biocompatible nature of norbornene is leveraged to evaluate the interaction of these amphiphilic polymers with protein. Thus, these amphiphiles have significant potential in biotechnology with promising future applications.

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## Silk Based Hydrogel Formulation For Transdermal Delivery Of Diclofenac

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### Abstract

Transdermal drug delivery methods have received a lot of interest because, in contrast to other drug delivery systems, they are valued for their capacity to provide precise and regulated drug administration. In this study, we investigate a brand-new hydrogel made of a Silk Sericin-Polycaprolactone blend developed for the transdermal delivery of Diclofenac. In-situ biodegradability, in-situ antibacterial capabilities, and antioxidant activity of the hydrogel were thoroughly characterized in this study. FTIR spectroscopy, rheological behaviour, porosity assessment, hydrophilicity, and swelling behaviour in distilled water and buffer, were also performed. Additionally, the hydrogel's matrix's drug release kinetics was examined. The findings suggest potential applications of our hydrogel as evidenced by the assessment of the various characterization techniques. Successful blending of Silk Sericin and Polycaprolactone was verified through FTIR spectroscopy, while SEM imaging unveiled the hydrogel's microstructure and surface morphology. Rheological analysis highlighted its suitability for transdermal applications, while porosity studies disclosed its networked structure. Remarkably, the hydrogel exhibited a propensity for water absorption, as indicated by hydrophilicity data, and showcased controlled swelling behaviour in both buffer solutions and distilled water, underlining its promise as a drug delivery system. Additionally, in-situ biodegradability, antibacterial experiments, antioxidant study and drug release kinetics established the hydrogel's potential utility in the context of infected skin conditions. In conclusion, the Silk Sericin-Polycaprolactone blend hydrogel exhibits promising attributes for the transdermal delivery of Diclofenac.

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## Histidine-Based Reduction-Sensitive Star-Polymer Inclusion Complex as a Potential DNA Carrier: Biophysical Studies Using Time-Resolved Fluorescence as an Important Tool

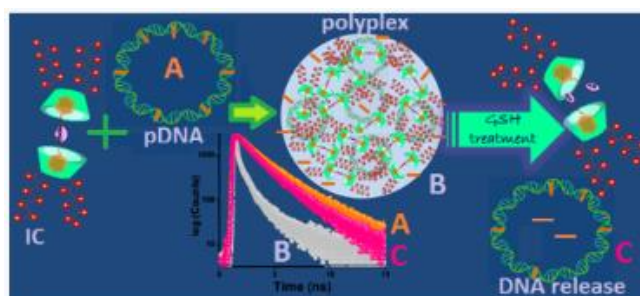
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### Abstract

Cancer is a global concern for substantial mortality issues. Rather than conventional drugs, artificial DNA can effectively destroy the cancer cell. For targeted DNA delivery, we have designed a novel stimuli-responsive polymeric carrier that can respond to cancer environment. An effective DNA carrier having optimum size and shape can condense and release DNA at the target site. We successfully designed a redox-responsive DNA carrier based on the host-guest interaction and established its behavior by time-Correlated Single Photon Counting (TCSPC) study. The acryloyl-incorporated histidine functionalized  $\beta$ -Cyclodextrin( $\beta$ -CD) undergoes RAFT polymerization and forms cationic star-shaped polymer. The disulfide containing bis-adamantyl group, as guest connected with the host  $\beta$ -CD, produces 2:1 inclusion complex (IC). We have used thiazole orange (TO) for the first time as DNA-intercalating fluorophore to investigate the DNA binding ability by dye displacement assays using time-resolved fluorescence spectroscopy technique. Analyzing fluorescence spectra of TO, pDNA and various concentrations of cationic polymer concludes that higher charge density enhances polyplex formation (pDNA & cationic polymer) and decreases fluorescence intensity of TO. The maximum lifetime of TO in IC-pDNA implies the strongest binding between IC and pDNA. The hydrodynamic size of IC-pDNA polyplex is  $\sim 230$  nm at low Glutathione (GSH) concentration providing stability in extracellular fluid. At high GSH concentrations, pDNA release was observed by time-resolved fluorescence spectroscopy<sup>1</sup>. The new carrier system developed by our group for DNA binding study at very low DNA concentration offers a new era for future cancer treatment.



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## **Fabrication of 3D bioprinted GelMA/methylcellulose hydrogel closely resembling the native corneal model with improved *in vitro* cytocompatibility and sustained keratocyte phenotype for enhanced stromal regeneration**

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### **Abstract**

Traditional treatment for severe corneal disorders involves corneal transplantation, a costly procedure prone to graft rejection and constrained by the global donor shortage. Enter 3D bioprinting with biodegradable polymers, a cutting-edge technique offering architectural replicas of tissues. Among these materials, GelMA stands out for its 3D scaffold structure, biocompatibility, robust mechanics, and optical clarity. Yet, its insufficient viscosity for precise printing at body temperature hinders progress. Our endeavor aims to craft 3D-printed GelMA/MC hydrogels for corneal stroma tissue engineering, exploiting MC's printability at room temperature and GelMA's irreversible photo-crosslinking under UV light. We meticulously tuned print parameters, examining thermal, morphological, and physicochemical features for two GelMA/MC hydrogel concentrations. Achieving a remarkable 78% transparency (at 700 nm), akin to normal corneas (80%), we conducted *in vitro* studies with goat corneal stromal cells, evidencing the hydrogels' capacity for cell adhesion and proliferation. Vimentin and keratan sulfate expression verified keratocyte phenotype retention. This 3D-printed GelMA/MC hydrogel successfully emulates native corneal stroma properties, holding promise for clinical corneal stromal tissue engineering

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## Cationic-porphyrin Incorporated Electrospun Fibers for Effective Photo-inactivation of Bacteria

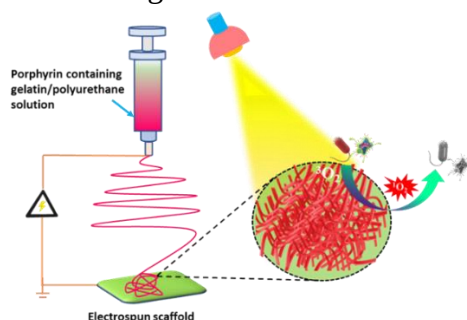
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### Abstract

Infectious diseases caused by pathogenic bacteria continue to be a persistent concern to public health. The introduction of new microbial diseases or the re-emergence of previously controlled diseases worsens the situation <sup>1</sup>. Antibacterial photodynamic therapy (APDT) is now gaining popularity in the scientific community due to its low susceptibility towards drug resistance, while bacteria often develop drug resistance rapidly in response to traditional antibiotic therapy <sup>2,3</sup>. The present work explores the possibility of combining a biodegradable gelatin/polyurethane electrospun polymer scaffold with a cationic porphyrin (GPP); to employ as a user-friendly photosensitizer in APDT. The membranes have been structurally characterized and the antibacterial action triggered by a visible light source has been investigated. The membrane GPP exhibited 97% and 96% inhibition against *E. coli* and *S. aureus* respectively in the presence of light.



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## Release profile of curcumin when loaded in bare form or in the form of an inclusion complex via hydrogel nanocomposite system

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### Abstract

Poor aqueous solubility of many known drugs is considered as one of the major challenges in drug development owing to low bioavailability and reduced therapeutic efficiency. One of the ways to deal with the solubility issue of a drug is formation of its inclusion complex. Curcumin (CUR) is one of the hydrophobic drugs having anti-inflammatory, anticancer and antioxidant properties which has wide applications in the biomedical field. However, the application of CUR is restricted due low aqueous solubility, low bioavailability and short half-life period. Also, it can be degraded by the enzymes present in the digestive system. Considering these difficulties of CUR, the present work aims to form an inclusion complex of CUR using  $\beta$ -cyclodextrin to improve the solubility of CUR by developing its inclusion complex. Also, CUR was loaded in a hydrogel nanocomposite system which would protect CUR from the enzymes and aid in its controlled release. Gelatin crosslinked polyacrylic acid incorporated with nanofiller was synthesized using a free radical polymerization method. The synthesized CURInc and hydrogel nanocomposite were characterized using various characterization techniques such as FTIR, XRD and FESEM. The *in vitro* drug release profile of CUR and CURInc was studied under different physiological pH conditions. CURInc loaded hydrogel nanocomposite exhibited more controlled release of CUR over CUR loaded hydrogel system.

Key words: Bioavailability, Curcumin, Hydrogel nanocomposite, Inclusion complex, Controlled release.

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## Antioxidant Polymers for the Mitigation of Cellular Oxidative Stress

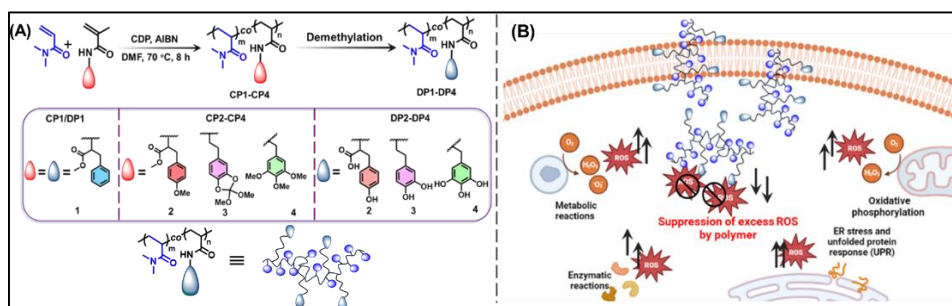
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### Abstract

Antioxidants are a class of compounds plays pivotal role in protecting cells from excess of reactive oxygen, nitrogen species (ROS, RNS) thus maintain cellular haemostatics.<sup>1</sup> ROS and RNS are produced in the cell through different cellular metabolic pathways and essential for metabolism as well as cellular signalling. However, an imbalance between elevated level of ROS, RNS and insufficient antioxidants creates oxidative stress,<sup>2</sup> which believed to closely associated with aging and several degenerative diseases.<sup>3</sup> Although, the existing small molecular antioxidants are often recommended as drug, however, many of these commonly used antioxidants suffer from low water solubility and low bioavailability, which limits their applications in clinical treatment. Among the various class of antioxidants, polyphenols have drawn immense attention as these are widely distributed in various renewable plant sources.<sup>5</sup> Herein, inspired from the polyphenol chemistry, we have designed a series of polyphenol containing polymers with various pendent group through reversible addition–fragmentation chain transfer (RAFT) polymerization. After successful characterisations of all the polymers we have analyzed radical scavenging properties among the similar molecular weight polymers through various methods such as 2,2-diphenyl-1-picrylhydrazyl radical (DPPH), 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) and hydroxyl (OH) radical scavenging assay, which depicts that polymer **DP4A** (Scheme 1) have shown excellent antioxidant properties than others. Moreover, the treatment of **DP4A** on H<sub>2</sub>O<sub>2</sub> induced macrophage cells capable to effectively arrest the cellular oxidative stress with negligible cytotoxicity. Altogether, this methodology has enabled the synthesis of biocompatible polyphenol pendent polymer with notable antioxidant property for various bioapplications.



**Scheme 1.** Schematic representations of (A) synthesis of polyphenol pendent polymers, and (B) suppression of cellular oxidative stress in the presence of antioxidant polymers.

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## Smart, 3D printed amyloid-based hybrid hydrogel of bovine serum albumin and hyaluronic acid as personalized treatment of diabetic wound healing

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### Abstract

Hyaluronic acid (HA) is a naturally occurring polysaccharide that is found in many tissues throughout the body, including skin, joints, and cartilage. It is effective in promoting wound healing by providing a moist environment for cells to migrate and proliferate, and by stimulating the production of collagen and other extracellular matrix components. However, there are several limitations such as short residence time, poor mechanical strength, short degradation time, and very high swelling behaviour that need to be considered when using HA hydrogel for wound healing. While on the other hand, protein-based amyloid fibrils tend to form self-assembled hydrogel under certain physiochemical conditions with exceptionally high and tuneable mechanical strength. Taken together, we have constructed a hybrid hydrogel of HA and amyloid fibrils. The combination of these two biomaterials in a hydrogel provides both excellent and tuneable mechanical properties as well as an active environment to support tissue repair and regeneration resulting in rapid wound healing. Overall, our results indicated that the hydrogel had the ability to promote cell migration and proliferation, reduce DNA damage, shorten the inflammatory period, and accelerate the deposition of collagen fibers and the formation of blood vessels in the model with diabetic skin injury, suggesting positive effects on diabetic wound healing. Thus our hydrogel might have great potential as a bio-ink in tissue engineering as a dermal substitute for customizable skin regeneration.

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## Photo-Switchable Smart Antibacterial Polypeptide Coating for Enhance Antibacterial Activity

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### Abstract

Antibiotic resistance to bacteria is one of the biggest problems in health care system. Most of the bacterial infections are caused by biomedical devices which poses to human health damage. Therefore, effective antibacterial surface coating agents is needed for overcome of this situation. A noble non-contact and noninvasive stimuli responsive photo switchable smart antibacterial surface based polymer has been developed to eradicate bacterial infection.<sup>1</sup> Polymeric based azobenzene has a more interesting photo-switchable stimuli responsive method to build smart surface. Hence, azo group in presence of UV light is reversibly converted into cis to trans form to disconnect the interaction.<sup>2</sup> Bacteria cell surface is negative in charge, thus polymer with positive charge containing ammonium group is greatly interacted the cell wall of bacteria and disrupted the cell wall. Therefore, polymer containing quaternary ammonium group and azo group has able to killed the surface bacteria and could be disconnected with UV stimuli to release the dead bacteria. Herein, we are developed a new non-contact and noninvasive stimuli responsive photo switchable smart antibacterial surface-based polypeptide polymer to enhance the antibacterial activity. Polymer is synthesized through ring opening polymerization of N<sub>6</sub>-carbobenzoxy-L-lysine N-carboxyanhydride (Cbz-L-Lys NCA) using primary amine containing azobenzene as initiator, after that deprotection of Cbz-L-Lys NCA and quaternary ammonium modification. Azo group and cationic ammonium group with various chain length on antibacterial polymer is investigated in details.

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## Redox-Responsive Norbornene Based Drug Delivery against Multidrug Resistance for Targeted Cancer Theranostic

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### Abstract

Multidrug resistance (MDR) is one of the major challenges for successful cancer chemotherapy due to the over expression of ATP-dependent drug efflux transporter protein such as P-glycoprotein (p-gp) and for the ineffective penetration of drug molecules into tumor. Hence, there is a essential need to develop multifunctional nano-prodrug system for site-specific delivery to inhibit P-gp mediated drug efflux and in situ monitoring the therapeutic response. Toward this goal herein, we have developed a GSH-redox-responsive norbornene based block copolymers grafted with avidin receptor, and mitochondria dual targeteting copolymers which are allowed to undergo self assembly phenomenon to produce nano-prodrug carrier PCT-TPS-CBT by using ring opening metathesis polymerization (ROMP) technique having diagnostic functionality. Three types of monomers were designed to incorporate i) anti-cancer drug camptothecin (CPT) along with S-S linkage, ii) over- expressed P-glycoprotein efflux pump inhibitor (D- $\alpha$ -tocopherol succinate polyethyleneglycol-1000) with mitochondria targeting segment (triphenyl phosphonium cation), iii) avidin cancer cell receptor targeting ligand (biotin), and cell penetrating peptide mimic (guanidyl cation) for improved delivery of drug to resistant cancer cell. These all substituted monomers were synthesized and thoroughly characterized by NMR, mass spectrum, and so on. After that, These nano-prodrug carrierers were subjected for self-assembly studies in aqueous media which can provide a prospective strategy to overcome multidrug resistance in cancer cell in synergistic manner to increase internalization and decrease efflux of therapeutic agent. Such a unique prodrug carrier have an attractive potential for the development of nanomedicine.

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## The Morpholinone Based Dual Drug Conjugated Polymer System: An Efficient Multi-Stimuli-Responsive Theranostic Nano-Material for Targeted Cancer Therapy and NIR Imaging

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### Abstract

The chemotherapeutic efficacy and consumption of complexity on healthy cells and tissues become one of the major objective for the treatment of cancer. Toward serve our goal, we developed a biodegradable, highly water soluble, triple stimuli responsive (esterase, pH, GSH) theranostic polymer NIR-SS-PolyMor-Gem-Btz-Biotin that was affixed with dual chemotherapeutic agent (gemcitabine and bortezomib), receptor targeting agent (biotin), a cationic charged near-infrared (NIR) fluorescence dye for mitochondriotropic agent and bio imaging purpose<sup>1</sup>. Our expectation is that the polymer will self-assemble and penetrate the endothelial membrane via EPR effect and enter in to cancer tissues by the process of avidin mediated endocytosis. Our strategy is taking favour of overexpressed esterase, low pH and the high glutathione (GSH) concentration in cancer cells, the ester bond will be cleave and disulfide bond will reduce in NIR-SS-PolyMor-Gem-Btz-Biotin respectively. As a consequence active anticancer drugs will release and a near-infrared (NIR) fluorescence dye will turn-on<sup>2</sup>. The proteasome inhibitor bortezomib will induce apoptosis and also enhance the efficacy of gemcitabine. Our glory of this project the drug delivery vehicle is newly synthesized backbone that having combination effect of bortezomib and gemcitabine will enhance the activities against the pancreatic ductal adenocarcinoma (PDAC)<sup>3</sup>.

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## Photopolymer Grafted Polyurethane as Controlled Drug Delivery Vehicle for Biomedical Application

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### Abstract

There has been a recent global drift towards modifying commercial photocurable resins to fabricate its mechanical, biological and polymerisation properties and thereby adapting these properties for biomedical applications. Previously acrylates have been utilised as pH responsive polymers, stimuli sensitive hydrogels, drug delivery vehicles. The advancement of resin based dental filling composites have greatly transformed the field of dentistry. Dimethacrylate polymers are usually employed in dentistry in fissure sealants, dental bonding agents and tooth restorative composites. The popularly used polymer is based on adducts of bisphenol A and glycidyl methacrylate, i.e., bis-GMA (Bisphenol A-glycerolate dimethacrylate). Herein, biocompatible polyurethane grafted Bis-GMA copolymers (PU-Ph) have been synthesised by in-situ polymerisation to balance its hydrophobicity and to assess its feasibility as a novel drug carrier for modulated delivery of anti-cancer drug, paclitaxel. Characterisation of developed copolymers was carried out using several spectroscopic techniques to ascertain their architecture and to understand the interaction between copolymer and drug molecules. Thermal and rheological properties have been analysed to evaluate polymer processing characteristics like degradation temperature, glass transition temperature, flow behaviour of polymer, material deformation and other properties like, loss modulus, storage modulus, viscosity, complex viscosity, etc. Drug release profile annotate the benefit of grafting and the evaluation of biocompatibility towards human cervical cancer cells (SiHa) exhibit its capability as drug carrier.

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## Synthesis and characterization of (3-acrylamidopropyl)trimethylammonium chloride *grafted* chitosan copolymers for controlled drug delivery applications

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### Abstract

Chronic non-healing wounds are one of the worst side effects associated with Diabetic mellitus which can cause severe morbidity and in worst cases lead to amputations. Hence, an effective wound care is essential for enhancing the patient's compliance and life.

Accordingly, we have synthesized series of graft copolymers of Chitosan-graft-(3-acrylamidopropyl)trimethylammonium chloride (APTMAC) containing antibiotics for controlled release in wound healing. The copolymers were characterized in terms of their molecular structure by <sup>1</sup>H and <sup>13</sup>C-NMR spectroscopy. The graft copolymers were cast into films and crosslinked using sodium tripolyphosphate. Swelling study of these cross-linked films were done and were externally loaded with an antibiotic. The release of drugs was studied in a buffer solution. The drug release profile was corroborated with the composition and swelling properties of the polymer films. It was observed that, films containing higher content of APTMAC could release the drug for a longer time which can help in better wound management.

This research highlights the potential of these chitosan-based films for controlled drug delivery and effective approach for wound management. Further details will be explained in the poster.

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## **Evaluation of antimicrobial activity of essential oils encapsulated in Polyvinyl alcohol/chitosan composite film.**

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### **Abstract**

In this research a study was conducted in which the incorporation of four essential oil nano-emulsion (thymol, geraniol, citral and carvacrol) into composite film composed of polyvinyl alcohol (PVA) and chitosan (CS). The objective was to assess the physical, mechanical, microstructural, and antimicrobial properties of these composite films. Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD), along with thermogravimetric (TGA) analysis, were employed to confirm the existence intramolecular interaction within the composite film matrix. Additionally, scanning electron microscopy (SEM) was utilized to gain insight into the surface characteristic of the composite films. The finding reveals that adding essential oil to the composite film led to an enhancement in water affinity (hydrophilicity) and tensile strength. The antimicrobial activity of films against *C. neoformans* and *C. luorentii* disc diffusion method, MTT assay and analysis of surface morphology by scanning electron microscop shown that the composite film increases antimicrobial property. Evaluated the cytotoxicity of composite films in HEK293 cell lines showed negligible cytotoxicity. Therefore, it could be promising as antifungal drug delivery. Composite film can be used for food and fruits packaging because these oils are safer according to the food and drug administration (FDA).

**Keyword-** PVA/CS, Antimicrobial, composite film, and cytotoxicity.

## Biobased biodegradable green polyurethanes and their nanocomposites

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### Abstract

Polymers are occupying a vital position in this civilized society and without their contributions further advancement of the society will be severely hampered. However, still now most of such polymers are obtained from fixed resources, which are declining day by day. Further, most of these synthetic polymers are non-biodegradable even after several years of their applications and hence cause environmental pollution upon discarding along with ecological imbalance. Thus, over the last two-three decades constant efforts have been made from the scientists and industrialists to replace fixed resources by renewable resources and transform the polymeric products to environmentally degradable. Now among various industrial polymers, polyurethane is the most versatile and showed excellent performance for a wide spectrum of applications. Under these circumstances, author's laboratory has been striving over the last more than two decades to produce biobased biodegradable green polyurethanes with high performance. The laboratory produced almost all types of biobased biodegradable polyurethanes including room temperature and elevated temperature curable resins for coating applications to advanced smart 3D printable scaffolds for biomedical applications. Author's group produced conventional and smart thermoplastic, elastomeric, solvent borne, waterborne, linear and special-architectural polyurethanes with greener attributes and desired performances. Further, to achieve the advanced performance with smart behaviors, these specially designed polyurethanes have been modified with different types of nanomaterials of zero, one and two-dimensional sizes. The smart behaviors including shape memory, self-healing, and self-cleaning have been explored. The potential fields of applications explored for them include stimuli-responsive biomaterials such as smart sutures, self-expandable stent, scaffolds for bone regeneration, etc., artificial muscle in soft robotics, self-healing materials in automobiles, wind energy blades, etc., self-cleaning surfaces in solar cells, auto-cleaning paints, etc. In this international conference, various aspects of such polyurethanes and their nanocomposites including concept, designing protocol, properties, and applications will be presented.

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## Self-healable disulfide-induced epoxy vitrimer with shape-memory, antioxidant, and UV shielding attributes

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### Abstract

One essential condition for the shift to a more circular economy is the manufacture of more environmentally friendly thermosetting polymers with a longer usable lifespan. The application potential for reusing materials that are long-lasting and very durable also tends to be constrained. Therefore, a thermosetting polymer such as epoxy that has been abandoned at this time contributes significantly to resource waste and seriously contaminates the environment. The combination of the covalent adaptable network (CAN) concept and the use of bio-based raw materials has ingeniously addressed this dilemma. In this scenario, we synthesized a dynamic disulfide-containing epoxy resin from an amide derivative of 2,2'-dithiodibenzoic acid, and it was then cured using poly(amido amine) and cystamine, two bio-based curing agents. The use of a reactive diluent decreased the production of volatile organic compounds while the epoxy resin was hardening. The epoxy vitrimer disulfide bonds and aliphatic moieties produced an exceptionally high strain along with good tensile strength attributes. The dynamic link allowed the vitrimers to have good self-healing and shape memory characteristics. The polymer chain architecture was able to topologically reorganize through the disulfide bond dynamic exchange reaction, making them reprocessable and degradable. Additionally, these epoxy vitrimers have strong chemical resistance qualities, may suppress oxidation, and can shield against UV radiation. Thus the studied epoxy thermoset has great potential to be used as a thin film durable material.

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## Green composite of yam starch-based bioplastic and its applications

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### Abstract

The unchecked use of plastic and its various forms in food packaging and other single-use applications has led to a variety of issues ranging from environmental pollution to human health [1]. Among various measures taken for the restriction and complete curbing of synthetic plastic, the development and application of bioplastic hold a particular interest as a bio-based biodegradable alternative [2]. The use of under-utilized starch source i.e. yam starch for the production of bioplastic and green composite has been explored through a simple solution casting method. The bioplastic showed impressive mechanical properties through the use of a minimum amount of plasticizer and cross-linker without any catalyst or curing temperature. Further, the property of the produced bioplastic was enhanced for pH-sensitive food monitoring with the incorporation of a natural dye in the bioplastic matrix [3]. Similarly, the green composite of unpurified yam starch was prepared using alkali-treated corn stalk fiber as filler for an overall improvement in their mechanical and thermal properties with additional UV protection features. Most importantly the produced bioplastic and its green composite showed excellent biodegradability under natural environmental conditions. Thus sustainable bioplastic and its green composite have great potential to be used as smart food packaging materials and for other advanced applications.

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## **Biobased flexible UV-shielding epoxy coatings from gallic acid derivative**

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### **Abstract**

The excellent thermal resistance, mechanical properties, and easy processability of epoxy resins have broadened their applicability in coating and paint industries. As the majority of the commercially available epoxy resins contain bisphenol-A (BPA) as the main constituent which is fundamentally derived from petroleum sources and also has potent toxicity, intensive research is being conducted in search of bio-based alternatives to BPA without compromising the thermomechanical properties. In this work, an epoxy resin has been synthesized by modification of gallic acid to obtain a biobased epoxy with high flexibility and UV shielding ability. Herein we incorporated long-chain flexible moieties in the polymeric network to alter the cross-link density and network rigidness in order to overcome the inherent brittleness and low-impact resistance of epoxy thermosets. The synthesized polymeric resin was characterized using Fourier transform infrared (FTIR), <sup>1</sup>H-NMR (Nuclear magnetic resonance), <sup>13</sup>C-NMR, GPC, etc. The bio-based epoxy thermosets were found to exhibit good mechanical properties and also displayed good thermostability at elevated temperatures. The obtained thermosets were also found to have satisfactory biodegradability attributes.

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## Starch-based hydrogel composite with wastepaper for agricultural application

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### Abstract

In recent decades, hydrogels have been considered as potential superabsorbent polymeric materials for agricultural applications due to their high-water absorption and controlled fertilizer release properties. Therefore, in this study, starch, itaconic acid and acrylic acid-based hydrogel composite was prepared by using wastepaper-derived cellulosic paper powder as the micro-reinforcing agent. The paper powder was obtained from printing wastepaper by applying simple alkali treatment. The FTIR, TGA and XRD studies revealed the formation of the hydrogel network structure and successful incorporation of reinforcing materials into the hydrogel matrix. Further, the porous structure of the hydrogel composite was confirmed from the FESEM images, which further revealed the formation of a three-dimensional network structure of the hydrogel. An increase in water swelling capacity was observed from 503 to 647 g/g when the amount of reinforcing agent was increased from 0 to 0.05% by weight. Further, the NPK release profile for the hydrogel composite was investigated for up to 20 days after incubation, showing the slow-release property of the formulation. The biodegradation property of the hydrogel was studied by soil burial method and confirmed from the FTIR and SEM image analysis. Moreover, the effect of NPK encapsulated hydrogel composite on okra seeds germination was investigated and found strong influence.

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## Facile Chemical Modification of Chitosan and Poly(vinyl alcohol) Using Chloroacetic Acids

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### Abstract

Poly(vinyl alcohol) [PVOH] was modified by simply mixing it with dichloroacetic acid and heating the mixture without employing any additional reagents/catalysts/solvents. This resulted in the formation of a random copolymer, poly(vinyl alcohol-co-vinyl dichloroacetate) [P(VOH-co-VDCAc)] copolymer, which was not soluble in water but was soluble in organic solvents such as acetone, methanol, and dimethylsulfoxide. Furthermore, the copolymer was inherently self-extinguishing, and did not melt drip or show glowing combustion. This copolymer could be used as a flame-retardant sizing agent for currency notes. In another reaction, chitosan was carboxymethylated by directly mixing it with monochloroacetic acid and heating the mixture without employing any solvents or catalysts. Contrary to the conventional solution-based strategies, the solvent-less carboxymethylation technique introduced extensive crosslinking in chitosan. These crosslinks occurred due to electrostatic interactions between the pendant carboxylic acid groups in the carboxymethylated repeating units and the amine groups in the repeating units that remain unmodified. Given the insolubility of crosslinked carboxymethyl chitosan in acidic pH, it can be used as an adsorbent for anionic dyes from acidic media.

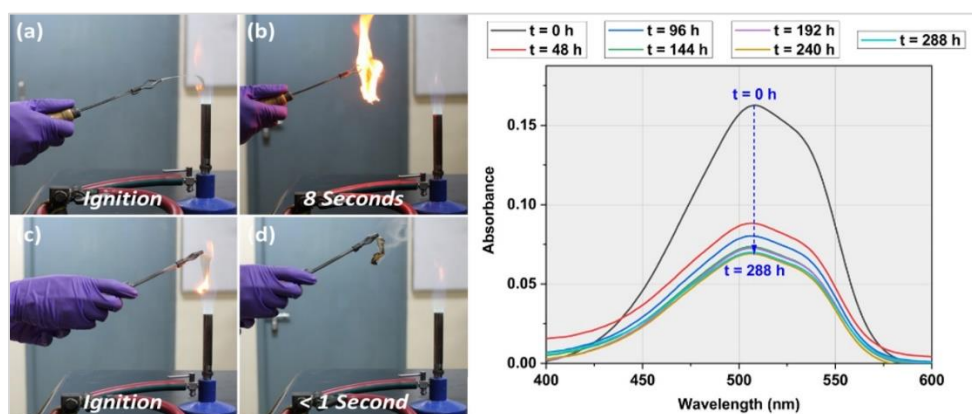


Figure: Left – Flammability of (a,b) PVOH, and (c,d) P(VOH-co-VDCAc) copolymer; Right – Adsorption spectra of 1 ppm of methyl orange solution in 0.025 M HCl with added crosslinked carboxymethyl chitosan at different times.

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## **Bio-based epoxy composite derived from Renewable Feedstock.**

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### **Abstract**

Agriculture wastes are derived from diverse sources such as vegetables, fruits, lemon peels, sugarcane bagasse, rice husks etc. Utilizing renewable feedstock and agricultural waste, can reduce our dependency on non-renewable resources and also contribute to a more environmentally friendly and sustainable future. Our findings have the potential to revolutionize the composite industry and pave the way for more eco-friendly materials for various applications. In the present study we developed bio-based resin for composite application. Bio-based epoxy was synthesized from renewable feedstock in order to use as reinforcing agent to fabricate composite. Here, the filler was mainly used from agriculture waste to develop an eco-friendly and sustainable composite. The composite was evaluated for its mechanical properties including tensile, flexural, impact, shear, and compression, further studies are expected to give more insight for addressing sustainability challenge.

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## Investigation of Coir fiber-reinforced Sustainable Geocomposites

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### Abstract

The emerging focus on eco-friendly natural fiber-based geocomposite systems are unequivocally raised from the current environmental concerns. In the face of escalating plastic pollution, especially the peril caused by the micro plastics, there is a growing urgency to explore the sustainable solutions. Geocomposites now being fabricated from non-biodegradable synthetic plastics easily disintegrates to microplastics that pose serious threat to marine ecosystems and human health. The pursuit of alternatives such as PLA, PBAT, PBS that are fully compostable<sup>1</sup> may not be cost-effective for this particular application. Coir, a notably robust natural fiber which presents an attractive option as a sustainable filler with these biodegradable polymers that enhances the mechanical properties. Higher loading of coir fiber in the polymer matrix resulted an increase in rigidity and hardness of the composite, while concurrently diminishing its strength and the ability to deform.<sup>2</sup> A comprehensive investigation of the mechanical strength assessments and evaluation of solvent resistance and water absorption characteristics of coir fiber-reinforced composites were conducted. Further, salt water immersion test, biodegradation test under soil burial and composting conditions are studied.

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## Advanced Reprocessable Thermosets Derived from Polybenzoxazines

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### Abstract

Polybenzoxazine is a new class of high-performance phenolic thermosetting material prepared by the ring-opening polymerization of benzoxazine monomers without needing any external catalyst. They outshine conventional thermosets due to their unique properties, high thermal stability, low water absorption, no or less volatile release during curing, and low volume shrinkage with excellent dimensional stability<sup>1</sup>. The permanent covalent crosslinks are responsible for the exciting properties of thermosets however, they hinder their reprocessability, generating huge waste which ends up segregated into landfill. Thus, a severe solution is the need of the hour to eradicate plastic pollution. The inclusion of dynamic bond for instance, sulfur-sulfur linkages into the polybenzoxazines networks, imparts reprocessability, repairability and recyclability to the material due to their dynamic nature at room temperature or under weak stimuli. Numerous approaches for incorporating sulfur-sulfur linkages include polymerization of disulfide-containing monomer<sup>2</sup>, polysulfides incorporation via inverse vulcanization<sup>3</sup>, Sulfur Radical Transfer and Coupling Reaction<sup>4</sup>, and Radical-induced aryl halide-sulfur polymerization. Conventional monomers and organic molecules copolymerized with high content of sulfur end up generating new age material with a variety of applications. These synthetic polymers are a matter of interest for their applications as self-healing material, reprocessable thermosets, cathode material for Lithium-Sulfur batteries, materials for high refractive index applications, and polymers to capture heavy metals with special binding affinity to mercury ions<sup>5</sup>.

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## **Expurgation of anionic dyes from contaminated aquatic sources by an organogel for a sustainable environment**

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### **Abstract**

With an expeditious increase in modernization and zeal for advancement, nature has always been a victim of human exploitation. The use of synthetic dyes in various industries has increased the ultimatum for the environment since waste generated from dyes is dumped onto aquatic resources.

To expurgate dyes from polluted water sources, an organogel composed of Montmorillonite-PAni has been explored. It was found that the gel attained high selectivity and would remove around 99.44% of an anionic dye. This makes the sorbent an effective source for dye treatment making it convenient for usage in practical applications.

## Castor polyol and Cellulose Polyol based biofoams for improved thermal insulation

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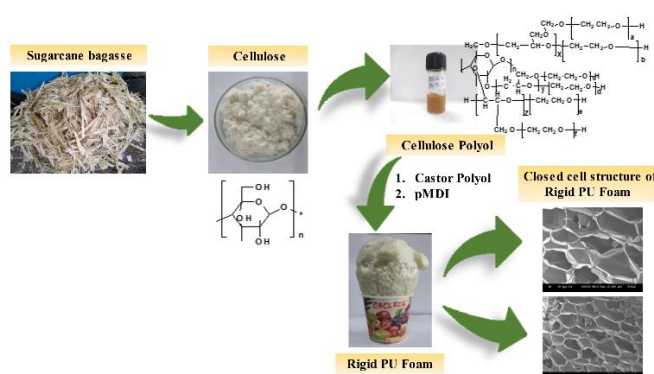
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### Abstract

The present research elucidates the synthesis and characterization of cellulose polyol derived from alpha cellulose and the subsequent development of rigid polyurethane foams using castor polyol and cellulose polyol blends. Alpha cellulose was converted into the semi-polyol first by reacting with glycidol, in the presence of sodium hydroxide, and water, followed by the reaction with ethylene carbonate in the presence of potassium carbonate yielding the cellulose polyol. Structural confirmation of the product was carried out using FT-IR, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR analyses. In order to prepare rigid polyurethane foams, a mixture of cellulose polyol and castor polyol at various ratios (castor polyol: cellulose polyol ratio of 100:0, 20:80, 40:60, 60:40, and 80:20) were blended. Each of these was formulated with pMDI, Tego8465 as a surfactant, DBTDL as a catalyst, and n-pentane as the blowing agent. The microstructure was examined using SEM which showed a closed cell structure. Density measurements indicated a positive correlation between the increased concentration of castor polyol and the resultant foam density. The flexural tests on the rigid PU foams indicated a positive correlation between the density of the fabricated foams and their flexural strength. Specifically, an increase in foam density resulted in a concomitant increase in flexural strength. Thermal conductivity data indicated that the foam generated through the utilization of a 60% cellulose polyol and 40% castor polyol blend exhibited the lowest thermal conductivity (0.04237 W/mk) at a temperature of 30°C. The integration of cellulose polyol into polyurethane foams confers improved performance.



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## Vitrimers derived from polybenzoxazines incorporating dynamic covalent bonds

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### Abstract

Polybenzoxazines have garnered significant attention recently due to their exceptional heat resistance, flame retardance, chemical resistance, dimensional stability, and high hydrophobicity. Unlike traditional thermosetting polymers that have irreversible cross-linked structures, polybenzoxazines incorporate dynamic covalent bonds (DCBs) into their networks. These DCB-based cross-linked polymers can be reprocessed through the reversible breaking and formation of dynamic covalent bonds, addressing resource loss and environmental pollution concerns. Various dynamic covalent linkages, including transesterification, disulfide, and boron ester linkages, have been explored in polybenzoxazine networks to promote self-healing and reprocessability. In particular, imine linkages have shown promise because of the availability of biobased monomers and the extensive knowledge of imine dynamicity. The integration of vitrimer properties with biobased materials offers a pioneering combination, allowing for the development of sustainable materials. The use of imine bonds as dynamic bonds in polybenzoxazines enables easy formation through a condensation reaction of aldehydes and primary amines, without the need for a catalyst. Overall, the concept of dynamic covalent bonds in polybenzoxazines provides a solution to the recycling challenges associated with thermosetting materials, making them ideal for renewable polymeric materials. [1] [2]

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## Epoxidized soyabean oil-based UV curable Epoxy – Acrylate resin for Digital Light Processing (DLP) 3D Printing

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### Abstract

Epoxy acrylates play a significant role in 3D printing (or additive manufacturing) due to a unique combination of properties, such as photopolymerization, fast curing, high resolution, and low shrinkage. However, most raw materials used in the synthesis are made from petroleum-based, non-renewable resources. The main objective of this project was to synthesize a bio-based alternative to epoxy acrylates.

In the present study, an UV-curable epoxy Acrylate resin oligomer was synthesized from Epoxidized Soyabean oil. The product obtained was characterized by Fourier transform Infrared (FTIR). Subsequently, a series of UV-curable resin formulations were prepared by combining Epoxy Acrylate with two different reactive diluents in various proportions. The effect of the properties was recorded. It was an overall observation that the addition of TMPTA imparted more stiffness while the addition of TPGDA imparted flexibility to the resin. This work presents a method to synthesize epoxy acrylates using renewable materials to be used in the 3D printing industry for innumerable applications ranging from intricate jewelry designs, and intricate architectural designs to automotive parts and smart materials.

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## Development of a Hybrid Emulsion from Plant based Acrylates for Adhesive Application

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### Abstract

With the ever increasing urge of renewable resources the demand for plant based acrylates has gained a lot of attention. Plant based acrylates have significant potential in paint, adhesives, ink and construction industries. The competence of these plant based acrylates with conventional petrochemical acrylates seeks more interest in finding new ways to match the performance of these plant based acrylates. In this study we have developed a hybrid emulsion containing high content of plant based acrylates along with least content of conventional acrylic monomers. The performance of this hybrid emulsion was tested on different substrates. The prepared emulsion showed promising adhesive performance, along with enhanced mechanical and physical properties

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## A phosphorus-based olefin linked fully conjugated polymeric ligand for palladium-catalysed *trans*-selective dicarbofunctionalization of internal alkynes

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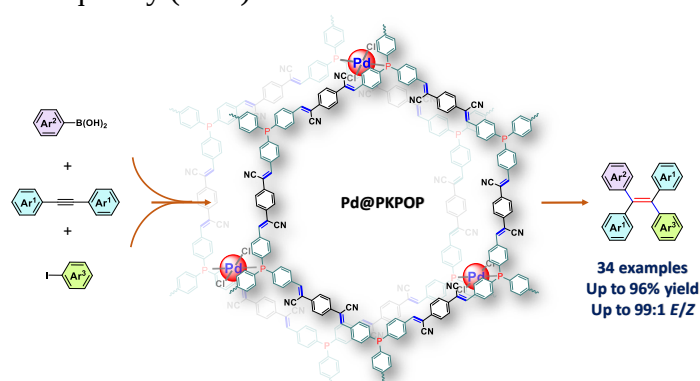
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### Abstract

Phosphorus is rarely introduced in  $sp^2$  carbon ( $C=C$ ) linked fully conjugated porous organic polymers (POPs) and has not been exploited in synthetically challenging and selectively competitive organic transformations. Herein, we synthesized a phosphorus-containing olefin-bonded fully conjugated organic polymer via a base-assisted Knoevenagel condensation reaction. Furthermore, we have metalated it with palladium chloride. Catalytically, this heterogeneous metal coordinated organic polymer has been employed on the challenging stereoselective multicomponent dicarbofunctionalization reaction on an unactivated internal alkyne using aryl iodides and aryl boronic acids as other reactants. *Trans*-selective tetra-substituted olefins were isolated with up to 96% yield and up to >99:1 *E/Z* selectivity for 34 examples. The catalyst tolerates enormous organic functional groups, including aldehyde, ketone, ester, nitrile, nitro, ether, halogens, alkyl, trifluoromethyl, and hetero-aromatic rings. Control and kinetic experiments were also performed to gain a mechanistic understanding. The polymer leveraging on multiple binding sites stabilized the palladium catalyst in different stages of the reaction that allowed the catalyst to be recycled for seven cycles with minimal product yield and selectivity loss. After recycling, the undamaged morphology of this polymeric material ensured further usability and made it more sustainable for catalysis. Turnover number (TON) and turnover frequency (TOF) are calculated to be 2561 and  $43\text{ h}^{-1}$ , respectively.



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## Effect of clove bud essential oil in guar gum-chitosan based edible coating on the postharvest shelf life of Khasi mandarin at ambient condition

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### Abstract

In the present study, Khasi mandarin has been taken as experimental material for enhancing the shelf-life to make sustainable economic development. For this purpose, the sustainable biopolymer for edible coating formulations has been developed using guar gum (0.7% w/v), chitosan (0.3% w/v), coconut oil, and clove bud essential oil. The effect of guar gum-chitosan composite edible coatings was investigated on the postharvest shelf life of Khasi mandarin up to 30 days of storage at ambient conditions. The postharvest characteristics such as weight loss, firmness, acidity, total soluble solids, and reducing sugar of control and treated fruits were evaluated at 5 day of intervals throughout the storage period. Results revealed that applying guar gum/chitosan-based edible coating with coconut oil and clove bud essential oil was more potential to prevent the shelf life of Khasi mandarin compared to other treatments and control, respectively. Guar gum/Chitosan/Coconut oil/Clove bud essential oil coating treatment had less weight loss (38%) and firmness (5.9N), as well as physicochemical characteristics like titratable acidity (0.29%), total soluble solid (10.8%), and total reducing sugar (5.41mg/mL). Further, the developed statistical model also confirmed the significance of the developed formulation in enhancing the shelf life of Khasi Mandarin.

**Keywords:** Guar-gum; Shelf-life; Khasi mandarin; Ambient conditions; Chitosan; Edible coating

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## Rice straw-based packaging film

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### Abstract

Rice straw makes up a significant portion of agricultural waste produced worldwide, and the proper disposal of this waste, currently managed through landfilling and incineration, is a significant global issue. This study modified rice straws using a strategic approach that integrates delignification and phosphorylation processes with cost-effective agricultural chemicals for producing films and cups on a larger scale. The developed films have a high charge content and exhibit enhanced mechanical durability in both dry and wet environments. They also demonstrate increased resistance to heat and flame retardancy and maintain their structural integrity even after being subjected to direct flame. The films were also heat-sealed to develop a pocket for storing and preserving perishable food items like apples, kiwis, and pears. Moreover, the developed gels were also moulded into cups, which display impressive stability when exposed to high temperatures, solvent-based conditions, and anti-fizzing properties for carbonated drinks. The proposed transformation of rice straws into packaging films and beverage cups, which offers reduced environmental impacts and economic viability, represents a sustainable alternative with great promise for achieving a world with less plastic dependency.

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## Proximity Enabled Photochemical C–H Functionalization using a Covalent Organic Framework Confined Fe<sub>2</sub> IV –μ–oxoSpecies in Water.

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### Abstract

Water has been recognized as an excellent solvent for maneuvering both the catalytic activity and selectivity, especially in the case of heterogeneous catalysis. However, maintaining the active catalytic species in their higher oxidation states (IV/V) while retaining the catalytic activity and recyclability in water is an enormous challenge. Herein, we have developed a solution to this problem using covalent organic frameworks (COF) to immobilize the (Et<sub>4</sub>N)<sub>2</sub> [Fe<sup>III</sup>(Cl)bTAML] molecules, taking advantage of the COF's morphology and surface charge. By using the visible light and [Co<sup>III</sup>(NH<sub>3</sub>)<sub>5</sub> Cl]Cl<sub>2</sub> as sacrificial electron acceptor within the COF, we have successfully generated and stabilized the [(bTAML)Fe<sup>IV</sup>–O–Fe<sup>IV</sup>(bTAML)] – species in water. The COF backbone simultaneously acts as a porous host and as a photosensitizer. This is the first time that the photochemically generated Fe<sub>2</sub><sup>IV</sup> –μ–oxo radical cation species has demonstrated high catalytic activity with moderate to high yield for the selective oxidation of the unactivated C–H bonds, even in water. To enhance the catalytic activity and achieve good recyclability, we have developed a TpDPP COF film by transforming the TpDPP COF nanospheres. We have achieved the regio and stereoselective functionalization of unactivated C–H bonds of alkanes and alkenes (3°:2° = 102:1 for adamantane with COF film) which is improbable in homogeneous conditions. The film exhibits C–H bond oxidation with higher catalytic yield (32-98%) and a higher degree of selectivity (cis:trans = 74:1; 3°:2° = 100:1 for cis-decalin).

## Catalyst Free Dynamic Covalent Adaptable Networks along with Recycling and Self-Healing Properties

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### Abstract

Dynamic covalent adaptable networks (DCANs) have emerged as a promising class of materials with the ability to undergo reversible chemical reactions, allowing for the adjustment of their properties in response to external stimuli. Catalyst-free DCANs represent a significant advancement in this field by eliminating the need for catalytic agents, simplifying the synthesis process, and reducing environmental impact. Here we explore the synthesis, recycling, and self-healing properties of catalyst-free DCANs, highlighting their potential for sustainable and resilient materials. The synthesis of catalyst-free DCANs relies on carefully designed dynamic covalent bonds, such as reversible imine or disulfide linkages, which enable rapid and reversible network reconfiguration. This property grants these materials the ability to adapt to changing conditions without the need for external catalysts, enhancing their versatility and applicability in various fields. One of the key advantages of catalyst-free DCANs is their potential for recycling. When subjected to controlled conditions, these materials can be depolymerized and reassembled multiple times without significant loss of their inherent properties. This recyclability not only reduces waste but also conserves valuable resources, making catalyst-free DCANs an environmentally friendly choice. Furthermore, the self-healing properties of catalyst-free DCANs make them ideal candidates for applications where durability and longevity are crucial. These materials have the innate ability to repair damage, such as cracks or fractures, through dynamic bond exchange processes. This property ensures the longevity and robustness of DCAN-based products, reducing maintenance and replacement costs.

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## **Fabrication and characterization of Cellulose-Acetate based polymeric films**

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### **Abstract**

The growing demand for efficient and sustainable gas separation technologies has led to a surge in research focused on the development of advanced materials for selective gas separation processes. Thus, the present study deals with the development of cellulose acetate (CA) polymeric films with different concentrations (2-15 wt%). The film was developed through a combination of solution casting and phase inversion techniques by optimizing its parameters, such as polymer concentration, to achieve the desired base film for the initial study. Different physical, mechanical, morphological, and biodegradability analyses have been performed for its characterization. From the tensile test, it was seen that 10 wt% CA achieves the highest tensile strength and elongation at break among different developed films. The SEM analysis also revealed fewer surface defects on the developed 10 wt% CA film. The barrier and bio-degradation analyses confirm that the film developed with 10 wt% CA concentration shows less water vapor permeability and maximum degradation. The results were validated with previous literature for a better understanding of our present study. Water vapour permeability, tensile strength and bio-degradability for best film were found to be  $5.6605 \times 10^{-5}$  g/m.h. Pa, 5.104 MPa and 31.65% (30 days) respectively. Thus, 10 wt% CA concentration shows a better film forming solution, which has the potential for the development of polymer nanocomposite membranes when incorporated with different nanofillers.

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## High-performance epoxy vitrimers based on Schiff base chemistry

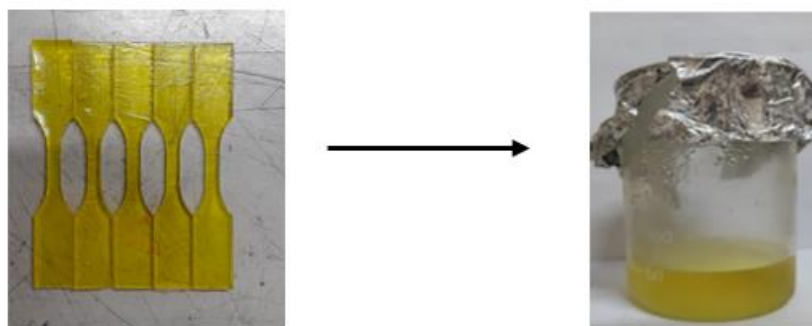
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### Abstract

The usage of fiber-reinforced plastic materials has increased tremendously, which has led to a huge increase in the creation of end-of-life waste materials, which are discarded mostly in landfills or incinerated. Growing sustainability challenges have urged researchers as well as technology developers to come up with sustainable solutions. One of the biggest challenges is the lack of recyclability of thermoset polymers, which contribute a large extent to plastic pollution worldwide. Vitrimers, proposed in 2011 by Leibler *et al.*,<sup>1</sup> bridge this gap. has been promising research development in a new class of dynamic polymers incorporating labile covalent bonds, which have the unique ability to activate the embedded dynamic chemistries upon external stimuli enabling the material to transition from solid to fluid-like flow. There is a vast array of organic molecules and chemistry at the disposal of the synthetic polymeric chemist to design tailor-made thermoset materials incorporating the dynamic CANs, thereby making them recyclable for a more sustainable economy.<sup>2</sup> In this work, the diamine curing agent monomer with a Schiff base structure was prepared and carbon fiber composites were prepared using the vacuum-assisted resin transfer molding (VARTM) method. The chemical structure was characterized using FT-IR and NMR techniques. The curing temperature of the commercial epoxy resin (DGEBA) with vitrimer hardener was determined from DSC studies. The cured epoxy thermoset showed high  $T_g$  ( $>120^\circ\text{C}$ ), Tensile strength ( $>50$  MPa), Young's modulus ( $>2$  GPa), and good thermal stability ( $T_i = 333^\circ\text{C}$ ). This thermoset exhibited typical vitrimer behavior by complete dissolution in acetic acid after 12 hr at  $50^\circ\text{C}$ , owing to the reversibility of imine linkages, making it a viable replacement for conventional thermosets in carbon fiber recycling.



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## Synthesis & characterization of an amphiphilic block copolymer derived from amino acid-based monomer using a xanthate RAFT, and its Impact on cell viability and cytotoxicity

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### Abstract

The development of amino acid-based polymers was due to their unique properties and structures like of biocompatible polymers having sensitive effects for numerous medicinal and biological actions like biochemical sensing and controlled release of drugs. To achieve this, poly (N-vinylpyrrolidone) (PNVP) and its block copolymer poly (N-vinylpyrrolidone)-b-poly (N-acryloyl-L-phenylalanine) (PNVP-b-PNALP) were synthesized by using a xanthate i.e., ethyl 2-((isopropoxycarbonothioyl)thio)-2-methylpropanoate (IPX), which exhibits good control RAFT polymerization. The plot between molar mass and conversion yields a linear line which confirms the pseudo-first-order kinetics, and molar mass distribution ( $\bar{M}_w/\bar{M}_n$ ) was found between (1.50–1.24). Both polymers were characterized by <sup>1</sup>HNMR, FTIR, DSC, TGA-DTA, GPC, and XRD analysis. TEM and DLS study of the aqueous solution of the block copolymer (PNVP-b-PNALP) exhibited self-assembly (119–160 nm with a few smaller particles of 91 nm). Different concentrations of polymers (200–0.75  $\mu$ M) were evaluated for their toxicities on macrophages (RAW 264.7) and cancer (MCF7) cell lines. The polymers were found to be nontoxic as we did not observe any significant changes in the rate of proliferation of both cells even at higher concentrations (up to 100  $\mu$ M). However, the polymers were found to induce apoptosis-like changes in the cancer cells up to 100  $\mu$ M, albeit not significant.

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## Development and Evaluation of Carboxymethyl Tamarind Kernel Gum-based pH-responsive Hydrogel for Release of Diclofenac Sodium

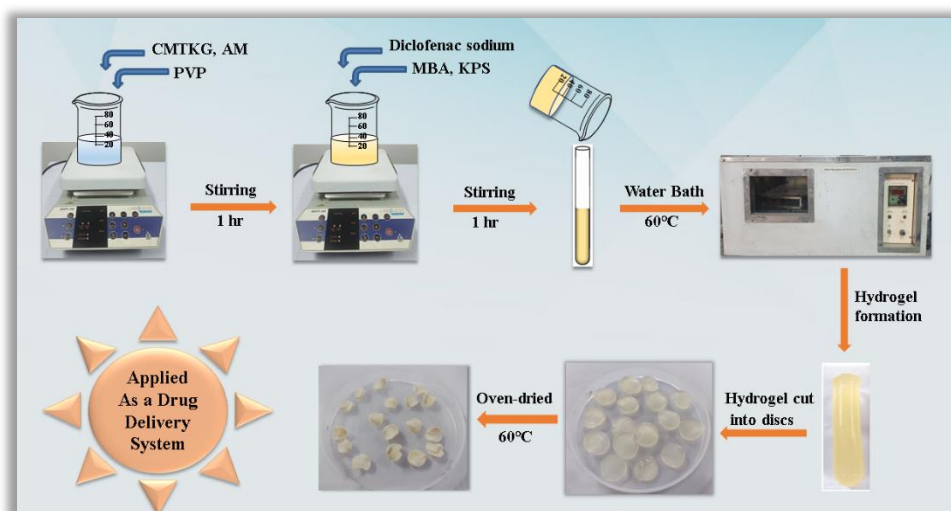
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### Abstract

The current research work focuses on the fabrication of biopolymer- based hydrogel and its loading was done with diclofenac sodium drug (DS) to obtain smart pH-responsive hydrogels. The synthesized hydrogels were characterized using Scanning Electron Microscopy (SEM), Powder X-ray Diffraction (PXRD), Thermogravimetry Analysis (TGA), and Attenuated Total Reflection-Fourier Transform Infrared spectroscopy (ATR-FTIR). ATR-FTIR confirms the successful formation of hydrogels, while PXRD and SEM indicate the amorphous and porous nature of the polymeric network. The TGA results indicate higher thermal stability for DS-loaded hydrogel than unloaded hydrogel. The swelling ratio as well as the release of DS were found to be higher under slightly alkaline conditions. The result of drug loading and release indicates that PVP increases drug loading(%) and release(%).The synthesized DS-loaded CMTKG/PVP/PAM hydrogels could be a promising substitute for prolonged delivery of sparingly soluble DS in pH 7.4.



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## Poly(disulfide)s by a Three Component Cascade Reaction Involving $\alpha$ -Lipoic Acid, Thiolactone and Amine: A Therapeutic Architecture for Stable Encapsulation and Controlled Release of Anticancer Drugs

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### Abstract

The utilization of nanoassemblies integrated with disulfide linker as drug delivery vehicles is attracting significant interest, attributed to their sensitivity towards the inherent redox gradients in biological systems.<sup>1</sup> Developing a comprehensive understanding of the variables influencing drug loading capacity, encapsulation stability, as well as proper control of cargo release kinetics holds tremendous promise for the advancement of redox-responsive materials for chemotherapeutic applications. Here, we reported a biocompatible, biodegradable, amphiphilic poly(disulfide)s using cascade polymerisation approach, wherein initiator thiolactone ring was activated by a primary amine, facilitating a nucleophilic ring-opening disulfide exchange polymerization (RODEP) of 1,2 dithiolane derivative under basic conditions.<sup>2</sup> In an aqueous environment, this amphiphilic polymer forms micellar nanostructure as examined by DLS and TEM experiment and exhibits excellent guest encapsulation stability, as demonstrated by the FRET experiment. The *in vitro* guest release experiment in presence of glutathione (GSH) has been investigated because the cancer cell (mM range) has higher concentration of GSH compared to the normal cells ( $\mu$ M range). The results revealed about 35% of guest release in 58 h of incubation in presence of 10  $\mu$ M of GSH, whereas about 84% release in the presence of 10 mM GSH under optimum micelle concentration of 0.3mg/ml. Examining the biological aspects of the doxorubicin (DOX) loaded nanocarrier unveiled a selective cellular uptake and cytotoxicity in cancer cells, facilitated by the modulation of surface charge that responds to the specific environment. In brief, this present work meticulously demonstrates a novel avenue to create amphiphilic nanocarrier using RODEP in one pot. The redox responsive polymeric nanocarrier can be used for tumor-targeted anticancer drug delivery due to their good biocompatibility, superior drug loading, high extracellular stability, and GSH induced intracellular drug release in a controlled fashion, which might have potential clinical utility in the field of chemotherapeutic applications.

The Synthesis, characterization, self-assembly, drug encapsulation, redox triggered drug release and biological evaluation will be the topic of this poster presentation.

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## Chiral and Achiral Modification to Tune the Helicity of Short-Peptide-Based Supramolecular Assemblies

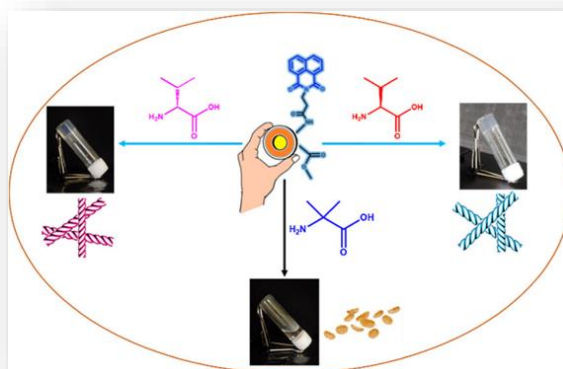
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### Abstract

Helical supramolecular architectures play important structural and functional roles in biological systems. However, the tuning of supramolecular helicity is very complicated and quite tricky. In this work, we developed two different strategies to tune the helicity of naphthalimide-capped peptide-based gel nanofibers. These are a) the alteration of the methylene unit present in the achiral amino acid<sup>1</sup> that is directly attached to the NMI group and b) changing the chiral part of the tail-ender amino acid in all possible ways<sup>2</sup>. The inversion of supramolecular helicity has been extensively studied by CD spectroscopy and morphological analysis. The density functional theory (DFT) study indicates that methylene spacers influence the orientation of  $\pi$ - $\pi$  stacking interactions of naphthalimide units in the self-assembled structure that regulates the helicity. This work illustrates a new approach to tuning the supramolecular chirality of self-assembled biomaterials.



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# Synthesis of PIL-OH Mediated Deacetylated Chitin and its Hydrogels: A Study on their Applications in Controlled Release of Paracetamol/Urea and dye entrapment

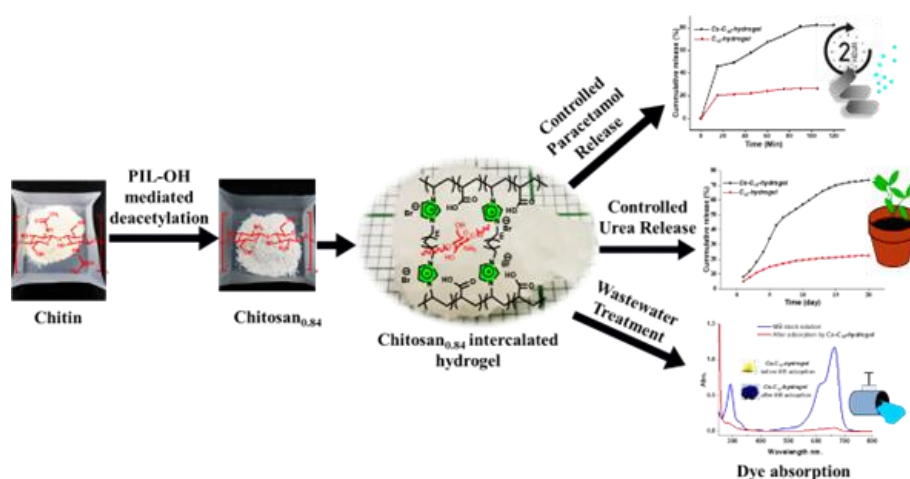
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## Abstract

Biopolymers are extensively used for preparing biocompatible and biodegradable materials. Chitin is the 2<sup>nd</sup> most abundant biopolymer, making it the best fit for many applications. However, the solubility of chitin was the main restriction in its application.<sup>1,2</sup> In this work, deacetylation of chitin is carried out with alkaline polyelectrolyte poly(DADMA-OH) that gave a higher amount of water-soluble chitin (with 84 % of the degree of deacetylation = chitosan<sub>0.84</sub>) compared to deacetylation using NaOH. The water-soluble chitosan<sub>0.84</sub> is used as intercalating chains for the preparation of acrylic acid and vinyl imidazole based hydrogels. 1,ω-Dibromoalkanes were used for the quaternization of imidazole groups to trigger the crosslinking in the above polymer network. A set of six hydrogels (three chitosan intercalated and three non-intercalated) were prepared and well characterized by IR, FESEM, EDX, TGA etc. As crosslinker chain length increases, hydrogel swelling ratio increases steadily. Chitosan<sub>0.84</sub> intercalated 1,10-dibromo decane crosslinked hydrogel showed excellent swelling (2330% swelling ratio) among six synthesized hydrogels. The multi-functionality of these hydrogels was explored towards -the controlled release of paracetamol, urea, and -waste-water treatment (dye absorption). These studies reveal that intercalation of water-soluble chitosan<sub>0.84</sub> in the hydrogels induces better swelling behaviour, paracetamol/urea loading, paracetamol/urea release and dye entrapment from water than that of their non-intercalated hydrogels.



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## Amphiphilic Fluorescent Well-Defined Living Polymer from Indole-3-Carboxaldehyde and 4-Bromo-1, 8-Naphthalic Anhydride: Synthesis and Characterization

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### Abstract

A well-defined amphiphilic fluorescent polymer bearing indole repeating units with naphthalimide pendants obtained by ATRP followed by chemical modification. The obtained polymer poly (N-allyl indole-2-(4-hydroxybutyl)-1, 8-naphthalimide) (PAIHN) was characterized by <sup>1</sup>H NMR, FTIR, and GPC. The polymer showed a specific fluorescence emission maximum at 538 nm excited at 435 nm in aqueous solution. The amphiphilic nature of the polymer was investigated in aqueous solution using two spectroscopic methods, namely, absorption and emission spectroscopy. The Critical Micellar Concentration values obtained by UV-visible and fluorescence are in good agreement with each other. The micelles were characterized by TEM at concentration of 0.014 mg/mL. The polymer PAIHN prepared after tweaking exhibits green fluorescence at 538 nm due to the significant effect of naphthalimide moieties, whereas before tweaking the polymer poly (1-allyl indole-3-carbaldehyde) (PAIC) exhibits blue fluorescence at 425 nm due to indole repeating units of the polymer.

## Tuning of Frontier Orbital Energy Levels of Fluorene Based Conjugated Porous Organic Polymer Through Introducing Electron Deficient Group for Improving Organic Photocatalysis

Raj Laxmi, Biplab K Kuila

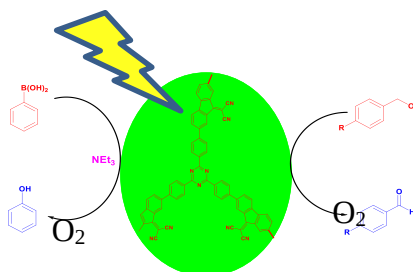
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### Abstract

Conjugated porous organic polymers (CPOPs) are multifunctional materials that combine high surface areas with extended conjugation and porosity, making them ideal for applications like degradation, catalysis, and gas adsorption separation.<sup>1-2</sup> Recently, photo-catalytic organic synthesis has drawn tremendous research attention due to its favorable environmental benefits, simple setup, and mild reaction conditions.<sup>3</sup>

Here, we have demonstrated a novel strategy to boost organic photocatalytic activity, by engineering donor ability based on triazine based CPOP through design of fluorene-based building blocks with electron deficient group precisely positioned in the structures. Both theoretical calculations and experimental studies revealed that the CPOPs that contains fluorene moiety with CN group at 9<sup>th</sup> position exhibited the best performance [TOF (mmol g<sup>-1</sup>h<sup>-1</sup>) = 13.33 and 10.9 in 3Watt blue and white light respectively] compared to others and also much higher than the state of art photocatalysts. The high performance can be attributed to the lower band gap, suitable positioning of the HOMO/LUMO energy levels, enhanced charge transfer efficiency, and low recombination rate of electrons and holes in CPOP3. The current work contributes a fundamental insight into the structure-property relationship for photocatalysis applications of CPOP and gives guidelines for the design of efficient photocatalysts for organic reaction by small structural modification of single monomeric unit of the polymer.



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## Design of a self-cleanable multilevel anticounterfeiting interface through covalent chemical modulation

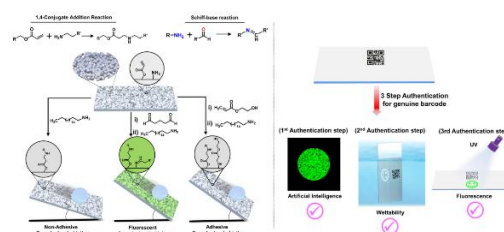
Manideepa Dhar and Uttam Manna\*<sup>1</sup>

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### Abstract

Counterfeit products have posed a significant threat to consumers' safety and the global economy.<sup>1</sup> Previous approaches used substrate structures, surface tags, embedded tags, and patterned interfaces to combat the growing challenges associated with counterfeiting.<sup>2-4</sup> Here we report a novel class of chemically functionalizable coatings with a combination of a physically unclonable porous topography and distinct physiochemical properties (e.g., fluorescence, water wettability, and water adhesion) obtained through orthogonal chemical modifications (i.e., 1,4- conjugate addition reaction and Schiff-base reaction at ambient conditions), as shown in Scheme 1.<sup>5</sup> The inherent porous topography of the prepared polymeric coating gives rise to unclonable features that can be decrypted using microscopy imaging-based machine learning. On the other hand, the reactive moieties in the coating, i.e., amine and acrylate, play an important role in determining the amount of air trapped in the coating, which confers both water-repellence and the condition-dependent appearance of patterns, such as being invisible in the air, but visible underwater. Moreover, the spatially selective postmodulation of the above coating through the formation of imine bonds embeds fluorescence that can be read out upon UV illumination. Overall, this novel class of anticounterfeiting interfaces can be decoded through multilevel authentication routes: besides the machine learning-based decryption of the random surface topography, the readout can occur through visual inspection during the exposure of the patterned interface to an aqueous phase or UV light.



**Scheme 1:** Design of multilevel anticounterfeiting interface based on chemically functionalizable porous polymeric coating

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## Surface modification of carbon dots via peptide covalent conjugation

**Niladri Hazra, Soumyajit Hazra, Subir Paul and Arindam Banerjee**

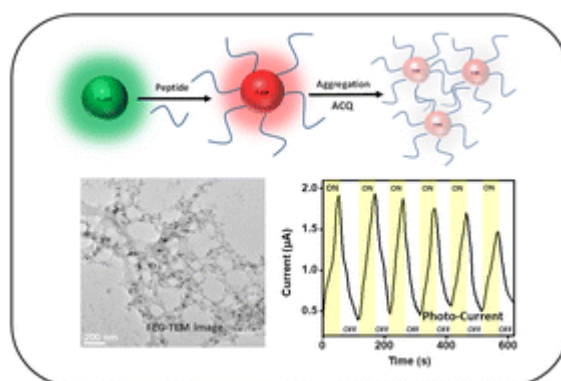
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### Abstract

Surface modification of carbon dots via covalent conjugation with a dipeptide resulted in a dramatic change in the fluorescence emission from green to red. The hydrophobic peptide units linked to the surface of the modified carbon dots helped them to aggregate by generating a nanodot-fabricated nanofibrous network. This nanofibrous network showed excellent electrical conductivity and photo-switching behavior, better than those of the non-aggregated dots.



Chem. Commun., 2023,59, 4931-4934



## Conversion of Waste PET into Bis(2-hydroxyethyl)terephthalate for the Synthesis of Value-added Co-polycarbonate via Melt Depolymerization Reaction using Recoverable Yttrium Oxide as a Catalyst

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### Abstract

Conversion of waste plastic into value-added chemicals or monomers is an innovative idea to address the problems associate with pollution waste management system. Polycarbonate is a class of polymers known for their diverse properties, including high strength, optical clarity, and resistance to heat and chemicals. In this study, we have investigated the depolymerization reaction of PET into Bis(2-Hydroxyethyl) terephthalate (BHET) monomer using yttrium oxide as a catalyst. Yttrium oxide is an effective and stable catalysts, which could be breaking down the polymer chains into its constituent monomers. Almost 100% of PET has been converted into BHET under atmospheric pressure and 190°C conditions for 180 minutes. The obtained BHET was used as a monomer for the synthesis of homo and co-polycarbonates with triphosgene and bisphenol- A. The structure of the homo and co-polycarbonates was confirmed by FTIR, NMR and XRD analysis and the thermal properties were investigated using Tg-DSC and TG analysis. The results of the Tg-DSC and TGA shows that the Tg and decomposition temperature of copolycarbonates has been improved than that of homopolymers. This research contributes to the growing body of knowledge of plastic waste management and the development of novel strategies for reducing environmental impact.

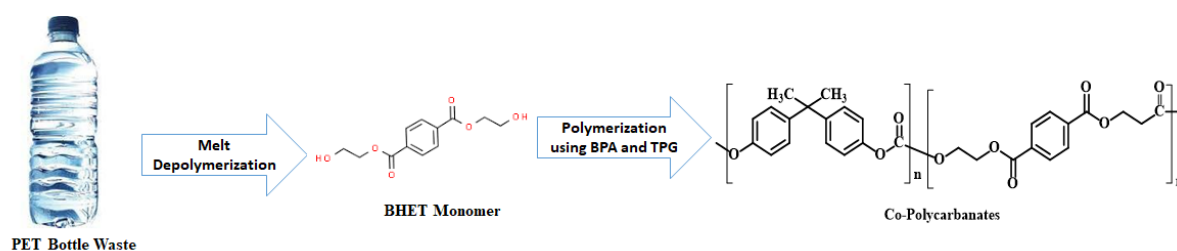


Fig.1. Melt depolymerization of PET followed by synthesis of value added co-polycarbonate

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**The exploitation of ionic and H-bonding interactions simultaneously for intrinsic quick self-healing at ambient conditions in poly(ionic liquids) consisting of imidazolium and sulphonium groups**

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**Abstract**

Poly(ionic liquid) based Self-healable electrolytes are getting tremendous attention owing to their quick self-healing ability at ambient conditions without external stimulus, prominent safety, high mechanical strength, appreciably good conductivity, and no electrolyte leakage. Ionic interactions are much stronger and more dynamic, capable of imparting faster healing ability to the electrolyte. To exploit ionic interactions and non-covalent hydrogen bonding simultaneously for faster self-healing at ambient conditions, Herein, we synthesized cationic and anionic Poly (ionic liquids). We blended them to form self-healable ionic polymer electrolytes (ShIPEs). The synthesized novel ionic polymer electrolytes exhibit appreciably good ionic conductivity with a maximum value of  $2.04 \times 10^{-5} \text{ Scm}^{-1}$  at 30 °C which reaches  $11.48 \times 10^{-5} \text{ Scm}^{-1}$  at 80 °C and these polyelectrolytes were characterized by <sup>1</sup>H, <sup>13</sup>C NMR, FTIR, DOSEY, GPC, TGA, DSC, etc. Interestingly, Poly (ionic liquid) based polyelectrolytes can heal only in 15 min at room temperature and 5 min at 60 °C. The designed Poly (ionic liquids) presents a new perspective to develop innovative and quickly self-healable polyelectrolytes for advanced electrochemical devices.

# Tetraphenyl-1,3-butadiene as AIE based building blocks, tethered with thiazolothiazole linker to construct different linear and branched polymers having excellent solid-state emissive property

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## Abstract

Polymers exhibiting efficient photoluminescence particularly in solid-state, have immense potential in the field of high-performance solid-state lighting applications.<sup>1</sup> Although numerous polymers are reported in the literature with strong photoluminescence quantum yield (PLQY) in the solution state, their efficiency drastically dropped when compared to the same in solid-state mainly due to profound aggregation effect. Incorporating AIEgens as the building blocks have emerged as one of the successful ways to construct polymers with good PLQY in solid-state where the AIE nature of the individual monomers is believed to transfer to the overall polymer backbone.<sup>2</sup> Of late, along with linear conjugated polymers, hyperbranched polymers and porous organic polymers (POP) having a three-dimensional orientation of the monomers are also achieved enough attention of the scientific world mostly because of their structural diversity, porosity and improved PLQY compared to the monomer or corresponding linear chain polymers.<sup>3</sup>

In this study, tetraphenyl-1,3-butadiene (TPB) one of the recently explored AIEgens<sup>4</sup> are utilized to construct series of linear chain polymers and a branched polymer. Initially, different -CHO derivatives of TPB moiety have been synthesized. Further these monomers are reacted with rubeanic acid where the -CHO group of the two adjacent monomers are converted to a thiazolothiazole ring which acts as a linker to construct the desired polymers. All the polymers are further characterized and their detailed photophysical studies revealed excellent PLQY in solution as well as in solid thin films. Successful synthesis of these solid-state emissive polymers creates an opportunity for us to explore their application as solid-state lighting devices.



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## $\beta$ -Amino-ester Linkage Assisted Design of Substrate, Process and Liquid-Independent Solid Slippery Coating

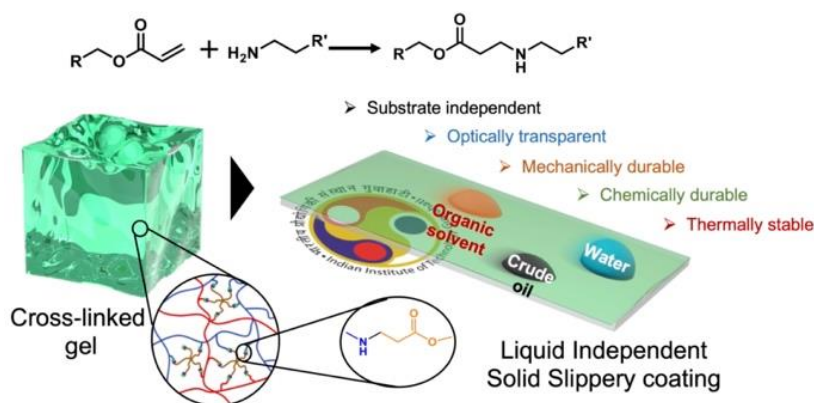
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### Abstract

The design of solid and smooth interface having ability for self-cleaning various types of liquid spills including water, polar/non-polar organic solvents, refined/crude oils and deposited solid particulates is essential to achieve energy-efficient and environment-friendly maintenance of various commercially relevant objects including solar devices<sup>1</sup>, window panels of buildings, etc. In this current approach, we have unprecedentedly demonstrated the ability of a covalent cross-linking chemistry in precisely modulating both essential surface free-energy and roughness of a solid interface for achieving liquid, substrate and process independent robust slippery property. The strategic choice of  $\beta$ -Amino-ester linkage through 1,4-conjugated addition reaction<sup>2</sup> between amine and acrylate groups of a three component (dominated with content (61 % (w/w)) of crosslinker) reaction mixture at ambient condition provided a facile basis for associating various important and relevant properties—including liquid self-cleaning ability<sup>3</sup>, anti-smudge property (against both water and oil-based inks), thermal stability (>300 °C), chemical stability, physical durability and optical transparency (~95 %) and so on. Thus, the prepared coating would be appropriate to maintain the unperturbed performance of commercially available solar cell modules and other relevant objects at outdoor conditions.



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## Functional Polymers based on Dynamic Boronic Ester Network

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### Abstract

Polymers containing dynamic cross-linking or networks are interesting class of smart materials that have the property of reusability and reprocessability owing to reversible nature of their networks. Boronic ester networks are such class of dynamic covalent networks formed as a result of condensation reaction between cis and trans 1,2 or 1,3 diols and boronic acid moieties and undergo facile bond exchange or reversibly due to transesterification and methathesis reaction. The resulting dynamic bonds shows exchange mechanism in response to water, pH, and temperature which results in the reformation of the chemical network once broken. Therefore, the (co)polymers bearing boronic ester linkages are useful for the preparation of multi stimuli-responsive and self-healable materials.

In our work, we have synthesized functional acrylate copolymers bearing pendant diol functionality and incorporated the boronic ester cross-linking through condensation of diol groups of the copolymers and boronic acid containing small functional molecules. The water responsive behavior of the resulting cross-linked copolymers were studied which showed dynamic bond exchange in presence of moisture as indicated by optical microscopy. It showed self-healing efficiency of 62 % measured using tensile properties measurement in UTM.

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## A New Class of Smart Mechanophoric polymers

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### Abstract

Recently, there has been tremendous interest among the materials community to prepare new functional smart materials, because of their wide range of specialty applications. Mechanophoric polymers are an interesting class of smart polymers which contain a special force-sensitive molecular motif that can lead to a chemical change within the polymer network in response to external stimuli<sup>1</sup>. In the literature, different types of mechano-responsive polymers are reported across multiple polymer systems having different mechanophoric moieties. Among different mechanophores, Spiropyran<sup>2</sup> has been widely used, but the synthetic procedure of this motif is multistep, complex, time-consuming process. There are tremendous efforts to introduce an easy and facile way to fabricate mechanoresponsive polymer with new mechanophoric motif. In reference to conquest of different smart polymers in my research group<sup>3,4</sup>, herein we report smart mechanophoric polymers by introducing different mechanophoric motifs based on Rhodamine as well as Coumarin. In this case, Rhodamine was suitably modified to prepare a tetra-functional core, and then it was used to polymerize acrylic monomers. The film of the resultant polymers exhibited excellent mechanophoric property under UV and stretching conditions. We have also prepared smart styrenic copolymers based on coumarin-based mechanophore. In this case, coumarin derivative was grafted to a tailor-made styrenic copolymer prepared via RAFT polymerization. The synthesized coumarin-based smart polymers showed excellent mechanoresponsive properties both under UV and ultrasonication. All the intermediate products were experimentally quantified via FT-IR and <sup>1</sup>HNMR analyses. The mechanophoric behavior and fluorescence switch-off and switch-on properties of these synthesized mechanophoric polymers were analyzed using a fluorescence spectrophotometer and XPS analysis.

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## Solvent Geometry Regulated J- and H-Type Aggregates of Azobenzene Based Organogelator: Phase-Selective Thixotropic Gelation and Oil Spill Recovery

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### Abstract

This article demonstrates the H-bonding mediated supramolecular polymerization and formation of 1D nanofiber of azobenzene based organogelator (AZO-4) in aromatic and aliphatic cyclic hydrocarbon solvents (toluene and methylcyclohexane). The AZO-4 molecule exhibits strong J- and weak H-type of aggregates in toluene and MCH respectively. The type of aggregate was governed by the geometry of the solvents used in the self-assembly process.<sup>1</sup> The J-type aggregates with high thermal stability in aromatic hydrocarbon, toluene is due to the enhanced interaction of AZO-4  $\pi$ - surface with the toluene  $\pi$ -surface, whereas H-aggregate with moderate thermal stability in MCH was due to the interruption of the cyclic hydrocarbon in van der Waals interactions of peripheral alkyl chains of AZO-4 molecule. The light induced reversible photoisomerization is observed for both J- and H-aggregates.<sup>2</sup> In the evaluation of macroscopic property, spontaneous and strong gelation was noticed in toluene preferably due to the strong interactions of the AZO-4 nanofibers with the toluene solvent molecules compared to the MCH. The viscoelastic property was quantified by the rheological measurements, which also established the thixotropic nature of the gels by step-strain experiments at room temperature. The thermodynamic parameter ( $\Delta H_m$ ) of gel-to-sol transition was determined for all the gels to get more insight into the gelation property. Furthermore, the phase selective gelation property was extended to the oil spill recovery application<sup>3</sup> using diesel/water and petrol/water mixture.

Synthesis, characterization, self-assembly, phase selective gelation property and oil spill recovery application of AZO-4 will be the topic of this poster presentation.

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## Development of cellulose-CNT-PVA intelligent films by incorporating anthocyanins of banana bract and their applicability as freshness sensors for fish during storage

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### Abstract

The smart packaging can provide real time quality of food for the consumers. This will avoid the food wastage and unnecessary transportation and storage. We have developed cellulose (CELL) reinforced pH sensitive films for food packaging applications by incorporating anthocyanin pigment extracted from banana bract (BBE) along with cellulose and carbon nanotube (CNT) into PVA films. In this work, the influence of BBE and the combination of nanocellulose and CNT on the structural properties of PVA films have been studied. The cellulose was crosslinked by epichlorohydrin and glycerol was used as a plasticizer. The mechanical properties, moisture resistance and UV-Vis screening properties of the modified PVA films have been studied. The structural characterization was carried out by XRD, FTIR and TGA. The PVA/CNT/CELL and PV/CNT/CELL/BBE exhibited higher barrier properties against water vapour and lower water solubility as compared to the pristine PVA films. The FESEM analysis indicated closely packed CELL on the PVA surface and dispersion of CNT on the surface. The anthocyanin added films exhibited significant antioxidant and UV shielding properties [1]. The transparency of the film decreased on addition of BBE. The fabricated films exhibited visually perceptible colour changes in the pH range between 1 and 12. These films were evaluated as intelligent pH indicators for monitoring the freshness of seafood samples. During the storage of fish food samples for 48h, the color of the film changed from light pink to green which is a clear indication of spoilage of food material.

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## Diketopyrrolopyrrole anchored A-alt-B type based metallopolymer as fluorescent probe for the selective recognition of amino acids.

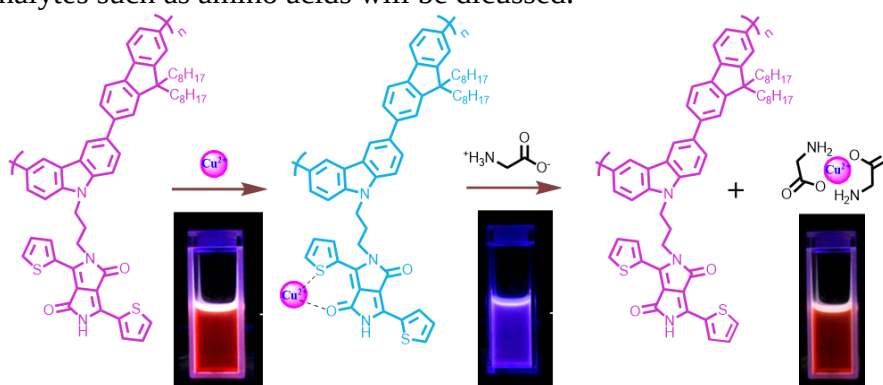
Chinmoy Kumar Behera,<sup>a</sup> Dipanjan Giri,<sup>a</sup> and Sanjib K. Patra<sup>a\*</sup>

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### Abstract

Emissive  $\pi$ -conjugated polymers are promising sensory materials for environmental and biological relevant species with advantageous property of *molecular wire* effect.<sup>1</sup> Our group is involved to develop  $\pi$ -conjugated polymer based probed for detection of environmentally and biologically relevant analytes.<sup>2,3</sup> In this work, a highly emissive and soluble poly(carbazole-*alt*-fluorene) (**P1**) based  $\pi$ -conjugated alternative copolymers with thiophene-diketopyrrolopyrrole as pendent unit have been designed and synthesized via Pd(0)-catalyzed Suzuki polymerization from the corresponding monomers 3,6-dibromo-9H-carbazol-3,6-di(thiophen-2-yl)pyrrolo[3,4-c]pyrrole and 2,7-bis-oxaborolan-9,9-dioctylfluorene. The well-defined copolymer **P1** has been characterized by multinuclear NMR spectra and the tetradetector GPC studies showing molecular weight ( $M_n$ ) of 15.6 kg/mol with the polydispersity indices of 1.38. The red emissive polymer has been explored for the detection of amino acids based on a secondary “turn-on” sensing approach. The thiophene-diketopyrrolopyrrole anchored carbazole-*alt*-fluorene based polymer shows high selectivity towards  $\text{Cu}^{2+}$  metal ions by varying the emission wavelength from strong red to blue due to the formation of the Cu(II)-coordinated polymers (**P1-Cu<sup>2+</sup>**). Most importantly and interestingly, the resulting metallopolymer, **P1-Cu<sup>2+</sup>** exhibits high sensitivity and selectivity towards amino acids specifically glycine with the detection limit of 90 ppb ( $\sim 1.21 \times 10^{-6}$  mol/L) along with relatively high association constants of  $1.83 \times 10^5 \text{ M}^{-1}$  over the other representative anions.<sup>4</sup> To unravel the sensing mechanism relying on photo-induced electron transfer (PET), we conducted comprehensive photophysical studies involving both the **P1** and its representative monomer, **M1**. Furthermore, fluorescence anisotropy studies were performed to investigate the molecular interactions between **P1-Cu<sup>2+</sup>** metallopolymer and amino acids. Our attempt on design and synthesis of  $\pi$ -conjugated polymers for detection of biological analytes such as amino acids will be discussed.



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## Design and Synthesis of Perylene Diimide (PDI) Based Donor-Acceptor (D-A) Type Polymers with Low Energy Band Gap Efficient for Energy Storage Application

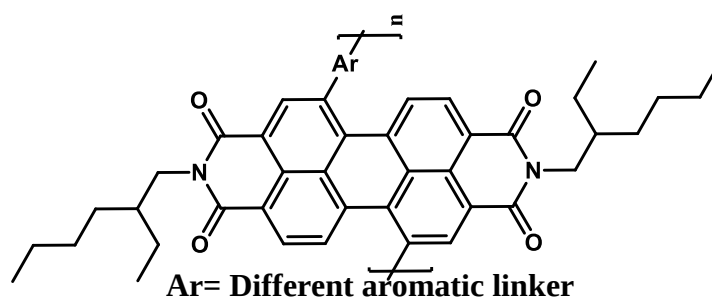
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### Abstract

Perylene diimide (PDI) based derivatives are widely used as a n-type semiconductive materials in optoelectronic and photovoltaic energy field because of following aspect such as high thermal and photochemical stability, excellent molar extinction co-efficient, good redox properties and bandgap tunability by substitution at 'bay' and 'ortho' positions of PDI<sup>1,2</sup>. Here in, we have designed and synthesized four PDI based polymers with different aromatic linkers at the bay position with increasing donor capability. All the four polymers were characterised by MALDI-TOF spectrometry and FT-IR spectroscopy. Study of thermal property using differential scanning calorimeters (DSC) and thermogravimetric analysis (TGA) revealed good thermally stability in each case. Furthermore, their optical properties were studied by UV-Vis absorption, photoluminescence (PL) spectroscopy and time dependent PL study using time-correlated single photon counting (TCSPC) method. Sharp peaks in the low angle region in the powder X-ray diffraction (PXRD) data indicates presence of crystalline nature in all the four polymers. To calculate the HOMO and LUMO energies, Cyclic voltammetry (CV) was performed. Calculated low band gap values of the synthesised polymers give us an opportunity to explore them as semiconductive materials in enegy storage application.



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## Photoreforming of Polystyrene Segmented Glycopolymer Architectures for Green Hydrogen Generation

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### Abstract

Sustainable H<sub>2</sub> generation from biomass photoreforming utilizing solar energy is promising way of green and cost-effective processes. Herein, mono-, bi- and tetra-functional photoiniferters were utilized in the RAFT polymerization process to design the block copolymer architecture using styrene and acetylated glucosemethacrylate monomer. The resulting polymers' weight average molecular weight, determined through SEC studies, ranged from 6763 to 22098 g/mol with 1.14-1.57 polydispersity (Đ). Deacetylated polymers' calculated molecular weights via <sup>1</sup>H-NMR spectra ranged from 4473 to 17059. Acetylated polymer architectures exhibited higher thermal stability compared to deacetylated polymers. Deacetylated polymers showed higher T<sub>g</sub> values than the acetylated polymers. In addition, a wide range of T<sub>g</sub> values (54-81 °C) and variations in the T<sub>m</sub> values of the acetylated polymers indicate the dependence on the nature of the pendent unit and macromolecular architecture. This work presents a mechanistic investigation of a series of polystyrene-based deacetylated macromolecular architectures over graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) and Pt/g-C<sub>3</sub>N<sub>4</sub> photocatalysts for hydrogen evolution reaction (HER) under visible light. The deacetylated macromolecule, LIN-PS-*b*-dPGM diblock copolymer exhibited higher HER (~753 μmol g<sup>-1</sup> h<sup>-1</sup>; ~1.84% quantum efficiency) than the polystyrene (53 μmol g<sup>-1</sup> h<sup>-1</sup>). This research unveils the significant influence of the glycopolymer segmented architectures, which adversely affects the efficacy of the HER process. This is attributed to the architecture of a polystyrene-segmented saccharide-based glycopolymer's prevalent surface coverage on g-C<sub>3</sub>N<sub>4</sub> and subsequently, photoreforming within the polymer architecture impacting the g-C<sub>3</sub>N<sub>4</sub> performance in photocatalytic H<sub>2</sub> production.

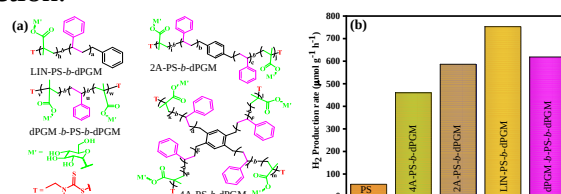


**Fig. 1.** (a) Chemical structures of the polystyrene-based glycopolymer architectures and (b) photocatalytic H<sub>2</sub> production using various polymer architectures.

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## RAFT-derived poly (vinyl alcohols) and its block copolymers

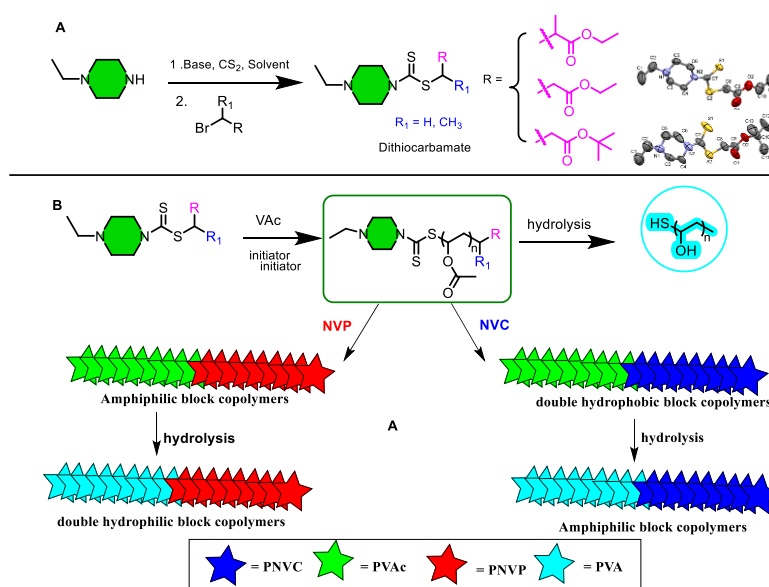
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### Abstract

Poly (vinyl alcohol) (PVA) is a widely used synthetic polymer derived from the hydrolysis of poly (vinyl acetate) (PVAc). A notable challenge in producing a well-defined high molar mass of PVA is the appearance of chain transfer reactions during the radical polymerization of PVAc. In this work, we present a novel approach to produce the controlled polymerization of vinyl acetate with a well-defined and linear structure using reversible addition-fragmentation chain transfer (RAFT) polymerization.<sup>[1,2]</sup> By employing this technique, we were able to significantly reduce chain transfer reactions. To achieve this a series of ethyl piperazine-based dithiocarbamate RAFT agents were prepared and utilized for the reversible deactivation radical polymerization of vinyl acetate (VAc), thereby achieving better control over the molecular weight distribution of PVAc. Some of the employed dithiocarbamate-based RAFT agents-02, 05 showed very good control over the polymerization of VAc with high molar mass and low dispersity. Here we report the synthesis of a variety of AB di-block copolymers, namely amphiphilic poly (VAc)-*b*-poly (NVP) and poly (VA)-*b*-poly (NVC), double hydrophobic poly (VAc)-*b*-poly (NVC); and double hydrophilic poly (VA)-*b*-poly (NVP).



Scheme 1. (A) Synthesis of ethyl piperazine based RAFT agents, (B). Homopolymerization of VAc by using dithiocarbamate RAFT Agents and its block copolymers.

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## Influence of Spacer Effect for Chirality Transformation during Helicity Induction in Chiral Polymers

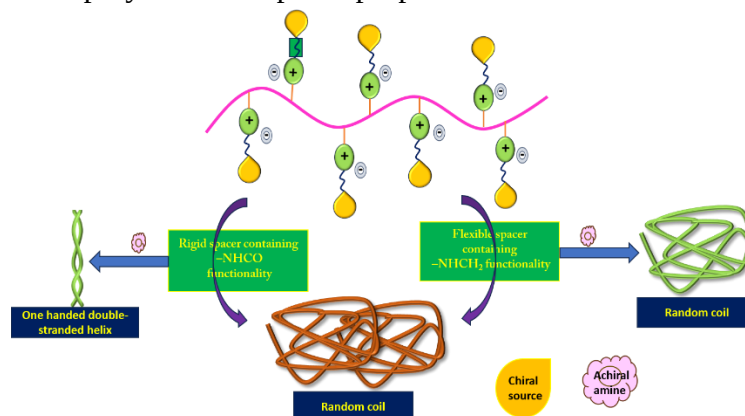
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### Abstract

Mimicking the self-arrangement helical properties from mother nature through synthetic organic polymers has been increasing significant interest due to its various potential applications in the chirality domain as well as to understanding the complicated bioarchitect functions at the molecular level.<sup>1</sup> Synthesis of helical polymers from chiral monomers is one of the interesting approaches as chiral pendants regulate the helical conformation.<sup>2</sup> Hence, here we have proposed newly designed chiral monomers and their corresponding chiral polymers via radical polymerization. The polymers exist as polyelectrolytes or poly(ionic liquids). Achiral amines act as helical inducer for inducing the helical chirality. Interestingly, it has been observed that the linker between chiral pendants to main chain highly influences the helical sense of the polymer.<sup>3,4</sup> In the present case, a rigid linker between the main chain and to stereogenic center showed a highly stable helical sense with one handed double-stranded helix, whereas the same polymers transfer completely to a random coil by changing the electronic rigid spacer to a flexible alkyl chain. There are significant remarkable changes also observed in the helical sense of polymer by increasing the length of the rigid chain, which are confirmed through CD absorption spectroscopy. In conclusion, here we have demonstrated the induction of helicity using external guest molecules in chiral polymers for a perfect helical sense. With these small structural changes in the spacer between the main chain to chiral pendants has a significant influence in polymers chiroptical properties.



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## Hybrid Network of Syndiotactic Polystyrene-Poly(3-octylthiophene-2,5-diyl); Spectral, Morphological, and Rheological Properties

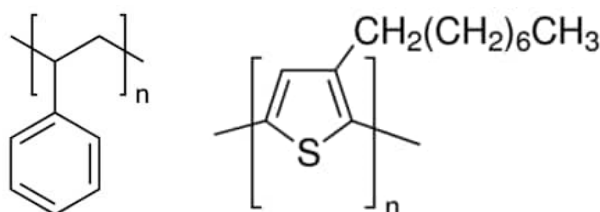
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### Abstract

This abstract contributes to the expanding knowledge of syndiotactic polystyrene-poly(3-octylthiophene-2,5-diyl) polymer hybrid network and their rheological behavior.<sup>1</sup> Comprehensive investigation of hybrid network composed of syndiotactic polystyrene (sPS) and poly(3-octylthiophene-2,5-diyl) (P3OT) is emphasizing their potential to enhance of material properties. By taking advantage of the fiber forming properties of both polymers in Anisole, sPS and P3OT are mixed at an elevated temperature to prepare a hybrid network. These sPS–P3OT networks have been intensively investigated by UV–Vis, AFM, and Rheology.<sup>2</sup> Absorption measurements indicate the occurrence of  $\pi$ – $\pi$  interaction between the P3OT chains and the sPS phenyl groups. The study delves into the intricate interplay between these distinct polymers, aiming to elucidate the impact of P3OT polymer fibre on the rheological behavior of the resulting hybrid network.<sup>3</sup> The objective of this research is to harness the synergistic effects between sPS and P3OT to tailor the rheological responses of the composite, unlocking avenues for versatile material design. The study employs a meticulous approach to composite formulation, focusing on achieving uniform dispersion of P3OT aggregates within the sPS matrix.<sup>4</sup> Furthermore, rheological assessments are conducted under varying shear strain and frequency to elucidate the composite's viscoelasticity, and shear thinning properties. The



anticipated outcomes encompass the revelation of novel rheological phenomena arising from the interaction between P3OT's polymer attributes and sPS's mechanical integrity.

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## Effect of Substituents of Naphthalene Diimide Derivatives On Electrochromic Behaviours Observed in Proto-type Devices

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### Abstract

Several triphenylamine (TPA) end capped to central naphthalenetetracarboxylic diimide based donor-acceptor-donor type electro-active monomers like TPA<sub>2</sub>NDI and TPA<sub>4</sub>NDI<sup>1</sup> were previously developed to explore the formation of electro-polymers and subsequent chromic effect of prepared films on the conductive surface. Our focus is shifted to evaluate the alterations in electrochromic properties by introducing diverse substituents (-Br, -CN, -Phenyl, Amino pyridine) into the central naphthalene moiety<sup>3</sup>. In three electrode configuration, reversible multiple colour changes from brown to deep blue by applying varying voltages (0 to 1.1 V) and also brown to deep pink<sup>fig 2</sup> with the voltage change from 0 to -2 V were investigated with relatively good response time, optical contrast, switching stability and coloration efficiency values. Polymer<sup>fig 1</sup> made of CNTPANDI can be switched up to 1200 cycles with the optimum coloration efficiency (560 cm<sup>2</sup>/C) in the anodic process and 300 cycles for the cathodic process in a three electrodes configuration. Proto type devices made of p-CNTPANDI demonstrated the electrochromism operated at a potential range of 0 to 2.2 V. Moreover, the device exhibited the EC memory in open-circuit condition with 50% retention of its coloured state until 27 min. The long EC memory as well as high coloration efficiency compared to other TPA based conjugated polymers<sup>2,4</sup> suggested the potentiality of this polymer film as a power-efficient EC material for modern display applications.

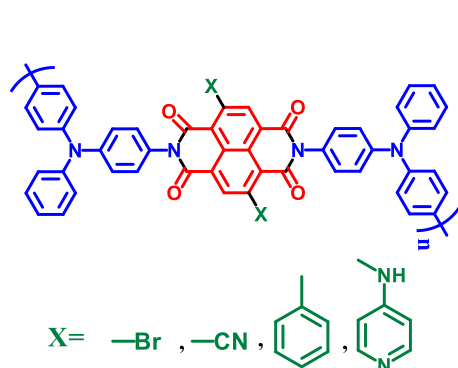


Fig 1: Structure of electropolymer

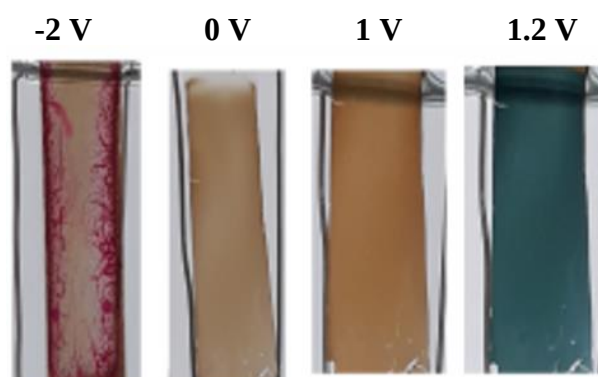


Fig 2: colour change of the p-CNTPANDI film with voltage

### References

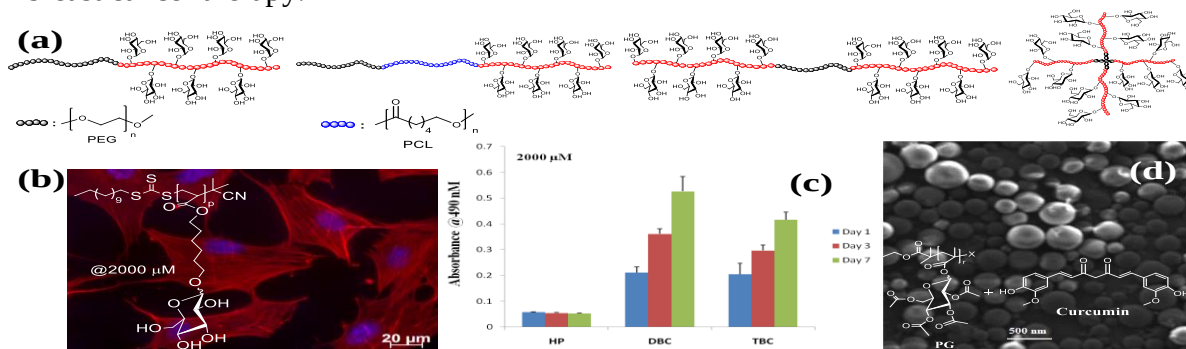
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## Glycopolymer Architectures for Improved Biocompatibility and Curcumin Delivery applications

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### Abstract

The adaptive versatility of tailored glycopolymers fostered by developments in precise and effective living radical polymerization techniques has broadened their scope for biological applications. We have reported the deacetylated RAFT synthesized glucose-based glycopolymer with 6-alkyl pendant spacer chain length at relatively higher concentration displays better biocompatibility on mouse osteoblast cells (MC3T3) than the 2- and 4-alkyl pendant spacers. Subsequently, upon the PEO/PEG functionalization of glucose-based glycopolymer synthesized *via* ATRP displayed reduced concentration-dependent variation in cell viability, improved the cell adhesion and biocompatibility with MC3T3 cells *in vitro* and can be pertinent as potential material for implant coatings. Further, the PEO-based di-block copolymer synthesized *via* RAFT displayed good osteoblast cell adhesion and viability response at moderate concentrations ( $\leq 100 \mu\text{M}$ ). Poly(methacryl-2,3,4,6-tetra-O-acetyl-D-manno-pyranoside) [PMAM], PEG-*b*-PMAM and PMAM-*b*-PEG-*b*-PMAM were employed to determine their biocompatibility with HBDCs leading to conclude that architecture, concentration and culture time are the limiting factors. Curcumin-loaded glycopolymer nanoparticles exhibited nano-dimensionality and uniform spherical morphology than their PEG-based di- and tri-block copolymer counterparts. Further, we present that the optimized formulation exhibited superior cytotoxicity, clonogenic inhibitory and cellular uptake potential in MCF-7 cell lines than the free curcumin, thereby improving curcumin's clinical manifestation in breast cancer therapy.



(a) Schematic representation of various glycopolymer architectures, (b) fluorescent microscopy images of actin stain osteoblast cells for assessing the expression of cytoskeleton protein with glycopolymers, (c) HBDCs proliferation with HP, DBC and TBC polymers and (d) SEM image of optimized curcumin loaded glycopolymer nanoparticles.

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## Synthesis & characterization of amino acid-based acrylamide derived amphiphilic block copolymer using a new xanthate and its influence on cell cytotoxicity & cell viability

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## Examination of Physiological Parameters of coated Strawberries by Deep Coating method with Chitosan and edible oil at ambient condition storage

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The objective of this study is to see how chitosan coating affects strawberries while stored at ambient conditions (18-22 degrees Celsius and 60-70% relative humidity) using cinnamon and coconut oil as functional components. Strawberries were coated with chitosan as a biopolymer(Matrix) containing essential oil, glycerol, and Tween-80 as functional ingredients at 2.5, 3.0, and 3.5 percent chitosan respectively. Among the coatings tested, 3.0% chitosan coating performed the best. To increase the shelf life of strawberries, many quality criteria such as quality attribute (colour, texture, sensory, pH, Brix), overall visual appearance, and fungal effect were evaluated. They govern the rate of exchange of gases of O<sub>2</sub>/CO<sub>2</sub> and water vapours, which is how this coating functions. These are semi-permeable in nature, so they only allow for the necessary amount of exchange, delaying fruit ripening and increasing shelf life. Chitosan contains antioxidant, antimicrobial, gel-forming, edible, nontoxic, and other qualities. Many studies have demonstrated that it established a defence mechanism against various bacteria and diseases in fruits and vegetables [1]. Coated strawberries were found to be far less susceptible to fungus attack than uncoated (only chitosan) strawberries. Fungus destroyed 23.33% of the uncoated samples, but only 6.66% of the 3% chitosan samples after day 6 of storage. The essential oil was also found to keep the colour of strawberries and prevent browning. There was very little change in attributes such as weight loss, pH, % brix, and titratability of coated strawberry significantly than uncoated one.

**KEYWORDS:** Strawberry, Shelf- life, Chitosan

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## Development of trifunctional polybenzoxazines coated hydrophobic cellulose paper for packaging material applications

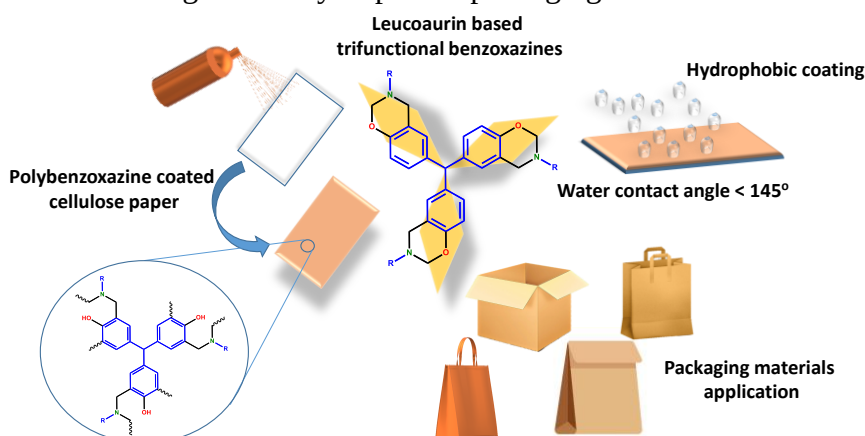
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### Abstract

A new type of tri-functional polybenzoxazines having symmetrical structure were synthesised using leucoaurin and five different aliphatic amines (i.e) butylamine, hexylamine, ethylhexylamine, dodecylamine and octadecylamine. The structure of the synthesized leucoaurin based benzoxazines was characterized using FTIR and proton NMR. The curing behaviour and thermal stability of the synthesized monomers and polymers were studied using DSC and TGA. Generally, polybenzoxazines are hydrophobic in nature and this property is dependent on the structure of the polybenzoxazines<sup>1,2,3</sup>. In this work, all the synthesized polybenzoxazines possess excellent hydrophobicity with water contact angle value above 145°. Among the polybenzoxazines synthesized, the leucoaurin with octadecylamine benzoxazine shows better water repellent property. The synthesized leucoaurin based benzoxazines were coated on the cellulose paper and their hydrophobic behavior was tested. In addition to that, the mechanical strength of the leucoaurin based polybenzoxazines coated papers were tested and the results were compared with the uncoated paper. The tensile strength of the coated paper were found to be increased than that of neat paper. The results obtained from the hydrophobic behavior study and tensile test, it is suggested that the leucoaurin based polybenzoxazines coated papers can be effectively used for packaging applications. Also the cellulose present in the paper allows the developed packaging material to be bio-degradable in nature. Data resulted from this study infers that the leucoaurin based polybenzoxazines coated cellulose paper can be effectively used as a bio-degradable hydrophobic packaging material for various applications.



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## Continuous Flow Synthesis of Defect-Free, High Molecular Weight P(NDI2OD-T2) by Stille and DHAP Polymerization

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### Abstract

Donor-Acceptor (D-A)  $\pi$  conjugated polymers are promising materials for optoelectronic applications.<sup>1</sup> The palladium catalyzed cross-coupling reactions like the Stille or Suzuki are the most commonly used methods to synthesize the conjugated polymer. They are unfeasible for scaling up the polymer for industrial purposes due to the requirement of pre-functionalization of monomers that are often toxic, difficulties in their purification, and most importantly the fact that it generates a stoichiometric amount of toxic trialkyltin (Stille).<sup>2</sup> One of the biggest challenges impacting the commercialization of the conjugated polymers is the difficulties in their scale up by the traditional method of batch-to-batch synthesis, which is prone to discrepancies in their molecular weights and molar mass dispersity. Such variation in the molecular weight has been shown to result in fluctuations in their device performance.<sup>3</sup> In this regard, we synthesized P(NDI2OD-T2) polymer by Direct heteroarylation polymerization in a continuous flow by green approach with reproducible results in molecular weight and device fabrication. P(NDI2OD-T2) was synthesized by continuous flow (CF) process using Stille as well as Direct Hetero Arylation Polymerization (DHAP) routes. The Stille Polymerization was modified to result in high molecular weight ( $M_n$ : 61kDa,  $\bar{M}_w$ : 1.7) polymers in a very short (<2.0h) period in both batch as well as continuous flow process. The polymerization by DHAP in the batch process was facilitated by a structural modification of the bithiophene monomer which activated the alpha C-H bond. The new monomer design involved flanking naphthalenediimide with bithiophene units in the bay position, which was further polymerized with bay substituted 1, 4-dibromo naphthalenediimide to afford the same polymer structure as P(NDI2OD-T2). The new monomer design resulted in a very high molecular weight ( $M_n$ : 99.5kDa,  $\bar{M}_w$ : 2.8) defect-free polymer by the DHAP batch process using 1,2,4-trichlorobenzene (TCB) as the solvent. The new monomer continuous flow polymerization (DHAP) where by reproducible molecular weights of  $M_n$ : 29.5 kDa,  $\bar{M}_w$ : 1.7 was obtained at much lower concentrations of reactant mixture compared to that for batch polymerization. Organic field-effect (OFET) mobility measurements indicated mobility values in the order of  $10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  for the Stille CF and DHAP batch polymer (using the novel monomer design).

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## **Synthesis of $\text{CuCo}_2\text{S}_4/\text{PANI}@r\text{GO}$ nanocomposite via hydrothermal method for high-performance supercapacitor application**

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### **Abstract**

In the current scenario, development of highly efficient energy conversion and storage technologies are at most important to meet the demand of the rapid development of modern society. Among the varieties of energy storage technologies, supercapacitors have drawn considerable attentions due to their multiple advantages of long cycling stability, high power density, fast charging capability as well as excellent rate performance.[1] Secondly, the ability of energy storage in the newly constructed device usually depends on the nature of electroactive material being used for electrode fabrication. Thus, developing high performance electrode materials and designing suitable structures are highly desired to solve the abovementioned shortcoming. Up to date, transitional metal-based compounds as battery-type electrode materials have drawn much attentions because of their high theoretical specific capacitance and excellent redox reversibility and are thus regarded as potential promising alternative Supercapacitor electrodes.[2] In this work,  $\text{CuCo}_2\text{S}_4/\text{PANI}@r\text{GO}$  nanocomposite was synthesized in different ratio using hydrothermal method. XRD, FT-IR, SEM, EDAX, and Raman spectroscopy were used to analyse the nanocomposite morphology, crystallinity, spectroscopic properties and chemical composition. As well, the cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectra (EIS) were used to investigate the electrochemical properties and performance of Supercapacitor for the synthesised  $\text{CuCo}_2\text{S}_4/\text{PANI}@r\text{GO}$  nanocomposite. Thus, the synthesised  $\text{CuCo}_2\text{S}_4/\text{PANI}@r\text{GO}$  nanocomposite could be promising potential electrode material for high performance supercapacitor.

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## **Solid Polymer Electrolytes Utilizing Catechol-Based Polyphosphates for 2D Channel Formation and Microstructure-Enhanced Li-Ion Conductivity**

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### **Abstract**

Electrochemical energy storage systems are essential technologies for potential utilization in renewable energy setups powered by intermittent sources like wind and solar and in portable applications like electric vehicles. This study outlines the production, analysis, and lithium-ion conductivity of a polyphosphate-based copolymer (P1–P4) integrated with catechol, intended for utilization as a solid polymer electrolyte (SPE) within lithium-ion batteries. The polymers synthesized exhibit notable thermal stability, high molecular weight, and porous structure, with their particles taking on a rod-like morphology. For instance, when employing P3 with 20% weight of LiTFSI, one of the SPEs displays a lithium-ion conductivity of  $1.4 \times 10^{-3} \text{ S cm}^{-1}$  at 80 °C, while P1, containing 40% weight of LiTFSI, showcases a conductivity of  $1.2 \times 10^{-3} \text{ S cm}^{-1}$  at the same temperature. The other polymers (P1–P4) demonstrate favorable conductivity at room temperature ( $\sim 10^{-4} \text{ S cm}^{-1}$ ). These findings highlight the most impressive lithium-ion conductivity recorded at 80 °C compared to existing literature. This elevated conductivity is attributed to the specific microstructure of polymer molecules due to the inclusion of bulky and rigid co-monomer groups, which create consistent gaps within the polymer framework. Furthermore, an assessment of coin cells employing SPE1 through galvanostatic charge–discharge cycling reveals consistent overpotential values and stable cycling performance for around 2000 cycles.

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## Mixed matrix composite PEM with super proton conductivity developed from ionic liquid modified silica nanoparticle and polybenzimidazole

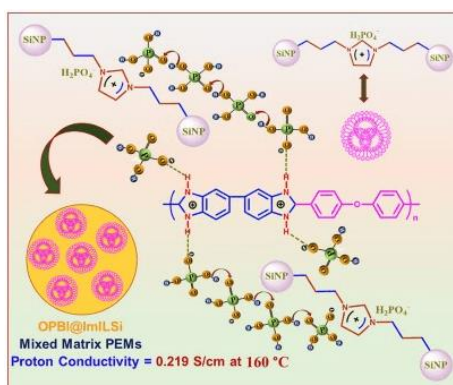
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### Abstract

Phosphoric acid (PA) leaching, low proton conductivity and weak mechanical strength of the polybenzimidazole (PBI) membrane need to be improved considerably for the development of proton exchange membrane (PEM). We have addressed these issues by preparing a mixed matrix composite (MMC) membrane comprising of oxy-polybenzimidazole (OPBI) and imidazole ionic liquid modified silica (ImILSi). Imidazolium based ionic liquid was synthesized and grafted to the surface of the silica nanoparticles (SiNP) to obtain ImILSi which further blended with OPBI to obtain OPBI@ImILSi. The uniform dispersion nature of the ImILSi in the OPBI matrix and the strong Hbonded interfacial interactions between nanofillers and polymers are found to be primary reason for significant improvement of various physical properties of the MMC. TGA, DMA and stress-strain studies exhibited significant enhancement in the thermal and mechanical properties of the MMC membranes. Most importantly, due to the loading of hydrophilic ImILSi, the MMC membranes resulted higher PA loading (~3-fold increase) which enabled the formation of facial proton transport nanochannels for their superior proton conduction under anhydrous environment and elevated temperature. For example, the OPBI@ImILSi-3% membrane showed proton conductivity value of  $0.219 \text{ S cm}^{-1}$  at  $160^\circ\text{C}$  which is a ~4-fold increase compared to OPBI membrane.



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## Photoreforming of carbazole and quinoline-based glucopyranoside macromolecules for green hydrogen evolution

Sandip Prabhakar Shelake<sup>1,2</sup>, Dattatray Namdev Sutar<sup>1,2</sup>, Saddam Sk<sup>2,3</sup>, Ujjwal Pal<sup>2,3\*</sup>, Annadanam V. Sessa Sainath<sup>1,2</sup>

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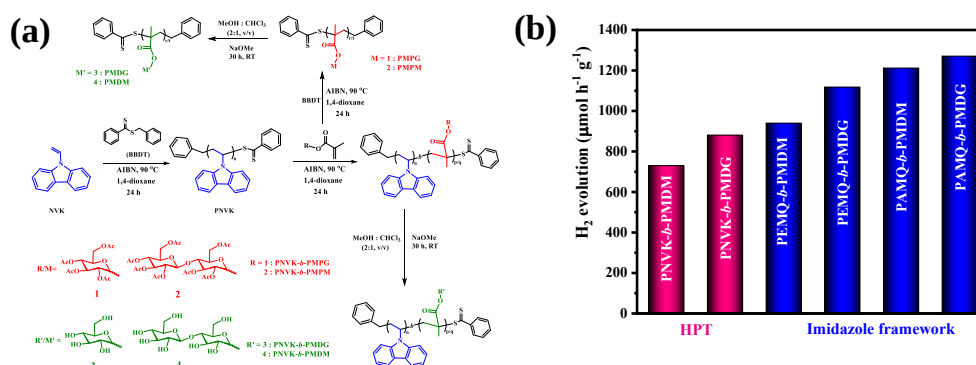
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### Abstract

Hydrogen evolution from renewable resources such as energy-rich biomass, water, and solar energy is possible and yet quite challenging. Herein, glucose- and maltose-based homopolymers and diblock copolymers from carbazole and quinoline-based monomers are reported by deacetylation of pendant acetylated mono- and di-saccharide moieties of the RAFT-generated glycopolymer segments. All the acetylated polymers showed both  $T_g$  (45–70 °C) and  $T_m$  (120–180 °C) transitions, whereas the corresponding deacetylated polymers exhibited only  $T_g$  (45–80 °C) transitions in DSC thermograms. However, in the case of acetylated diblock copolymers, the  $T_g$  and  $T_m$  values were decreased compared to the carbazole- and quinoline-based homopolymers. In addition, we employed the synthesized carbazole- and quinoline-based glucopyranoside macromolecules as sacrificial electron donors under visible light illumination for  $H_2$  production by photoreforming using hierarchical porous  $TiO_2$  (HPT) and imidazolate framework photocatalyst, respectively. The quinoline-based deacetylated diblock copolymers (900–1270  $\mu\text{mol g}^{-1} \text{h}^{-1}$ ) showed higher hydrogen generation than the carbazole-based polymers (730–880  $\mu\text{mol g}^{-1} \text{h}^{-1}$ ). Therefore, we report an advanced photoreforming property of the saccharide-based glycopolymers over modulated  $TiO_2$  and imidazolate framework photocatalyst that results in contributing to the hydrogen economy.



Scheme 1. (a) Schematic representation of polymers synthesis by RAFT process and (b) histogram of photocatalytic  $H_2$  production at different diblock copolymer media.

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## Synthesis and characterization of sulfonated polytriazoles utilizing 1,4-bis(4-azido-2-(trifluoromethyl)phenoxy)benzene for the proton exchange membrane applications

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### Abstract

Semi-fluorinated aromatic hydrocarbon-based sulfonated polytriazoles have gained a reputation as a high-performing polymer because of their outstanding set of properties.<sup>1</sup> This study demonstrates the synthesis of a new semi-fluorinated diazide monomer, that is, 1,4-bis[4'-azido-2'-(trifluoromethyl)phenoxy]benzene (BATFB), and exploiting this non-sulfonated bisazide monomer, a series of semi-fluorinated aromatic hydrocarbon-based sulfonated polytriazoles (BABPSSH-60, -70, -80, -90) was synthesized utilizing the Cu(I)-catalyzed "Click" cycloaddition polymerization reaction along with the sulfonated bisazide monomer, 4,4'-diazido-2,2'-stilbenesulfonic acid disodium salt tetrahydrate (DASSA) and the terminal dialkyne monomer, 4,4'-(propane-2,2'-diyl)bis((prop-2-yn-1-yloxy)benzene) (BPAAL). Those copolymers are readily soluble in DMF, DMSO, DMAc, and NMP. The chemical structural characterization of those monomers and the copolymers was carried out by spectroscopic techniques (FTIR and NMR). Then, the membranes were fabricated by the traditional solution-casting method. Thereafter, the degree of sulfonation (DS) and the ion exchange capacity (IEC) values of those as-synthesized copolymers were confirmed using the <sup>1</sup>H NMR spectrum and the titration method. These copolymer membranes demonstrated admissible thermal and mechanical stabilities, balanced water absorption properties, and reasonable chemical stability in Fenton's reagent. The morphological analysis of those as-fabricated membranes was investigated by the AFM, SAXS, SEM, and TEM techniques. The morphological investigation confirmed a well-separated nano-phase morphology, which provided a fruitful proton conduction pathway.<sup>2</sup> The proton conductivity of the BABPSSH-XX copolymers was found to be in the range of 19-104 mS/cm at 90 °C. Among all of them, BABPSSH-90 (IEC<sub>w</sub> = 2.46 mEq/g) showed the highest proton conductivity of 104 mS/cm at 90 °C.

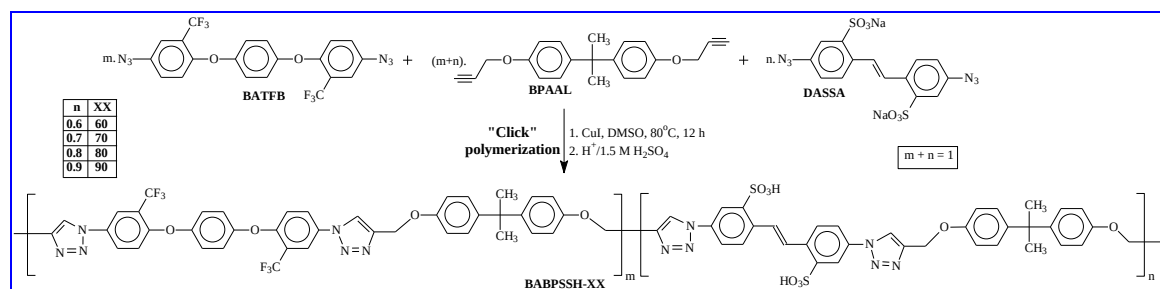


**Figure:** Synthesis scheme of BABPSSH-XX copolymers by the "Click" polymerization.

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## Schiff's Base crosslinker enabled PANI hydrogel synthesis and its electrochemical performance for supercapacitor applications

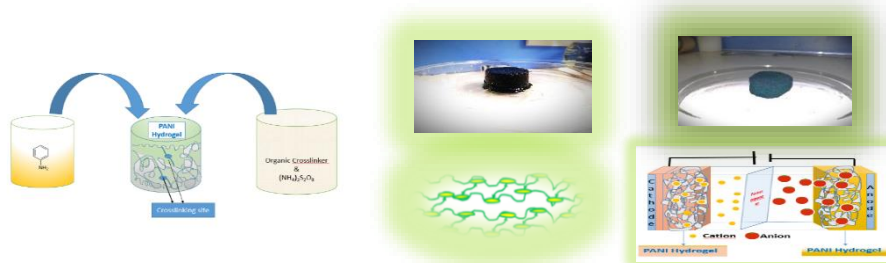
S.Ghosh, J. Majhi, Kaushik Parida\* and Anasuya Bandyopadhyay\*<sup>1</sup>

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### Abstract

In recent years one of the most essential research fields is to develop an efficient electrical energy storage system to battle climate change and energy crisis. Strong demands for portable, wearable, and smart electronics called for the rapid development of smart energy storage systems. The automobile sector is shifting towards hybrid engine vehicles to reduce the emission of greenhouse gases. Longer cycle life, high power density, and low maintenance cost make supercapacitors a potential competitor against other energy storage devices. Conductive polymer hydrogels have gained research attention as unassailable energy storage systems, particularly in flexible and, smart supercapacitors. Inherent porosity, hydrophilicity, flexibility, and other chemical functionalities favor conductive polymer hydrogel as a potential energy storage material to substantially improve the electrochemical and mechanical performance of energy storage systems, specifically in supercapacitors. The design of conductive polymer hydrogel synthesis contributed significantly to the electrochemical performance of the final product. Here we have synthesized a novel crosslinker molecule and have through a Schiff base reaction. After the successful synthesis of the crosslinker molecule, we prepared PANI hydrogel by using the synthesized crosslinker molecule through chemical oxidative polymerization. Then PANI hydrogel was dried through lypholizer and all the structural and electrochemical characterization was carried out with the PANI Xerogel. Our synthesized PANI hydrogel demonstrated excellent specific capacitance as compared to previously reported pristine PANI hydrogel.



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## **Development of flexible polymer substrate for organic solar cell application**

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### **Abstract**

There is a worldwide search for an alternative source of energy to replace fossil fuel as it generate greenhouse gases. To satisfy the global energy demand, harnessing solar energy by utilizing photovoltaic cells is a promising alternative that will produce zero carbon emissions[1]. As India is situated within the Sunbelt region of the earth[2], thus it is an ideal place to utilize solar energy resources. Although Si-based solar cells are installed in large quantities in industrial areas and on rooftops of multi-storeyed buildings[3], owing to its high cost, and space-intensive rigid structure, it is not suitable for indoor and domestic purposes. Flexible organic solar cells have emerged as a promising alternative for indoor applications. Here we have developed a novel polymer PDMS-co-Styrene as the substrate material for flexible organic solar cells as a result it can withstand sunlight and other weathering conditions for a long period without degradation. Since siloxane is too flexible to be used as a substrate[4]; we have introduced styrene to the backbone to incorporate stiffness. As a result of which the developed solar cell will be foldable, rollable, less space-intensive, and easy to install. In the absence of sun, it can be folded so that air can come through (vide Figure 1). Because of the low cost and simple installation of this organic solar cell, this has a chance to get higher popularity for domestic use.

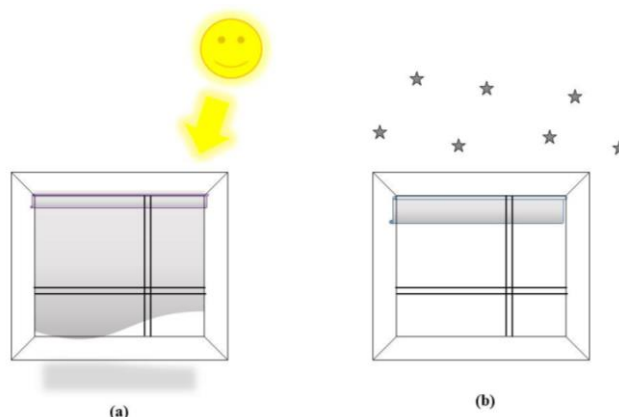


Figure 2 Depiction of Solar curtain (a) used as a solar cell in the daytime (b) folded during night

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## Synthesis and Characterization of a Conducting Copolymer Electrode for Energy Storage Applications

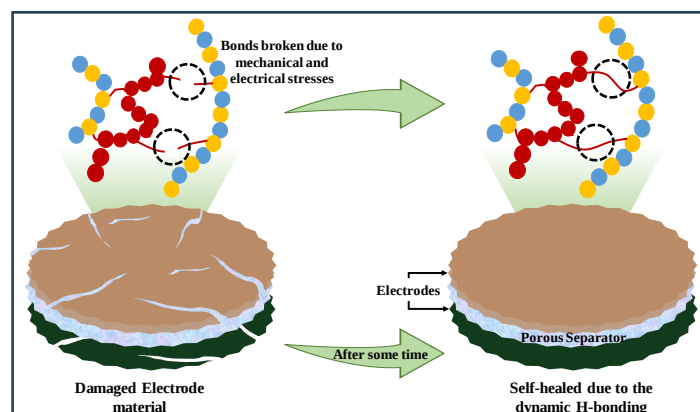
K. Priya<sup>1</sup>, S. Sharma<sup>1</sup>, S. Ghosh<sup>1</sup>, J. Majhi<sup>1</sup>, and Anasuya Bandyopadhyay<sup>1\*</sup>

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### Abstract

To fulfill the energy demand, there is a quest for alternative energy storage technologies that would lead to using cleaner, more durable, eco-friendly, sustainable, and efficient energy storage technologies and innovative systems. The continuous development and demand in power supply systems require versatile energy storage devices offering a wide range of energy density and power density [1]. Electrode development is currently the focus of researchers around the world. Therefore, we aim to synthesize a novel flexible electrode material with improved electrochemical properties and a wide range of energy density and power density. Firstly, we have tried to synthesize a thiophene-based alternating copolymer by using a Suzuki cross-coupling reaction [2]. However, the amount of mechanical stress is massive on each component of flexible devices as they continuously expose to mechanical deformations such as stretching, compression, twisting, folding, scratching, and accidental cutting, which may lead to degradation in their performance and lifetime. Thus, we are aiming to induce nature-inspired self-healing properties in the electrode material which will help it repair itself by employing the unused functional groups present in the polymer backbone [3]. The same mechanism will also help to repair externally caused damage in the structure and will increase the lifetime of the device. A gelator will be used for the purpose that will induce dynamic bonding between the polymer chains forming a self-healing copolymer gel which will be used as an electrode material.



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## Translating conformational-controlled solution structure into solid state and their application in Organoelectronics

S. Samanta and Raj Kumar Roy\*

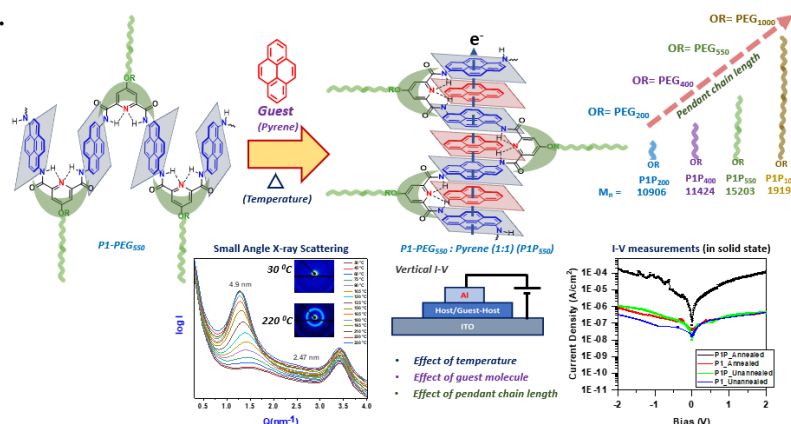
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### Abstract

In recent years, the ability to engineer and fine-tune molecular conformations in solution has laid the foundation for innovative smart materials. However, a good strategy is required to bridge the gap between solution-based feasibility and solid-state functionality. This transition is crucial to explore the potentials of conformational-controlled systems, very specifically the idea of through-space charge transfer, where the effective transportation of charges takes place through space between the interacting aromatic  $\pi$ -surfaces.<sup>1</sup> This is extremely important not only to understand the electron transport across conformationally organized  $\pi$ - $\pi$ -stacked systems in biochemical redox processes but also to design new materials and electronic devices with enhanced electronic properties.<sup>2</sup> In this presentation, I will discuss the impact of translating conformationally guided solution structures into the solid state on through-space charge transfer phenomena in Organoelectronic applications.

Previously, we demonstrated the synthesis and characterization of polyethylene glycol (PEG) functionalized aromatic polyamides, exhibiting an intrachain  $\beta$ -sheet-like conformation (in solution) via the cooperative effect of H-bonding and  $\pi$ -stacking.<sup>3</sup> In this work, we successfully transformed the solution structures of these periodically grafted aromatic polyamides to the solid state, resulting in a 1D stacked arrangement of aromatic  $\pi$ -surfaces. Furthermore, the effect of various factors influencing bulk state phase separation, such as (a) temperature, (b) guest molecule, and (c) pendant chain length, was investigated experimentally. These folded polyamides have effective through-space charge transport channels between the cofacially interacting aromatic  $\pi$ -surfaces, offering potential Organoelectronic applications. This is validated by current-voltage (I-V) measurements, successfully reproducing the previously observed effects.



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## A Novel approach to synthesize ferrocene grafted hydroxyl terminated polybutadiene

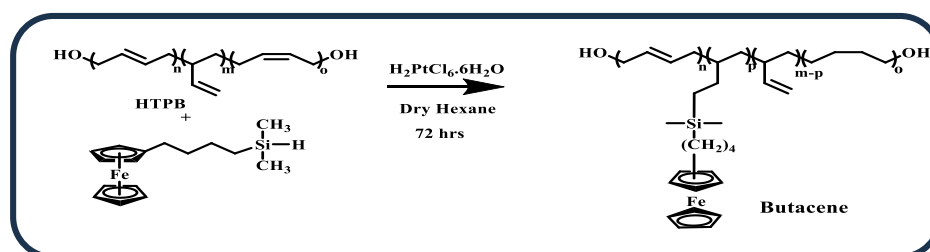
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### Abstract

Synthesis of 4-(dimethylsilyl)butylferrocene grafted hydroxyl terminated polybutadiene, which is commercially known as Butacene with control iron remains a significant challenge due to the difficulty in finding the appropriate grafting methodology. In the present work, we have developed a new grafting methodology for the synthesis of Butacene with control iron content. More particularly, the present reported work relates to a simple and cost effective industrially scalable process for the synthesis of Butacene. Further, Polyurethane (PUs) were prepared by coupling HTPB and Butacene with isophorone diisocyanate (IPDI) in THF media. The obtained PUs were showed similar thermal profile and glass transition temperature ( $T_g$ ) but their tensile properties are different. Butacene-PU was showed more tensile strain than the parent HTPB. We believed that our developed polymeric binders can be used as burn rate modifier in composite solid propellant for aerospace applications.



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## Multicationic alkaline anion exchange membranes of Polybenzimidazole

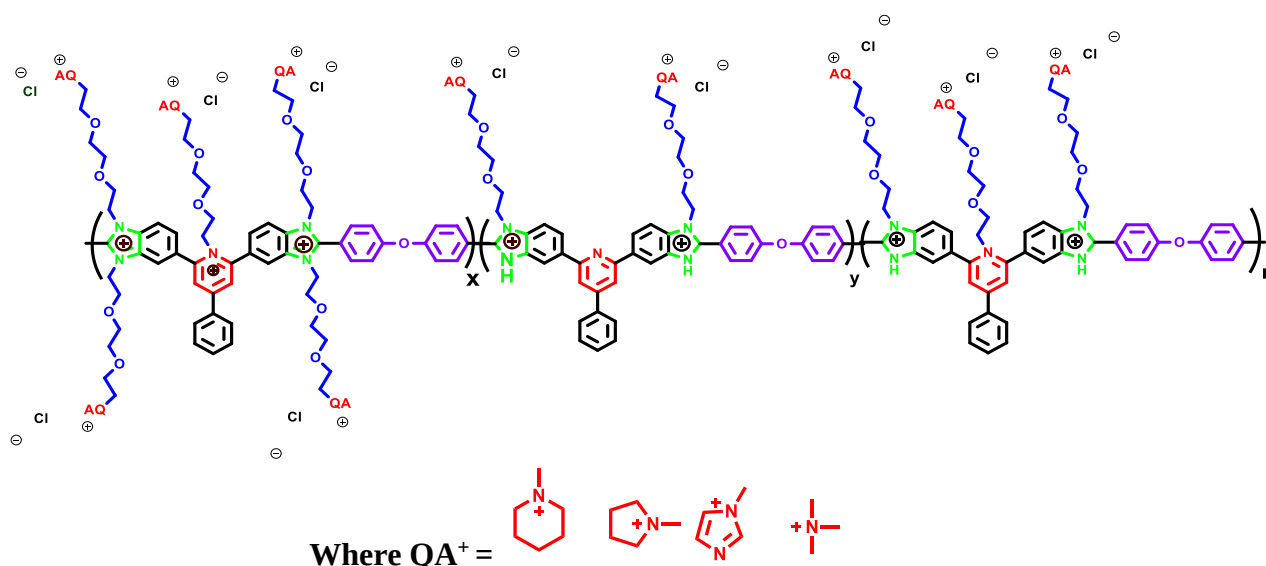
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### Abstract

Multiquaternary ammonium cationic sites with high ion exchange capacity and high alkaline stability are crucial for the performance of anion exchange membrane (AEMs). In this study, polybenzimidazole based anion exchange membranes are synthesized in which non-cationic ether containing linker is attached to different heterocyclo-aliphatic rings as pendant moieties. The major aim is to identify degradation reactions undergoing in membranes when kept in alkaline media and to establish heterocyclo-aliphatic based cation design principles. It is found that the alkaline stability of these cations depends upon their position in polymer structure and ring size. The N-methyl piperidine grafted membrane reached hydroxide conductivity of 75 m  $\text{Scm}^{-1}$  and represent a new class of anion exchange membranes.



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## Side-Chain Modification in Conjugated Polymer Frameworks for the Electrocatalytic Oxygen Evolution Reaction

Neelam Gupta, Biplab Kumar Kuila

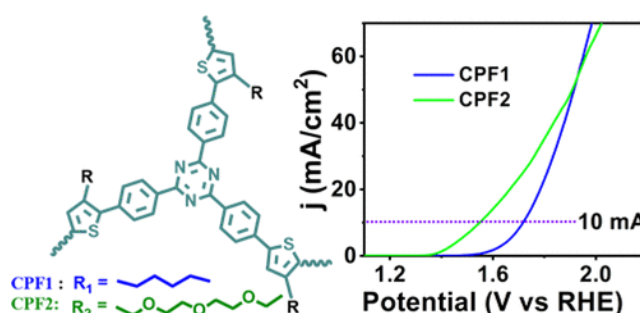
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### Abstract

Conjugated polymer frameworks (CPFs) have recently emerged as an alternative metal-free nanometer-scale porous framework with extended conjugation, making them ideal for various applications such as gas adsorption and separation<sup>1</sup>, catalysis<sup>2</sup>, and energy storage<sup>3</sup>. These organic framework materials are ideal for electrocatalysis due to their high surface area, tuneable structures with appropriate building blocks, porous structure, and surface redox active group<sup>4</sup>.

we have developed two novel triazine and thiophene-based conjugated polymer frameworks CPF1 and CPF2 which show superior self-supported metal-free OER electrocatalysis. Depending on the side chain functionality, CPF displays different electrocatalytic performances. CPF2 with ethylene glycol side chain attached to thiophene moiety shows a current density of 10 mA/cm<sup>2</sup> at an overpotential of 328 mV superior to CPF1 (10 mA/cm<sup>2</sup> at an overpotential ( $\eta$ ) of 488 mV) having hexyl sidechain. The achieved OER activity by CPF2 in an alkaline medium is comparable to or even better than that of other well-reported metal-free catalysts with excellent durability. So, these materials are the strong contender for the metal free electrocatalysis for future energy conversion from abundant water resources. The present study also sheds some light on designing better electrocatalysts based on framework materials through side-chain modification.



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## The cooperative enhancement of a novel -MnSe/ppy composite OER catalyst in alkaline media

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### Abstract

Hydrogen (H<sub>2</sub>) is unable to emerge from water because of the water-splitting process's extraordinarily sluggish kinetics. Enhancing the creation of effective oxygen evolution reaction electrocatalysts is thus important in order to understand the primary barrier to the OER. This study synthesizes, describes, and electrochemically evaluates Nickel cobaltite with polypyrrole heterostructure as an efficient electrocatalyst for OER. A number of methods, such as powder x-ray diffraction (PXRD), scanning electron microscopy (SEM), and fourier transform infrared (FTIR), are used to characterize the unique material that was synthesized. By commencing the OER at an astonishingly low voltage of 125 mV (Vs. reversible hydrogen electrode [RHE]) at 10 mAcm<sup>-2</sup>, with a Tafel slope of 36 mV dec<sup>-1</sup>, the novel NiCo<sub>2</sub>O<sub>4</sub>/ppy composite catalyst is demonstrated to be incredibly effective. The NiCo<sub>2</sub>O<sub>4</sub>/ppy electrocatalyst outperforms its NiCo<sub>2</sub>O<sub>4</sub> and ppy equivalents for OER in an aqueous KOH (1.0 M) solution when electrochemical conditions are identical. These outcomes outperform benchmark Ni and rare earth metal electrocatalysts. With this invention, a desirable non-noble metal that performs admirably as an OER electrocatalyst is made available.

## Poly(pyrrole) supported NiCo-Benzimidazole on Ni foam for high performance supercapacitor application

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### Abstract

This piece of study demonstrate the bimetallic imidazolate frameworks for energy storage application. The decreasing of energy sources in modern society, developing new and sustainable energy storage devices on ecological environments. Compared with fuel cells and secondary batteries, electrochemical supercapacitors (SCs) have drawn extensive attention in energy storage systems because of their rapid charging speed, desirable power density, satisfactory cycling life [1] . NiCo-BIM/PPY on Ni-foam as a electrode for supercapacitor, demonstrates a remarkable electrochemical performance with a high specific capacitance and a good rate capacity of retention. Supercapacitors are deemed as reliable power sources for portable devices and electric vehicles [2]. Metal organic frameworks (MOFs) comprising metal ions and organic linkers possess the merits of high porosity, low density and tunable pore size. In recent years, zeolite imidazolate frameworks have also received extensive attention. Due to the unique framework and structural flexibility of ZIFs, they have been regarded to be suitable sacrificial templates for electrodes with high activity life . This study affords an easy and effectual protocol for construction of integrated ZIFs based electrodes, which will find broad applications in supercapacitors and electrocatalysis [3]. The materials were characterized by XRD, XPS, SEM, TEM, FTIR, BET, RAMAN & UV spectroscopy and CV, GCD, EIS are the different type of techniques for supercapacitor application. The synthesized nano-composite is maximized to obtain the best performance.

**Keywords:** Ni-Co-Benzimidazole; Poly(pyrrole); Metal-organic framework; supercapacitor.

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## Heteroatom-enriched polybenzoxazine as a precursor for N, O codoped carbon structures for supercapacitor application

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### Abstract

Conventional carbon electrodes in supercapacitors suffer from kinetic problems due to in-pore ion transport resistance, leading to reduced electrochemical performance<sup>1</sup>. To overcome these shortcomings, electrochemically active sites in the form of chemical dopants can be incorporated resulting in physicochemical changes in the carbon structure. In particular, N-doping results in a significant enhancement in the electrochemical activity due to the presence of lone pair of electrons, making it more electronegative than carbon atoms. In addition, the presence of nitrogen heteroatoms also enhances the electric conductivity and wettability of the carbon structure. Recently, polybenzoxazine has emerged as an advanced phenolic thermoset with amine as a chief raw material, thereby becoming the source of nitrogen functionality in the polymer backbone. Moreover, it offers other unique properties, including high crosslinking density, high char yield, the flexibility of precursor choice, low water absorption, and low volume shrinkage with exceptional dimensional stability, making it an ideal candidate for deriving inherently heteroatom-doped carbon materials<sup>2</sup>.

A facile one-pot strategy was adopted for controlled synthesis of polymer particles via an integrated approach of template-free dispersion polymerization and benzoxazine chemistry<sup>3</sup>. Polybenzoxazine particles were attained by in situ ring-opening polymerization of the multifunctional heteroatom-rich precursors. The uniform particles were achieved via careful tuning of reactant ratio, precursor concentration and solvent ratio. The obtained polymer particles when subjected to carbonization conditions resulted in heteroatom-doped carbon spheres. Furthermore, in order to demonstrate their applicability, the uniform and highly heteroatom-doped carbon structure was utilized as the active component of the supercapacitor electrode<sup>4,5</sup>.

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## Metal–Organic Framework–Derived ZnO-Assisted $\beta$ -Phase-Stabilized High-Performance PVDF/ZnO-PDMS/rGO Nanocomposites as Piezo–Tribo Hybrid Nanogenerator

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### Abstract

Triboelectric and piezoelectric nanogenerators are being investigated to harness the electrical energy contained in mechanical vibrations. These two effects are investigated as a piezo-tribo hybrid nanogenerator (PTNG). Herein, polyvinylidene fluoride (PVDF)/ZnO nanocomposite where ZnO is synthesized is fabricated using metal–organic framework precursors. As-fabricated polydimethylsiloxane/reduced graphene oxide nanocomposites are coupled with PVDF/ZnO nanocomposites to create PTNG. ZnO is incorporated into the polymer matrix to boost piezoelectricity by stabilizing the  $\beta$ -phase of PVDF. The as-fabricated PTNG has an output of  $\approx 185$  V open circuit voltage,  $\approx 14.5$   $\mu$ A short circuit current, and  $\approx 338$   $\mu$ W/cm<sup>2</sup> of power density, which is enough to light up 40 red light-emitting diodes (LEDs) in series and 22 red LEDs in parallel. Daily portable electronics like a digital watch and calculator can also be powered by it. This PTNG and its piezoelectric component can generate power from various bodily motions, like walking, pressing the heel, bending the elbow, etc.

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## Copper Doped Polyaniline Wrapped Graphene Oxide for Energy Storage Application

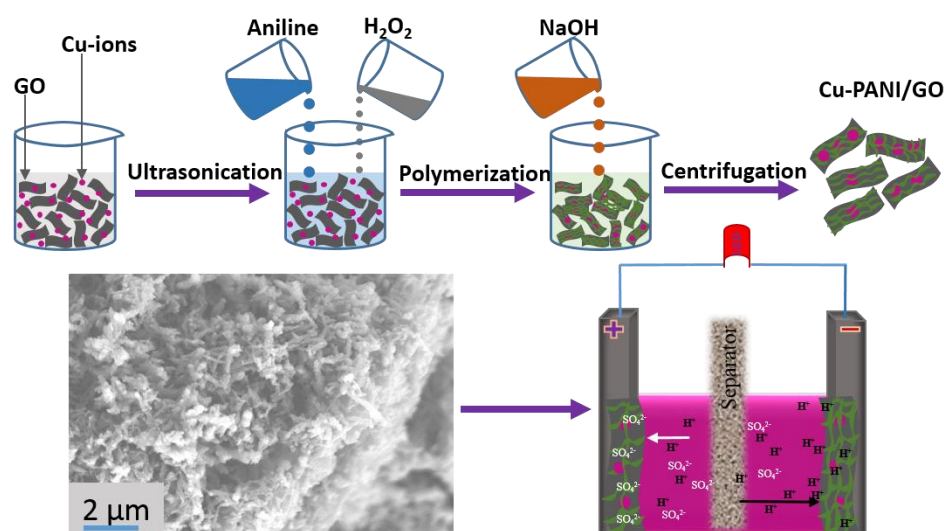
S. Kumar and D. Pradhan\*<sup>1</sup>

<sup>1</sup>Materials Science Centre, Institute of Technology Kharagpur, 721302, West Bengal, India

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### Abstract

The demand of high energy storage devices has surged in recent times due to the rapid advancement of technology, especially development of portable electronics devices and hybrid electric vehicle<sup>1</sup>. Researchers are now focused on exploring lightweight, flexible, inexpensive, and environment-friendly energy storage solutions with high power, high energy, and long cycle life<sup>2,3</sup>. Among various energy storage device supercapacitor (electrochemical capacitor) have gained significant attention due to their high-power density, comparable energy density, fast charging capability and easy effective fabrication process<sup>4</sup>. This study presents the development of transition metal doped polyaniline/graphene oxide composites as promising electrode materials for supercapacitors. Graphene oxide is utilized to stabilize the polymer backbone, thereby mitigating volume changes during counter ions intercalation and deintercalation leading to enhanced cycle stability. Additionally, Copper incorporated into polyaniline/graphene oxide composite to improve electrical conductivity and tailored the electrochemical active sites. The physicochemical properties of the prepared electrode materials are studied by different characterization techniques. The electrochemical performance of these electrode materials is evaluated through cyclic voltammetry (CV), galvanic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) analysis. The Cu-PANI/GO exhibit excellent supercapacitor performance with an enhanced specific capacitance of 437 F/g at a current density of 1 A/g.



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## Synthesis of Metal complex immobilized conjugated Polymer and its application to Supercapacitors

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### Abstract

The storage of the energy resources in this technological world we live in, is at high stake. In order to store energy efficiently, researchers have been exploring new materials and methods recently. The conversion and storage of energy for a constant supplication with special attention for storing electrochemical energy is highly in demand. Where Supercapacitors with high power density, quick charge–discharge time, low input resistance, extended cyclic stability are promising candidates to store electrical energy as solid-state device which may overcome many of the drawbacks in batteries. Thus, synthesis of new electrode materials with efficiency is considered to be paramount significance and order of the research retrospective literature survey reveals that in supercapacitors, organic conjugated polymers based on Transition Metal complexes had displayed remarkable multifunctional characteristics. This research offers insight into the synthesis of terpyridine-derived polymer (Polyoctyloxyterpyridine) with metal complex incorporation. The as synthesised polymer was characterised using XRD, FT-IR, SEM, RAMAN, and NMR spectroscopic techniques which revealed the Morphology, Structure, Surface area, Crystallinity of the material. Studies using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectra (EIS) were conducted to investigate the electrochemical characteristics and capacitance of the same. Thus, the results of the application could be highly perfomable, which would become the future of energy storage devices.

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## **Phthalonitrile – Cyanate ester Blend Resin Infused Carbon Foam Systems with Superior Electromagnetic Interference Shielding Performance**

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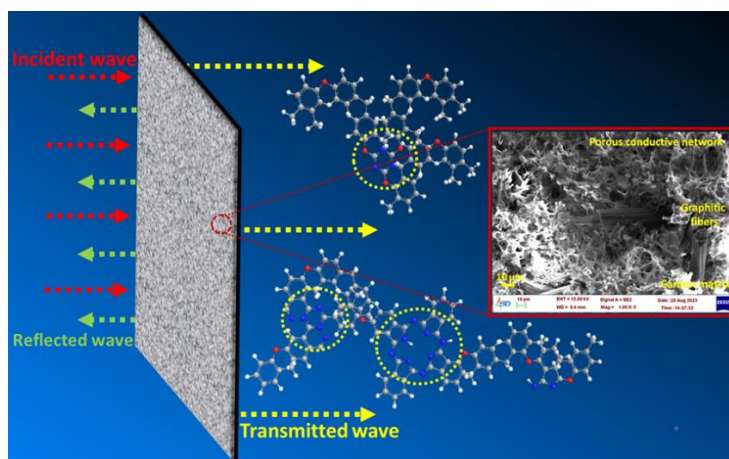
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### **Abstract**

The growing concern over electromagnetic pollution issues brought on by the expanding demand for electronic and electrical equipment has drawn a lot of attention to the requirement for electromagnetic interference (EMI) shielding materials. The desirable features are lightweight with excellent mechanical properties which could provide superior shielding effectiveness (SE). In this work, low density EMI shielding carbon foams were fabricated by infusing a resin blend of phthalonitrile (PN) and cyanate ester (CE) into a rigid graphitic board, followed by carbonization. The high nitrogen content of high performance PN-CE blend and the superior thermal stability of the resulting triazine and phthalocyanine rings produced from the ring formation polymerization of nitrile groups make it a suitable material for shielding applications<sup>[1]</sup>. The low density (0.3 -0.4 g/cc) carbon foams achieved a high EMI SE of ~ 40 - 45 dB, indicating efficient shielding of incident EM waves. The primary EMI shielding mechanism was determined to be absorption and the foam structure provided thermal stress relief upon pyrolysis. Both the conductive carbon matrix created after complete carbonization and the polarization effects brought on by the intrinsic nitrogen-containing structure contribute to high EMI SE. These carbon foams can be potential material for EMI shielding and are anticipated to be helpful in directing the development of EMI shielding materials in the future.



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## Directional Freezing-Induced Self-Poled Piezoelectric Nylon 11 Aerogels as High-Performance Mechanical Energy Harvesters

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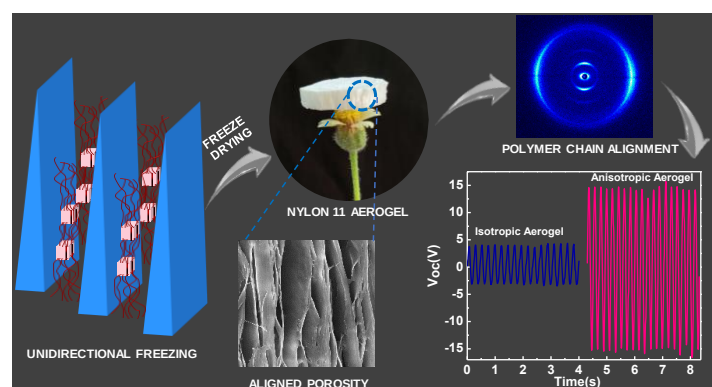
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### Abstract

Polymeric piezoelectrics have been widely applied for energy harvesting applications due to their rapid processability, mechanical flexibility, and self-poling capability.<sup>1,2</sup> Besides the dominantly used polyvinylidene fluoride and its copolymers, odd-nylons crystallized into the piezoelectric phase attracted interest in energy harvesting applications owing to their better thermal stability.<sup>3</sup> However, realization of the piezoelectric phase with the preferred crystal orientation for self-poling in nylons has remained elusive under mild conditions. Herein, we demonstrate the facile preparation of unprecedented isotropic and anisotropic nylon-11 aerogels, and such aerogels are used to fabricate piezoelectric nanogenerators. The nylon-11 solution was frozen isotropically to yield isotropic aerogels, while unidirectional freezing resulted in anisotropic aerogels. The unidirectional freezing of nylon-11 solutions enabled the orientation of polymer crystals along the freezing direction. The as-fabricated aerogels crystallized predominantly into the polar piezoelectric  $\gamma$  crystals and exhibit high thermal and mechanical stabilities. The mechanical energy harvesting performance of nylon-11 aerogels is studied by fabricating piezoelectric nanogenerators, among which the anisotropic aerogel delivers a higher peak-to-peak open circuit voltage of  $\sim 30$  V, which is 4-fold as compared to that of the isotropic aerogel. Furthermore, the developed piezoelectric nanogenerators with anisotropic aerogels delivered an excellent peak power density of  $0.1 \text{ W/m}^3$  and demonstrated for powering various electronic gadgets. This strategy provides a practical avenue for the self-poling of semicrystalline piezoelectric polymers, which is an efficient and readily scalable approach for energy-harvesting applications.



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## Preparation of sodium alginate based conducting hydrogel material and its conductivity studies

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### Abstract

Herein we have reported single sodium ion conducting pseudo solid polymer electrolyte material, was synthesized successfully using sodium alginate (ALG) and sodium salt of polyacrylic acid (SPA) in the water as solvent via solution cast technique. This pseudo-solid polymer material allows  $\text{Na}^+$  cation transport inside the matrix. The FTIR technique confirmed the appreciable interaction between the sodium alginate and sodium polyacrylate polymer. This amorphous polymer material has good flexibility, tensile strength, and good elasticity which provides a better electrode-electrolyte interface. The material shows electrical conductivity in the range of  $10^{-5}$  S/cm at room temperature and  $10^{-4}$  S/cm at higher temperatures ( $>40^\circ\text{C}$ ). The material shows electrochemical stability of 2.18V owing to a very good amount of current density with  $\approx 97\%$  ionic transport number for the sodium ion. The material shows drift ionic velocity in the range of  $10^{-4}$  m/s and ionic mobility in the order of  $10^{-6}$   $\text{m}^2/\text{Vs}$  at room temperature. It shows the matrix ionic diffusivity constant in the order of  $10^{-7}$   $\text{m}^2/\text{s}$ . It possesses low activation energy for ionic movement inside the matrix of 0.465 eV. The polymer matrix shows the correlated type of hopping. A very large amount of capacitance is associated with polymer matrix with minute electrode contribution.

**Keywords:** solid polymer electrolyte, sodium ion hydrogel, sodium alginate, energy storage material.

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## Studies on the Impact of Variation in Nickel Nitride Nanocatalyst Concentration on the Electrocatalytic Bifunctional Efficiency of Sustainable Electrodes for Alkaline Water Splitting

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### Abstract

Green hydrogen is eco-friendly and often referred to as the future fuel. The synthesis of transition metal nitride (TMNs) based nanocatalyst and their subsequent utilization for fabricating sustainable electrodes for water splitting have garnered much attention nowadays. Herein we report the synthesis of a set of concentration varied nickel nitride based nanocatalysts and the electrodes fabricated using the same for the purpose of alkaline water splitting. The electrodes Ni<sub>3</sub>N-8, Ni<sub>3</sub>N-16 and Ni<sub>3</sub>N-32 were fabricated and each one of them was subjected to electrochemical analysis in 1M KOH electrocatalytic conditions. During electrochemical analysis, it was found that the electrodes showed OER and HER overpotentials in decreasing order with increasing nickel nitride content. Ni<sub>3</sub>N-32 with the lowest OER and HER overpotentials behaved as the best bifunctional electrode among the three different electrodes tested and was much more stable than the other two electrodes in harsh alkaline conditions. The XPS and XRD spectra analysis confirms the presence of nickel nitride in the samples. The FE-SEM images and EDX mapping also confirm that the hexagonal nanostructures formed on the electrode surface are basically nickel nitride nanoparticles. It is presumed that these nanostructures are perhaps responsible for the enhanced electrocatalytic activity of the electrodes. Hence this promising electrocatalytic efficiency as noticed can be attributed to the structure and conductive property of nickel nitride whereas the stable nature of the electrodes is probably due to the presence of the NC layer. The method may possibly be extended to prepare similar bifunctional electrodes with other transition metals.

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## Development and characterization of MPU/CA/nHA composite films as flexible tribo-piezoelectric nanogenerators

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### Abstract

The development of novel polymeric piezoelectric composites for energy harvesting applications is a potential research field. These materials offer the convenience of mechanical flexibility, lower manufacturing cost, and rapid processing compared to ceramic-based composites<sup>1,2</sup>. In this work, we propose the development of flexible tribo-piezoelectric polymer composite films based on a millable polyurethane (MPU)/cellulose acetate (CA) blend reinforced with nanohydroxyapatite (nHA). Polymer-nanocomposite films have been fabricated through a solution casting technique. The morphology, mechanical strength, chemical features, and crystalline characteristics have been evaluated through SEM, UTM, FTIR, and XRD respectively. The butterfly-shaped amplitude curves from DC-EFM confirmed the piezoelectric nature of the composite films. Ferroelectric features have been studied through P-E hysteresis curves. Dielectric properties have been analyzed by employing an impedance analyzer. A device prototype has been fabricated and tribo-piezoelectric responses and resultant voltage generated by random finger tapping were evaluated by means of a digital oscilloscope. The results suggest a promising possibility of fabricating highly functional piezoelectric nanogenerators for a spectrum of applications<sup>3</sup>.

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## Design principle of high-performance SPEEK/QMPSF-based bipolar membrane for water splitting application

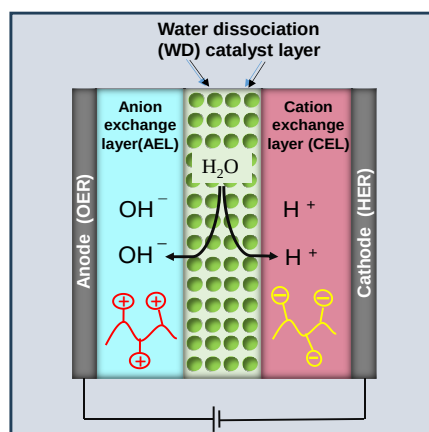
S. K. Maiti<sup>1</sup>, N. Ali<sup>1</sup>, M. Ray<sup>1</sup>, and Sujay Chattopadhyay \*

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### Abstract

The water dissociation potential of bipolar membranes (BPMs) is gaining interest in various electrochemical energy conversion technologies such as fuel cells, photo-electrochemical CO<sub>2</sub> reduction, and electrolyzers<sup>1</sup>. BPM, a special type of polymeric ion exchange membrane, comprises a positively charged anion exchange layer (AEL), a negatively charged cation exchange layer (CEL), and sometimes an interfacial catalyst layer (ICL). ICL of BPM helps in enhancing the water dissociation into proton and hydroxyl, which migrate respectively through CEL and AEL of BPM in reversed bias potential. However, water must be transported via the AEL or CEL, in reverse to the flow of hydrated  $H^+$  and  $OH^-$  simultaneously. This combined operation is one of the intrinsic BPM architectural challenges restricting the flow of current through the bilayers<sup>2</sup>. The water transportation across the membrane layers must be sufficient enough into the junction layer so that it never dries up during the operations. This undesirable condition may lead to an increase in membrane potential along with membrane degradations. In this study, we investigated the impact of optimum CEL thickness for effective water dissociation. In addition, the various physico-chemical properties (ion exchange capacity, dimensional stability, water uptake), mechanical properties, and electrochemical properties (IV curve, impedance spectroscopy) were also determined for sulfonated poly(ether ether ketone) (SPEEK) and chloromethylated polysulfone (QMPSF) membranes which were synthesized for CEL and AEL, respectively<sup>3</sup>. Furthermore, a balanced electric field between ICL and varying monolayer thickness has been studied for efficient water splitting of BPMs in electrolyzer applications for hydrogen generations.



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## Enhanced dielectric properties of MoWO<sub>3</sub> metallate fabricated on Polyvinylidene fluoride for efficient supercapacitor application

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### Abstract

An efficient electrochemically active hybrid material viz., MoWO<sub>3</sub>@PVDF has been prepared with appropriate composition and was coated on Nickel foil with optimum experimental conditions. Thus the fabricated MoWO<sub>3</sub>@PVDF electrode was characterized by employing several spectroscopic and microscopic techniques such as FTIR, RAMAN, XRD, SEM, EDAX, and TGA. The electrochemical performance of the hybrid material was investigated by Cyclic Voltammetry (CV), Galvanostatic charge-discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS) techniques. The significance of this hybrid is the enlarged lattice space between Mo<sup>6+</sup> and W<sup>6+</sup> in the crystal structure of MoWO<sub>3</sub> which facilitates higher specific capacitance and cycling stability than Molybdenum oxide and Tungsten oxide (MoO<sub>3</sub> and WO<sub>3</sub>). The hybrid electrode unveils higher specific capacitance (C<sub>sp</sub>) than Individual metal oxides (MoO<sub>3</sub> and WO<sub>3</sub>) at 1 A g<sup>-1</sup> leading to rapid electron transfer and low charge transfer resistance. The hybrid also has the capacity to retain its capacitance even at high current density, high energy density, and cyclic stability which proves to be an efficient nanohybrid for energy storage applications in the case of electrical and electronic devices.

**Keywords:** PVDF, Metallate, Molybdenum-Tungsten Oxide, Current density, Capacitance

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## Energy Harvesting from real wastewater using biodegradable polymer based Microbial fuel Cell

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### Abstract

To resolve an increasing global demand in energy, a source of sustainable and environmentally friendly energy is needed. Microbial fuel cells (MFC) hold great potential as a sustainable and green bioenergy conversion technology that uses waste as feedstock. Development of an effective small-scale MFC for energy generation from different types of real waste water collected from different areas like industry, oil mills, municipal areas. An innovative miniature MFC was developed, using microfabrication technique unique with structural features like heart-shaped flow channel at both cathode and anode chamber of the MFC. The miniaturized MFC device due to its high surface area to volume ratio the proportion of electrode-coupled cells in microliter chamber increases. Moreover, the current generation is associated with local electron transfer at microbial -electrode interface. The number of electrically addressable cells should scale down with electrode area so that measurement can be done in uniform local environment. Lab fabricated low cost membrane has been used. Maximum voltage of 800mV has been achieved. It has got wide application as remote sensor where MFC can act as low power sensor that collect data from remote areas. It can act as small robot where the tummy of the robot will be filled with waste water also for power devices like mobile phones. The miniaturized MFC has also got its application in heavy metal detection in waste water.

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## Non-toxic CuInS<sub>2</sub> quantum dots sensitized solar cell with functionalized thermoplast polyurethane gel electrolyte

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### Abstract

Functionalization of multi-walled carbon nanotubes (CNTs) was carried out through ultrasonication in acidic medium followed by chemical attachment of thermoplastic polyurethane and subsequent chain extension using butane-diol to obtain CNT-tagged polyurethane (PU-CNT). PU-CNT was functionalized by using propane sultone as a sulfonating agent to attach the pendent sulfonate moiety on urethane linkage. The functionalization of CNTs, tagging of CNTs with polymer chain, chain extension and subsequent functionalization of polymer have been confirmed through spectroscopic techniques such as NMR, FTIR, UV-vis, and Raman spectroscopy. Thermal stability and the nature of interaction is explored through thermal measurements to understand the effect of CNT functionalization. Electrical conduction has been improved by the chemical attachment of CNTs with polymer ( $1.61 \times 10^{-6}$  S/cm) which further increases through functionalization ( $1.37 \times 10^{-4}$  S/cm) and thereby make them suitable for gel electrolyte. Quantum dot of CuInS<sub>2</sub> has been synthesized using DDT as capping agent and its characteristic properties and the dimension are worked out for their suitability as active materials in solar cell. Optical band gap of quantum dots and HOMO/LUMO band structure of functionalized polyurethanes have been measured through UV-vis and cyclic voltametry, and thereby, draw the overall energy diagrams of possible combination of materials. Solar cell devices have been fabricated using the appropriate materials and found improved power conversion efficiency of 0.81% with Au (gold) as counter electrode. The reason behind the better efficiency is understood from the lesser energy gap between HOMO energy level of prepared gel electrolyte (SPU-CNT) and Au (gold) counter electrode, better conductivity and higher rate of hole transportation, to reduce the electron-hole pair recombination.

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## Polyether sulfone base Janus membrane for osmotic energy conversion device

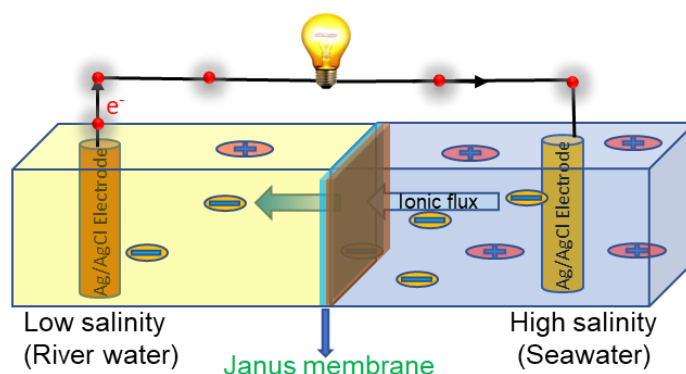
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### Abstract

Environmental concerns have encouraged researchers to investigate renewable energies, which involve transforming ambient energy into electrical energy. The osmotic energy outputs from the salinity gradient are consistent and predictable among other renewable energy-generating systems. It can produce 1.4-2.6 TW/year by combining sea and river water, and 18 GW by mixing sea and municipal sewage<sup>1</sup>. It may be recovered using reverse electrolysis (RED) and pressure retarded osmosis (PRO) technologies. RED technology outperforms PRO because of its cheap investment cost and less membrane fouling<sup>2</sup>. RDE is comprised of an ion exchange membrane that selectively allows and restricts the ions, resulting in a potential difference against the membrane. In such a system, the Gibbs-free energy generated by mixing electrolytes of various salinities creates electricity<sup>3</sup>. Ionic flow and counterion selectivity are critical considerations for membrane performance. Here we created the S-PES-based Janus membrane for RDE applications, which has a microporous sulfonated channel and a highly selective quaternary layer. The positively charged layer is responsible for anion conductivity and selectivity, whereas the anionic layer rectifies the conductivity by avoiding concentration polarization. The  $\text{Cl}^-$  ion conductivity of the developed membrane is double that of the commercial FAA-3-50 membrane, and the resulting power density was  $0.6 \text{ W/m}^2$  under a 50-fold KCl gradient, which was also higher than the FAA-3-50 membrane. This result demonstrates that the manufactured membrane has a high potential for harvesting osmotic energy using a membrane-based energy conversion device.



### Osmotic Energy Harvesting

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## Incorporation of MOF based superior proton conductive fillers and antioxidants in SPEEK for enhanced performance and stability in PEM fuel cells

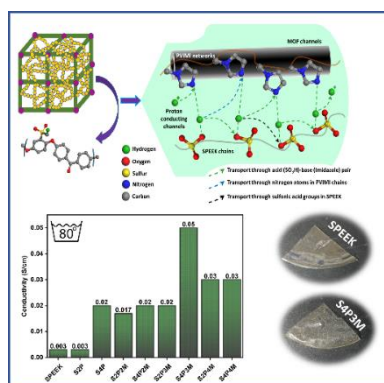
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### Abstract

Metal-organic Frameworks (MOFs) are an interesting class of solid-state crystalline, porous materials with significantly high surface areas. Zirconium based microporous MOF 808 constructed from  $Zr_6$  nodes ( $Zr_6O_4(OH)_4$ ) and BTC (benzene-1,3,5-tricarboxylate) has been synthesized in this study. Further modification of the MOF was carried out by radical in situ polymerization using vinyl (1-imidazole) to design novel structures that were incorporated as hybrid fillers in sulfonated poly (ether ether ketone) (SPEEK) matrix to formulate composite PEMs by solution casting. The samples were also enriched by natural antioxidants in low percentages to check their long-term durability in fuel cell. The composite membranes displayed higher thermal stability, proton conductivity, durability and fuel cell performance than pure SPEEK. The filler generates abundant proton conducting channels through the MOF pores and interacting sulfonic functional groups of SPEEK matrix causing the proton conductivity to increase by 5.13-fold higher than pure SPEEK. Furthermore, peak power density achieved by the membrane at 80°C is comparatively higher than many other reported literatures on SPEEK based membranes. The antioxidants worked to reduce the chemical degradation significantly and contributed to long term stability of the membrane in single cell. The results give an overall insight that this kind of modified membranes can be potentially applied in PEM.



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## Molecular Architectonics Guided Carbon Nitride Polymers for Boosting Sunlight Absorption for Photocatalysis: A Combinatorial Approach

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### Abstract

Humans have tried to harness the solar power since a long time. Researchers across the globe intend to translate solar energy into chemical energy form like hydrogen, from photocatalytic splitting of water or methane or methanol from photoreduction of CO<sub>2</sub> which have high calorific values as fuels and are clean by nature as well. Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) has stood up as a highly potent photocatalyst for artificial photosynthesis, primarily due to its high chemical and thermal stability, low toxicity, cost-effectiveness, visible light absorption capacity and ingeniously tuneable synthetic routes as compared to other semiconductors. Nevertheless, lesser electrical conductivity, fast recombination of photoexcitons and narrow visible light absorption window hinder the application of this photocatalyst for practical utilization. To address the aforementioned issues and to modulate the photochemical and photophysical properties of g-C<sub>3</sub>N<sub>4</sub>, molecular doping has been a widely employed strategy. Radiative recombination losses and narrow visible light absorption in g-C<sub>3</sub>N<sub>4</sub> can be mitigated by disrupting the regular triazine and heptazine repeat units, introducing disordered zones in the framework using rationally chosen non triazine based molecular precursors like pyridine, pyrazine, pyrimidine, pyrazine and other heterocyclic or carbocyclic moieties in a combinatorial fashion. A simple solvent mediated supramolecular assembly of precursors followed by pyro-polymerization approach can be taken as a holistic platform for the synthesis of different molecular architectures of carbon nitride type polymers having a plethora of desired photo-physicochemical properties and varied C/N ratios and connectivities. This combinatorial platform enables the tuning of molecular architectures in CN polymers instigating extended visible light absorption for artificial photosynthesis.

**Keywords:** Carbon Nitride, Combinatorial Supramolecular Assembly, Molecular Architectonics, Molecular Doping, Photocatalysis

## Fabrication of H-bonding Assisted Soft Multifunctional Liquid Metal Integrated Elastomer Architectures for Soft Matter Engineering

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### Abstract

Liquid metal (LM)-based polymer composites are currently new breakthrough and emerging classes of soft multifunctional materials (SMMs) having immense transformative potential for soft technological applications. However, the challenge that remains in the fabrication of such promising materials lie in the fundamental problems of phase incompatibility and lack of interactions between the polymer and the LM, eventually emanating sedimentation of LM resulting in failure in fabrication. In this work, we report an innovative soft bi-phasic composite system by integrating eutectic gallium-indium LM alloy into a chemically modified block copolymer matrix, resulting in a soft and ultra-stretchable elastomeric material architecture by exploiting the H-bonding interaction of LMs with block copolymer with outstanding multifunctional attributes. The influence of microstructure and interfacial interactions on multifunctional properties have been established and also validated with various mathematical models such as Eshelby's approach, Cole-Cole model, and effective medium theory to understand the origin of the unique attributes of these soft materials. The resulting composites exhibit a substantial 4-fold enhancement in the dielectric permittivity and over 350% improvement in thermal conductivity over neat polymer while preserving the deformability, with more than 1400% strain at break. This work provides a cost-effective, facile and scalable approach to construct soft multifunctional materials for soft matter technological applications.

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## Breathable, Fast charging and Self-Powered Piezo-Supercapacitor for health monitoring

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### Abstract

Developing a smart interface that connects plants with their environment is crucial for actively monitoring the well-being of plants, with particular emphasis on its potential for enhancing agricultural productivity. Despite the advancement of numerous sensors, providing a sustainable power source for these electronic devices remains a tough problem. Herein, a waterproof and breathable, fast self-charging, self-powered electrochemical energy storage device (WB-PSC) is designed using polyvinylidene fluoride (PVDF) nanofibers embedded with ZnO hollow spheres, which was realized by electrospinning[1]. Under the influence of ZnO, the combination of intense supersonic impact and shear flow caused a conversion of nonpolar  $\alpha$ -phase PVDF into the polar  $\beta$ -phase with a catastrophic effect. The combination of ZnO hollow spheres with built-in nanorods and  $\beta$ -phase-rich PVDF can help enhance generated charges at interfacial sites under an applied force. The electrospinning of PVDF/ZnO nanofibre exhibited a 33% increase in the  $\beta$ -phase compared to that exhibited by pure PVDF. Using activated carbon as the electrode, the WB-PSC shows high conductivity and impressive EDLC-type electrochemical performance, breathability, and hydrophobicity[1]. This work realises the concept of establishing a WB-PSC with environment adaptability and energy scavenging capabilities, demonstrating the tremendous potential for developing a self-powered agro system.

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## A new Synthetic Polymer-Based Bifunctional catalyst for Water and H<sub>2</sub>S Splitting

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### Abstract

Polymer-based catalysts have developed as a promising avenue in the quest for sustainable hydrogen production through the splitting of water (H<sub>2</sub>O) and hydrogen sulfide (H<sub>2</sub>S). This abstract provides an overview of the state-of-the-art developments and key insights into the utilization of polymer-based catalysts for water and H<sub>2</sub>S splitting. Polymer-based catalysts offer a unique combination of advantages, including high catalytic activity, tunable surface properties, and remarkable stability, making them highly desirable for these energy conversion reactions. The choice of polymers, functional groups, and synthesis methods significantly influences the catalyst's performance. Polymer matrices can be tailored to accommodate various catalytic species, such as transition metal complexes and metal nanoparticles, enhancing their catalytic activity and selectivity. In the case of water splitting, polymer-based catalysts have demonstrated exceptional promise for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and sulfide oxidation reaction (SOR). Their compatibility with proton-conductive polymers further improves their performance, allowing for efficient proton transport and reducing overpotential. The utilization of earth-abundant catalysts within polymer matrices holds immense potential for sustainable hydrogen generation. For H<sub>2</sub>S splitting, polymer-based catalysts offer a green and economically viable route to produce hydrogen and elemental sulfur. Through tailored polymer design, the catalysts can efficiently facilitate its decomposition into hydrogen and sulfur. This process not only generates hydrogen, a clean energy carrier but also mitigates the release of harmful hydrogen sulfide gas, addressing environmental and safety concerns. Here we elaborate on recent advances in polymer-based catalysts for water and H<sub>2</sub>S splitting, emphasizing their catalytic mechanisms, performance metrics, and potential applications. Additionally, challenges such as catalyst stability, long-term durability, and scale-up considerations are discussed. The utilization of polymer-based catalysts for these vital reactions offers a sustainable and environmentally responsible approach to hydrogen production, contributing to the ongoing global efforts to transition towards a clean energy future.

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## Unraveling Mechanistic Insights in Covalent Organic Frameworks for Highly Efficient Sequestration of Organic Iodides from Simulated Nuclear Waste

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### Abstract

Throughout the last couple of decades, considering the impending global energy and environmental crisis, paramount development in nuclear energy has been widely observed as an alternative high power density and low-carbon energy source. However, problems associated with nuclear reactors include the emission of volatile radioactive substances like organic iodides and iodine, which must be eliminated before releasing the off-gas. These substances include methyl iodide (CH<sub>3</sub>I), ethyl iodide (CH<sub>3</sub>CH<sub>2</sub>I) and iodine, which are exceedingly harmful to both environment and human health. Considering this, even though several porous solid adsorbents have been successfully employed to sequester organic iodides (generally CH<sub>3</sub>I) from the vapor phase, majority of the earlier investigations have largely focused on the saturation capacity and kinetic study of CH<sub>3</sub>I capture. However, the importance of the porous adsorbents' strategic functions in the binding interaction with organic iodides has been underappreciated and poorly understood. Herein, we demonstrated a systematic strategy to understand the role of framework integrated functionalities towards organic iodide sequestration by varying the number of N-heteroatomic sites in a series of chemically robust porous covalent organic frameworks (COFs). The CH<sub>3</sub>I adsorption capacity was found to positively correlate with the porosity as well as the N-heteroatomic or heterocyclic functionalities such as imine, pyridine and triazine sites of these COFs. Under both static and dynamic condition the COFs exhibited high CH<sub>3</sub>I sorption capacities through N-methylation reaction. This work present fundamental importance to understanding the CH<sub>3</sub>I adsorption mechanisms, and also offer direction for the design and development of novel adsorbents for relevant applications.

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## **Design, Synthesis and Characterization of Redox-Active Heteroatomic Azo Based Ligands and their Ru (II) polymers as Novel Functional Materials**

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### **Abstract**

Smart materials have gathered attention worldwide due to their numerous applications in various areas, such as memory devices [1], smart coatings, chromic materials [2], antimicrobial agent [3], optoelectronics materials, and sensors [4], etc. Today, the major challenge is to design novel smart materials effectively so that they can produce visible and reversible effects in the system in the presence of one particular external stimulus. As a result of this, research has been diverted toward synthesizing novel metallopolymer to design smart materials. As in these metallopolymer, organic moiety (ligand) is bonded directly to the metal ion with coordination and covalent bonds through the complexation process, producing the synergistic effect of both the constituents in 1D straight-chain polymer. As most of the functional metallopolymer are synthesized with either terpyridine or bi-pyridine moiety, so our research objective is to explore azo moiety as a new functional precursor. We have designed and synthesized two novel azo ligands, and their structures are confirmed with the help of  $^1\text{H}$  NMR, XPS, SC-XRD, ATR-IR, and HRMS techniques. One ligand is monotopic, while the second one is ditopic in nature. Both of them are showing solvatochromism and fluorescence properties. Ru(II) based metallopolymer with aromatic azo ligands were synthesized. The cyclic voltammetry study indicated that both conjugated ligand and metallopolymer are electrochemically active. The field emission scanning electron microscopy (FESEM) and atomic force microscopy (AFM) micrographs showed the amorphous nature of the polymer.



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## Amplifying Plasmonic, Chiroptical, and Magnetochiral Effects via Peptide-Derived Chiral Conjugated Polymers

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### Abstract

Chiral polymers consistently hold a competitive advantage over their achiral counterparts by harnessing asymmetry effectively, enabling them to emulate natural systems across various dimensions. The homogenously ordered macroscopic assemblies of chiral  $\pi$ -conjugated polymers, adopting adaptive morphologies, present a multitude of possibilities within chiral photonics.<sup>1</sup> These possibilities extend to applications in electronics, spintronics, and sensing, eventually culminating in the potential for seamless integration into device fabrication. Recent surge in the development of chiral conjugated polymers and organic-inorganic hybrid systems across research domains encompassing plasmonics, and chiroptics, has garnered significant attention, positioning it as an emerging and pivotal field with the potential to drive advancements in metamaterial applications.<sup>2</sup>

In this study, we employ well-known diacetylene and thiophene-based systems to develop novel chiral conjugated polymers, utilizing peptides as readily functionalizable chiral precursors. Additionally, we are incorporating photo-tunable azobenzene moieties to introduce a photocontrol element that enables further manipulation of the system through photoisomerization. These structural modifications in the polymer backbone instigate mesoscopic alterations within the system, which subsequently manifest in the resulting macromolecular properties. We extend our exploration of diacetylene and thiophene-based polymers towards the realms of chiral plasmonics, and spintronics. The peptide tethered diacetylenes were effectively used for tunable thermo-, halo-, -solvatochromism.<sup>3</sup> Further modification of the system lead to enhancement of SPR properties of chiral gold nanoparticles.<sup>4</sup>

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## Vis-to-NIR Multistate Electrochromic Switching with Covalent Organic Framework Film

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### Abstract

Multicolored electrochromic organic materials have attracted significant research attention for their application in low-energy-consuming optoelectronic devices.<sup>1</sup> Small organic molecules have been extensively investigated in this context due to their high brightness and color tunability.<sup>2</sup> However, the inadequate film-forming ability and long-life durability hinder the device application. Recently, covalent organic frameworks (COFs) have been demonstrated as new materials for electrochromic devices due to the high specific surface area and unimodal pore channels that facilitate electrolyte percolation rendering fast response time.<sup>3</sup> On the other hand, the designable pore architecture with redox functionalities and robust covalent bonds lead to high electrochemical stability and color tunability.<sup>4,5</sup> Herein, we developed a two-dimensional electrochromic COF (EC-COF) based on bis(triphenyleneamine)-containing moiety as a redox-active building unit. EC-COF films show a three-state anodic electrochromism with a high color contrast of ~60% in the NIR region with fast response time (4.9 s for coloration and 10.6 s for bleaching at 1100 nm). The highly porous nature of EC-COF facilitates ion movements through 1D pore channels. A prototype device has been fabricated with the EC-COF film and integrated with a customized cellphone application for monitoring the safety of electronic sensor systems.

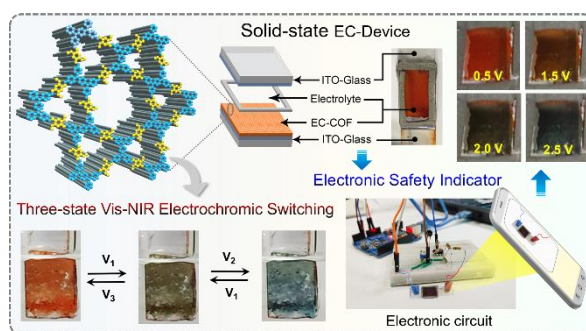


**Figure 1.** Schematic representation of a three-state electrochromism of covalent organic framework (EC-COF) film and its device performance.

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## Covalent Organic Framework Thin-film Photodetectors from Solution Processable Porous Nanospheres

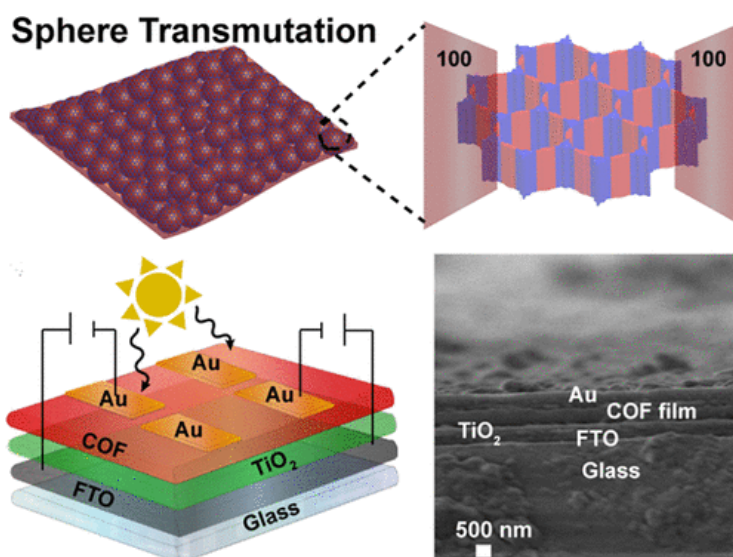
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### Abstract

The synthesis of homogeneous covalent organic framework (COF) thin films on a desired substrate with decent crystallinity, porosity, and uniform thickness has great potential for optoelectronic applications. We have used a solution-processable sphere transmutation process to synthesize  $300 \pm 20$  nm uniform COF thin films on a  $2 \times 2$  cm<sup>2</sup> TiO<sub>2</sub>-coated fluorine-doped tin oxide (FTO) surface. We have synthesized four COF thin films (TpDPP, TpEtBt, TpTab, and TpTta) with different functional backbones. The TpEtBr COF film showed the lowest optical band gap (2.26 eV) and highest excited-state lifetime (8.52 ns) among all four COF films. Hence, the TpEtBr COF film can participate in efficient charge generation and separation. We constructed optoelectronic devices having a glass/FTO/TiO<sub>2</sub>/COF-film/Au architecture, which serves as a model system to study the optoelectronic charge transport properties of COF thin films under dark and illuminated conditions. Visible light with a calibrated intensity of 100 mW cm<sup>-2</sup> was used for the excitation of COF thin films. All of the COF thin films exhibit significant photocurrent after illumination with visible light in comparison to the dark. Hence, all of the COF films behave as good photoactive substrates with minimal pinhole defects. The fabricated out-of-plane photodetector device based on the TpEtBr COF thin film exhibits high photocurrent density ( $2.65 \pm 0.24$  mA cm<sup>-2</sup> at 0.5 V) and hole mobility ( $8.15 \pm 0.64 \times 10^{-3}$  cm<sup>2</sup> V<sup>-1</sup> S<sup>-1</sup>) compared to other as-synthesized films, indicating the best photoactive characteristics.



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## Polymer Crystallization Enabled Excimer Emission in Anthracene-Appended Poly(L-lactide)s

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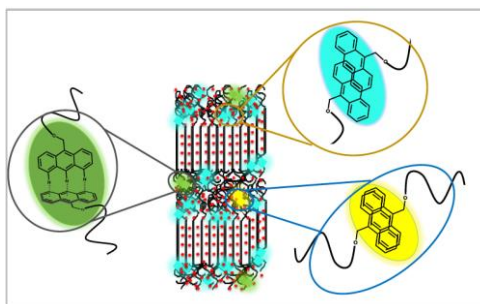
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### Abstract

The design and development of solid-state excimer-emitters bear great potential for attaining efficient solid-state luminescent materials. In this study, we have synthesized anthracene-appended poly(L-lactide)s (AAPs) to regulate the arrangement of anthracene moieties by controlling the crystallization and polymorphic form of covalently linked poly(L-lactide) (PLLA). In the high molecular weight AAP, the fluorescence intensity mainly arises from the monomeric anthracene moieties, whereas in the low molecular weight AAP, the excimer emission was observed depending on the structure and morphology of covalently-linked PLLA. The monomeric emission is predominantly observed in amorphous polymer due to the molecular level dispersion of covalently-linked anthracene moieties throughout the polymer matrix. When the polymer was crystallized under different conditions, covalently-linked anthracene moieties were excluded from polymer crystals or crystalline lamellae and are located on the surface or at the interface, which is advantageous for regulating the geometry of anthracene moieties. In the case of single crystals of PLLA, covalently-linked anthracene moieties assemble on the surface and emit mainly in their monomeric state due to the lack of  $\pi$ -stacking. In the melt-crystallized sample ( $\alpha$  form), covalently-linked anthracene moieties reside at the interface of crystalline and amorphous domains by either dipolar interactions or  $\pi$ -stacking and fluorescence arising from anthracene excimers and monomers. In the gel state ( $\epsilon$  form), only the excimer emission was observed due to the effective interactions between the anthracene moieties in the presence of excess solvent in the amorphous domains. In this way, polymer crystallization played a significant role in determining the arrangement of covalently-linked anthracene moieties in AAP.



Schematic illustration of anthracene moieties arrangement and emission of AAP-1/DMF gel at room temperature( $\epsilon$  form)

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## Functionalized Polymer using PET-RAFT polymerization

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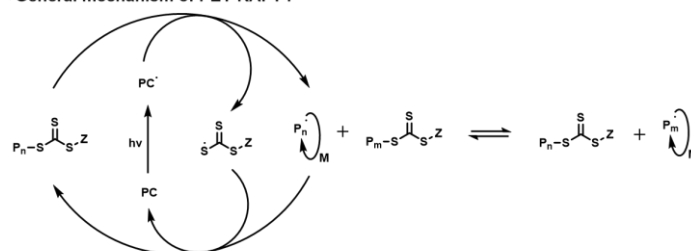
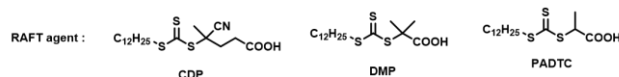
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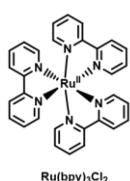
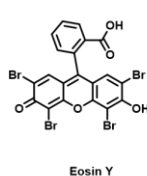
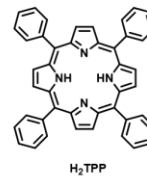
### Abstract

Due to the effort in the past two decades, reversible addition-fragmentation chain transfer (RAFT) polymerization has developed into one of the most versatile and powerful living radical polymerization (LRP) for preparing polymers with different architectures. However, challenge remains because the requirement of high temperature and presence of oxygen will quench the initiation and propagation radicals. In recent years, photoinduced electron/energy transfer-RAFT (PET-RAFT) polymerization has been developed. This technique uses visible light to initiate the reaction and is compatible with ambient condition and green solvents. It also maintains the ability of producing well-defined polymers and possess high potential as an alternative of conventional RAFT technique. In this project, we propose using a photosensitizer like  $\text{Ru}(\text{bpy})_3\text{Cl}_2$ ,  $\text{H}_2\text{TPP}$  or Eosin Y as a catalyst and a RAFT agent which could be CDP, DMP or PADTC to facilitate the polymerization, which is again with using UV or in visible light. These combinations of photocatalyst and RAFT agent is applicable for the polymerization of a broad range of monomers, including styrenic, methacrylates, acrylamides, and acrylates monomers. This abstract briefly describes PET-RAFT techniques and highlights their potential uses in optoelectronics, bioimaging, and 3D/4D printing. Understanding the full potential of PET-RAFT polymerization and its ever-expanding goals in both academic- and industrial-scale applications.

#### • General mechanism of PET-RAFT :



#### Photoinitiator :



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## **A review on metallization techniques for additively manufactured polymer antenna**

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### **Abstract**

The rapid advancement of additive manufacturing (AM) technology has resulted in a revolution in the manufacture of complex structures made of a range of materials. Furthermore, the combination of AM and metallization techniques has emerged as an innovative method for creating functional and customizable metal-polymer hybrid structures with lightweight, high strength, complex geometrical structures, and added characteristics such as electrical or thermal conductivity and higher surface quality. As a result, these approaches are frequently employed for antennas used in aircraft and space technology. Much study has been conducted globally in this growing field. So, the purpose of this work is to explore the ways for increasing the performance of 3D printed polymer antennas through the use of various metallization processes by reviewing literatures available. To create comparisons indicating the most efficient use of material for producing an antenna, metallization processes are analyzed, along with a categorization based on materials employed. The major emphasis here is on the effectiveness of various approaches in terms of deposition, adhesion property, electrical conductivity, and characteristics of metallic coatings formed on polymers. As a consequence, this will give insight into the materials used for 3D printed antennas, as well as the numerous common and non-traditional metallization processes used. This article examines current advancements in 3D printing and metallization processes as they apply to polymer antennas. It investigates the field's possible uses, problems, and future possibilities.

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## Conducting Polymer Based on Dibenzofluorene and Anthraquinone Moiety for Optoelectronic Device Application

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### Abstract

Conducting polymers or synthetic monomers have revolutionized the world and are at the heart of scientific research having a scope of vast diverse applications in many technological fields. The conducting and redox polymers have been investigated as energy storage systems because of their better sustainability, ease of synthesis, and environmental compatibility. Blue light emitting conjugated co-polymers with alternating alkyl/allyl dibenzofluorene and substituted diphenyl anthracene units were synthesized by aromatic nucleophilic substitution reaction. The characterization and synthesis of light emitting -polymers derivatives connected via ether linkage reported in present work. The obtained polymers were stable solid and soluble in various organic solvents like THF, DMSO, CDCl<sub>3</sub> etc. The structural and optical characterization was done by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, FTIR, XRD, UV-Vis and photoluminescence spectroscopy respectively. The thermal study of polymer showed that they were thermally stable to varying degree. The electrical and optical properties of the polymer derivative showed the properties promising for the fabrication of efficient blue light emitting devices.

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## Bio-Based Bisphenol Containing Built-in Alkoxy Groups as a Building Block for Synthesis of Aromatic (Co)poly(ether sulfone)s Bearing Functional Groups via Post-polymerization Modification

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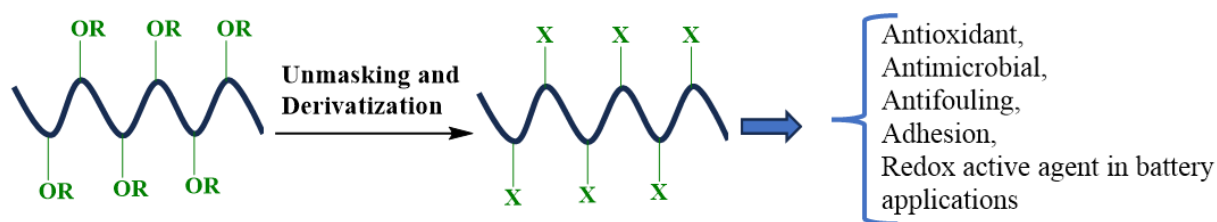
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### Abstract

A new bisphenol monomer containing built-in alkoxy groups was conveniently synthesised by acid-catalysed single step reaction of biobased aldehyde and phenol. Aromatic nucleophilic substitution polycondensation of biobased bisphenol or varying compositions of biobased bisphenol and bisphenol A with bis-(4-phenyl sulfone) in a solvent mixture of N,N-dimethyl acetamide and toluene afforded (co)poly(ether sulfone)s fitted with alkoxy groups. The formation of random copoly(ether sulfone)s was inferred from <sup>13</sup>C NMR spectroscopic studies. Inherent viscosity and number average molecular weight values of (co)poly(ether sulfone)s were in the range 0.80–1.30 dL g<sup>-1</sup> and 80000–110000 g mol<sup>-1</sup>, respectively indicating formation of reasonably high molecular weight polymers. (Co)poly(ether sulfone)s could be cast into clear, transparent and flexible films. TG analysis indicated their good thermal stability while T<sub>g</sub> values decreased with increase in mole % incorporation of bio-based bisphenol monomer. The built-in alkoxy group present in (co)poly(ether sulfone)s were conveniently deblocked resulting in the formation of (co)poly(ether sulfone)s possessing pendent functional moieties. By virtue of the presence of functional groups in the constituent repeating units of bio-derived (co)poly(ether sulfone)s, these functional polymers are anticipated to exhibit characteristic properties such as antioxidant, antimicrobial, antifouling, adhesion to dissimilar surfaces and could find applications as redox active agent in battery applications, speciality coatings and as membrane materials.



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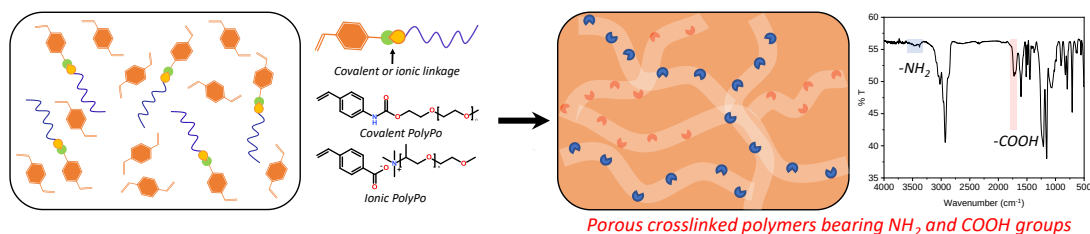
## Polymerizable Porogens: Synthesis of multifunctional porous polymers and the influence of branching in the porogenic segment of structure of porous polymers

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### Abstract

Porous materials have been recently used for gas storage for catalysis, sensors, precursors of carbon materials, photonic bandgap materials, filtration membranes, chromatographic packing materials, electrode materials for energy storage, and for many other such applications. Control of porosity, pore size, pore connectivity, and pore functionalization are primary parameters that define the functionality and utility of porous polymers. The preparation of porous polymers with a high density of functional groups lining the internal pore walls can be achieved by the use of polymerizable porogen (PolyPo), wherein the porogenic segment is linked to the polymerizable moiety either via a readily cleavable covalent bond<sup>1</sup> or is electrostatically bound as a counterion.<sup>2</sup> The pore size varied with the size of the porogenic segment in both cases. More recently, we explored an exciting possibility of preparing mesoporous monoliths, carrying both amine and carboxylic acid groups, in a single step;<sup>3</sup> here, polymerization of DVB was done in the presence of a covalently linked PolyPo (source of amine) and an ionic PolyPo (source of carboxylic acid), as shown in the schematic below.



It was noticed that the porogenic segments of the two porogens do not collocate, but microphase separate independently during the polymerization and hence leave behind amines and acid groups in distinct pores within the same matrix; this approach opens up an opportunity to design multifunctional catalytic matrices. The pore size and structure of porous polymers is expected to be influenced the molecular structure of the porogen; in order to examine this aspect, we prepared a series of ionic PolyPo, wherein the topology of the ammonium counter-ion is varied in while keeping its molecular weight constant. This permitted us to examine examined the influence of branching in the porogenic segment of the PolyPo on the nature and and porosity of the porous polymers that are generated.

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## Inulin based crosslinked superabsorbent hydrogel: Synthesis and characterization.

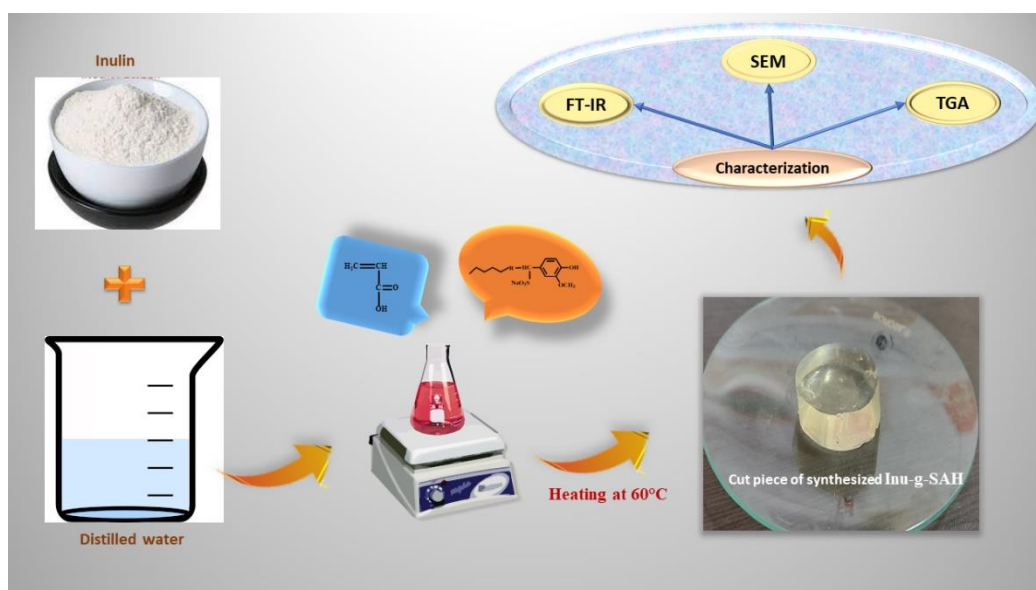
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### Abstract

Inulin (Inu) is a natural, highly abundant storage fructan polysaccharide with  $\beta$ -D- (2  $\rightarrow$ 1) fructosyl fructose units with chain length varying between 2 to 65 fructose units. It is biocompatible, biodegradable, and nontoxic. It has the potential to survive the acidic environment. In consideration of these beneficial effects, in recent years, the interest in inulin has been concentrated on its chemical derivatization to obtain systems suitable for various purposes. The aim of this work is the preparation and characterization of new hydrogel based on Inulin and acrylic acid via chemical cross-linking agent N,N'-Methylenebisacrylamide (MBA) for its application in highly acidic conditions. The prepared Inulin-g-poly(acrylate) hydrogel (Inu-g-SAH) was thoroughly characterized by FT-IR, SEM, and TGA to observe the structural, morphological and thermal changes occurring during the synthesis process. The influence of the amount of initiator and cross-linker on the swelling property was also assessed. FT-IR confirmed the grafting obtained in Inu-g-SAH through MBA. The thermal and morphological analyses revealed that the hydrogel exhibited improved thermal properties, with a 32.4% improved residual mass and porous and visibly crosslinked appearance compared to pure inulin. The hydrogel showed remarkable swelling in distilled water (20642%) and the degree of swelling was found to be inversely proportional to the cross-linker concentration. Due to its unique properties, this synthesized hydrogel is anticipated to be an efficient adsorbent for dyes even in acidic conditions of industrial wastewater.



## Moringa oleifera gum-cl-acrylic acid/polyethylene glycol-based hydrogel: Future scope for wound healing application

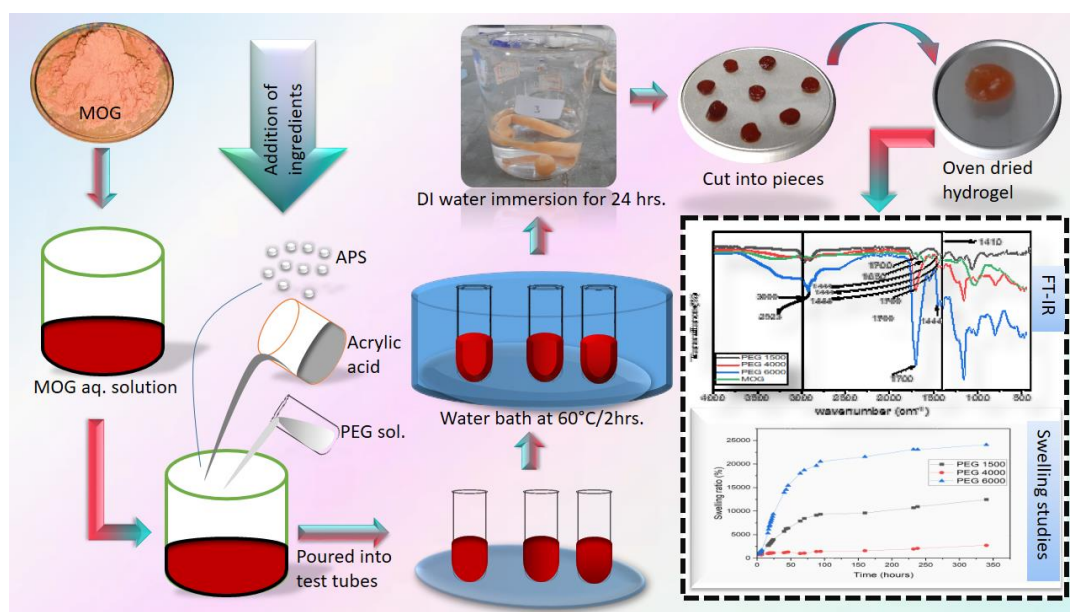
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### Abstract

A chronic wound is difficult to heal, repeated bacterial infection may lead to complex clinical problems. In the wound healing progression drug delivery using hydrogel was found very impactful. Hydrogel fabrication using natural gum is a promising candidate to strengthen the healing process and resist bacterial infection. Hydrogels synthesized from natural gum include characteristic features like low cost, biodegradability, and biocompatibility. The present study focuses on the synthesis of a novel hydrogel using *Moringa oleifera* gum and acrylic acid. Polyethylene glycol (PEG) of different molecular weights was used as a cross-linker in the presence of ammonium persulphate as an initiator. *Moringa oleifera* gum-cl-acrylic acid/polyethylene-based hydrogel was further characterized for FT-IR evaluation. Results from FT-IR confirmed the formation of a polymeric network with successful crosslinking. Thermal behavior was studied using TGA in which three-step degradation was observed. A rheological study was carried out using a rheometer, in which amplitude sweep data reveals a higher storage modulus than loss modulus at every strain value. *In vitro* swelling studies data displayed, the hydrogels cross-linked with higher molecular weight of PEG provide maximum swelling percentage (24091%). Furthermore, the synthesized hydrogel was assumed to be useful in wound healing applications.



## Phthalate Free Electron Donors for Ziegler-Natta Catalyst and Propylene Polymerization

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### Abstract

Industrially, phthalate based Ziegler-Natta catalysts have been used extensively for the commercial production of Polypropylene (PP) and use of electron donors lead to improved performance of Ziegler-Natta catalyst systems.<sup>1</sup> As phthalate based systems has caused regulatory and human health concern, so it has become obvious to replace the phthalate-based catalyst systems with non-phthalate systems. In this regard, novel non-phthalate based Ziegler-Natta catalyst have been synthesized. The non-phthalate molecules synthesized in lab is from bio-based precursor. Phthalate free Ziegler-Natta catalyst is synthesized using these bio-based internal electron donors. Catalyst performance is evaluated in propylene polymerization and found to be active and showing good stereo-specificity.

This work represents a synthesis of novel Ziegler-Natta catalyst comprising bio-based derivative as internal electron donor. The Ziegler-Natta catalysts has non-toxic, environment friendly internal electron donor and afford production of polypropylene with excellent isotacticity.<sup>2</sup>

## Controlled Synthesis of PVDF based Affinity Membrane and insight to the Mechanism of Activation

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### Abstract

A new “grafting from” strategy for grafting of different monomers covalently on commercially available poly(vinylidene fluoride) backbone is designed using ATRP for the fabrication of affinity membrane. Random copolymers of Furfuryl Methacrylate, Oligoethyleneglycol Methacrylate, Di(ethyleneglycol)methylether Methacrylate and n-Butyl Methacrylate are covalently grafted on PVDF backbone by ATRP. The initiation mechanism of controlled grafting of these polymethacrylates from PVDF backbone has been established for the first time by XPS analysis using C-F bond activation via halide exchange technique. The reactive furan rings present in the substitution of grafted PFMA chains are subsequently used as ‘dienes’ for Diels-Alder cycloaddition reaction with maleimides. This allowed installation of specific H-bonding capable moieties showing preferential immobilization of adenine, melamine and uracil. Analysis of polymerization kinetics, molecular weight with monomer conversion and Size Exclusion Chromatography has shown a nicely controlled graft copolymerization initiated by PVDF backbone as macroinitiator. <sup>1</sup>H-NMR spectroscopy has been used for structure elucidation and calculation of absolute molecular weight of the graft copolymers. The FTIR analysis indicates shift of PVDF crystallites from  $\alpha$ -polymorph to  $\beta$ -polymorph with grafting of polymethacrylate chains. A spherulitic morphology of the PVDF which gets shifted to self aggregated spherical morphology in the graft copolymers as observed from FESEM and AFM analysis of the DMF casted solvents. Membrane fabrication by the synthesized graft copolymers are conducted following ‘*breath figure*’ followed by ‘*immersion precipitation*’ techniques. This results in development of membranes having temperature dependent porous surfaces enriched with polar/hydrophilic graft copolymeric chains resulting better anti fouling property with lysozyme and BSA.

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## Synthesis and Characterization of Oligoglycerol based Dendronized Amphiphilic Polythiourethane

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### Abstract

The micellar and liposomal structures are sensitive to dilution as their stability depends on a critical micellar concentration (CMC) for self-assembly. Leaching of the encapsulated drug in the bloodstream is a major inherited problem in micellar systems due to stability and infinite dilution during intravenous application.[1] In this regard, amphiphilic polymers are more advantageous than small molecule-based amphiphiles due to their low CAC and high stability in aqueous solution. Polyurethanes (PUs) are known for ease of synthesis and intra/inter molecular H-bonding, leading to the folding of the polymer backbone, resulting in different nanostructures ranging from polymersome to spherical micelles. PUs are traditionally synthesized by the polyaddition of diols with diisocyanates in the presence of a catalyst. [2] It is challenging to get rid of phosgene which is used for the preparation of diisocyanates. Due to such toxicity and reactivity of isocyanates to moisture[3], greener approaches were developed to synthesize PUs. Among these, the non-isocyanate (and thus phosgene-free) PUs (NIPUs) are mostly explored using the polyaddition reaction of di- or polyfunctional cyclocarbonates with di- or polyfunctional amines. Such ring opening leads to the formation of primary or secondary hydroxyl groups. But the post-modification or reactivity of these hydroxyl groups is difficult, limiting the further scope of functionalization in the backbone. During polythiourethane synthesis, more reactive free thiols are produced, further being utilized to functionalize the backbone.[4,5] In this project, oligoglycerol based AB type polythiourethane synthesized in one pot using dithiocarbonate and diamine as monomers. In addition, self-assembly of such polymers will be shown as well.

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## Photoinduced Electron Transfer-Reversible Addition–Fragmentation Chain Transfer (PET-RAFT) Polymerization by New Organic Photocatalysts under Blue Light Irradiation

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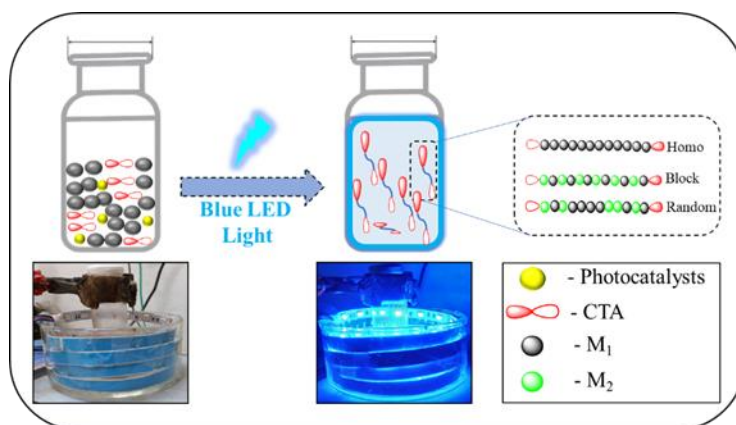
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### Abstract

Photoregulated controlled polymerizations are mostly conducted in the short wavelength region such as UV region. It is neither friendly to the environment (the greener approach) nor to the human body. In chemical reactions, the short wavelength source does not have deep penetration and may cause unreacted starting material or unwanted side products. The organic photocatalysts (PCs) have the advantage of easy operation in ambient environment and low toxicity when compared with metallic catalysts. We herein report new organic small molecule PCs for photoinduced electron transfer-reversible addition–fragmentation chain transfer (PET-RAFT) polymerization of various acrylates and methacrylates, which can be activated by irradiation with visible (blue) light ( $\lambda_{\text{max}} = 522 \text{ nm}$ ), that is the “ON and OFF” reaction having the temporal control on polymerization can be effected. The precision polymers were thus synthesized within hours under blue light irradiation with excellent control over the molecular weight and polydispersity. The kinetics study of polymerization revealed the pseudo-first-order reaction, indicating good control by the studied PCs.



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## Acryloyl-L-Serine Derived Polypeptides with Stimuli-Responsiveness, Amphiphilicity and Gelation

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### Abstract

Development of synthetic polypeptides with functional diversity is one of the most important area of research over many years as their structural conformations and functional behaviors are similar to natural proteins. Incorporation of specific functional groups introduces stimuli-responsiveness to the polypeptides and makes them potentially important materials for applications in biomedicine and advanced biotechnology. Thus, the aim is to develop such kind of functional polypeptide materials, which involves designing and synthesis of a new NCA monomer based on L-serinylacrylate (SerA NCA) and subsequent ring-opening polymerization to obtain poly(acryloyl-L-serine) [P(AcSer)]. The functionalization of P(AcSer) produces zwitterionic polypeptide, amphiphilic polypeptide and polypeptide-based crosslinked organogel and hydrogel materials employing thiol-ene Michael and radical polymerization reactions respectively. The covalent grafting of L-cysteine with P(AcSer) embellishes zwitterionic polypeptide, P(AcSer)-g-Cys, which exhibits dual pH- and UCST-type thermo-responsiveness in water. Moreover, the P(AcSer)-g-Cys molecules associated together at the pHs of 2.2-41, forming insoluble spherical nanoaggregates which further aggregate among themselves into different shaped dendrimeric morphologies. The efficient tailoring of P(AcSer) with thiolated triethyleneglycolmonomethylether (MTEG-SH) introduces amphiphilicity to P(AcSer)-g-MTEG, which resulting in a LCST-type phase behaviour in water and formation of vesicles as confirmed from DLS, FEG-TEM and cryo TEM. The crosslinked polypeptide gels with remarkable swellability in organic solvents are prepared by crosslinking P(Ac-Ser) with thiol-based crosslinkers (HDT and PETMP). The crosslinking of P(AcSer) chains with ionic liquid crosslinker develops a hydrophilic polypeptide gel capable of efficient removal of anionic dye.

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## Alkyl Side-Chain Functionalization of Poly(L glutamate) can Introduce Thermoresponsiveness, Self-Assembly and Semicrystallinity

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### Abstract

The proper functionalization is prerequisite for synthetic polypeptides to incorporate amphiphilicity and responsiveness towards external stimuli.<sup>1</sup> In solution, the amphiphilic character allows their self-assembly into nanostructures such as micelles and vesicles, which find applications as drug carriers and tissue engineering scaffold.<sup>2</sup> This study reveals the functionalization of poly(L-glutamate)s with long chain alkyl groups for introducing stimulus-responsiveness, self-assembly behaviour and semicrystallinity. The synthesis involves ring-opening polymerization (ROP) of  $\gamma$ -propargyl-L-glutamate N-carboxyanhydride to yield poly( $\gamma$ -propargyl-L-glutamate) (PGlu-Pr). Subsequently, the pendant propargyl groups of the PGlu-Pr are clicked with as-synthesized long-chain alkyl azides through Cu-catalyzed alkyne-azide-cycloaddition (Cu-AAC) reaction, resulting in the formation of alkyl-grafted poly(L-glutamate)s [PGlu-C<sub>n</sub>(s), n = 10, 12, 16, 20]. Both PGlu-Pr and PGlu-C<sub>n</sub>(s) exhibit helical secondary conformations in solution phase (THF) and in solid state, with decreasing degree of helicity as the alkyl chain length increases. In comparison, the proper array of control monomeric analogs, alkyl grafted L-glutamates (Glu-C<sub>n</sub>s), reveal the formation of birefringent crystals due to the presence of long alkyl chains, as confirmed through differential scanning calorimetry and polarized optical microscopy. Notably, PGlu-C<sub>n</sub>(s) with n  $\geq$  12 exhibit partial crystallinity in the solid state. Intriguingly, unlike Glu-C<sub>n</sub>(s), CHCl<sub>3</sub> and THF solutions of PGlu-C<sub>n</sub>(s) exhibit upper critical solution temperature (UCST)-type phase behaviour with an adjustable cloud point. The vesicular nanoaggregates are generated by the self-assembly of PGlu-C<sub>n</sub>(s) in these solvent as confirmed via dynamic light scattering and transmission electron microscopy. These nanoaggregates demonstrate the ability to encapsulate organic dye, as observed through fluorescence spectroscopy and confocal microscopy.

## Gallic Acid Based Rust-Conversion and Corrosion-Resistant Coating Through Mini Emulsion Process

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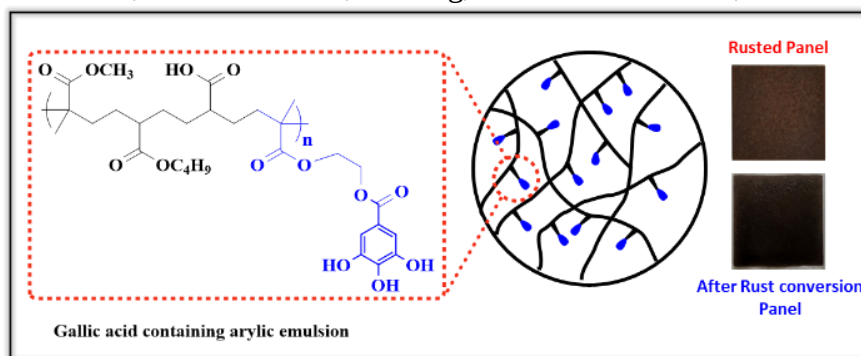
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### Abstract

The term "corrosion" refers to the process of material qualities degrading as a result of numerous electrochemical processes. It is a natural, unavoidable process that affects the strength and longevity of the materials as well as costs money and time. Gallic acid, a naturally occurring polyphenolic compound found in plants, possesses inherent properties that make it effective for rust conversion as well as for corrosion resistance when applied on metal surfaces due to the phenolic hydroxyl groups which can chelate it with the metal ions. In this work, we have incorporated the gallic acid functionalities in the back bone of an acrylic polymer matrix in a high solid acrylic emulsion through mini emulsion polymerization and studied its rust conversion and corrosion resistance performance. Initially gallic acid was modified with 2-hydroxy ethyl methacrylate (HEMA) to get a polymerizable gallic acid ester (GAHEMA) and characterized using NMR, FTIR and LCMS. This GAHEMA was incorporated in a high solid acrylic emulsion of methylmethacrylate/butyl acrylate/acrylic acid with varying weight percentage (0-2.5%) of GAHEMA to get rust conversion and corrosion resistant coating. The average solid content was 58.6 wt% and these emulsions are stable for more than 6 months which was characterized using particle size analysis. We observed that 0.5 % reaction showing very good rust conversion performance while 1 wt% reaction showing best corrosion resistance performance, studied using EIS and PDP studies. Thermo-mechanical properties have been analyzed using TGA, DSC and UTM. This novel coating showed best in class performance compared to the reported gallic acid-based systems.

**Keywords:** Gallic acid, rust conversion, coating, corrosion resistance, and metal protection,



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## Multi-stimuli Responsive Smart Polymeric Materials bearing Reactive Pendant Functionalities

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### Abstract

Designing multi stimuli responsive smart polymer material bearing reactive pendant functionalities has gained attention among the scientific fraternity and could serve as a potential alternative in various applications. poly(glycidyl methacrylate) (PGMA) is one of the most versatile reactive scaffolds in polymer chemistry due to the general adaptability of these functionalization. Numerous functionalities can be added to the reactive scaffold through post-polymerization modification of poly(glycidyl methacrylate) (PGMA) using nucleophilic ring opening reactions of the pendent epoxide groups.[1,2] In all circumstances, if many functionalized polymers are desired, consecutive post-synthesis modification processes can also be carried out. Which brings a wider versatility to the material and enhances its applicability. In the present work, we present the development of magnetically recyclable iron-catalyst mediated photoRDRP of glycidyl methacrylate (GMA) and synthesis of well-defined dual stimuli responsive PGMA containing diblock copolymers thereof via iron-mediated sequential photoRDRP followed by post-polymerization modification. Detailed investigation of the physicochemical properties of the synthesized polymers were carried out to understand their potential applications.[3]

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## Imine Thiophene-Ligated Cr-Complex as Single Site Catalyst in Ethylene Polymerization<sup>†</sup>

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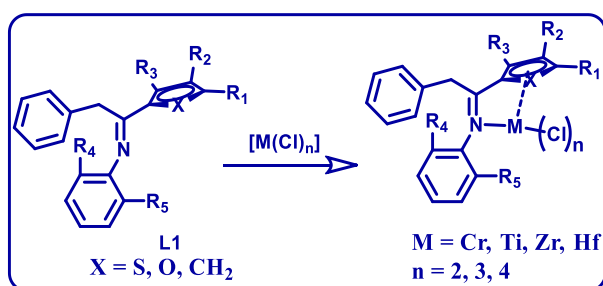
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### Abstract

Polyethylene is the single largest volume polymer produced globally. Majority of this is produced using Ziegler type catalysts. However, Ziegler-type (ZN) catalysts are known to produce polyethylene (PE) with broad PDI. Sometimes, broad PDI is unacceptable and therefore production of PE with narrow PDI is desired.<sup>1</sup> On the other hand, single site catalysts such as titanocene or zirconocene can produce PE with narrow molecular weight distribution. Such PE shows property enhancement, for example, metallocene PE has better puncture resistance than ZN PE.

In our attempts to prepare single site catalysts, we report designing and synthesis of an imine-thiophene ligand L1.<sup>2</sup> The ligand L1 was treated with early transition metals (Cr, Ti, Zr) to generate single site homogeneous catalysts. The identity of these catalysts was unambiguously ascertained using a combination of NMR, ICP-AAS, and ESI-MS, etc. Subsequently, these catalysts were tested in ethylene polymerization using MMAO as cocatalyst and produced high-density polyethylene (HDPE) with a narrow polydispersity index (PDI) of 1-2. The PDI suggests single-site behavior, reflecting precise control over polymerization. Interestingly, the chromium-based catalyst exhibited superior activity compared to Ti and Zr counterparts, indicating its efficiency under optimized conditions. Thermal properties of synthesized polymer were assessed using differential scanning calorimetry (DSC), which revealed melting temperatures in the range of 139-143°C and crystallinity surpassing 50%.



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[†] We acknowledge GAIL India Ltd. for financial support for this collaborative R&D work.



## Comb like polymer poly(alkyl methacrylate) as polymer additive and its rheological study for waxy crude

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### Abstract

Polymers with various alkyl chains have a wide range of applications in petroleum industry as a pour point depressant (PPD)/flow improvers (FI) for crude oil. Reversible Addition Fragmentation Chain Transfer (RAFT) polymerization technique has been employed to synthesize poly(octadecyl methacrylate) (POMA) of different molecular weights (MW) using 2-cyano-2-propyl-4-cyanobenzodithioate as a chain transfer agent. The effect of various reaction parameters on MW and molecular weight distribution (MWD) of POMA has been investigated. Analytical techniques such as FT-IR and NMR spectroscopy confirm the formation of POMA whereas MWs were obtained from Size Exclusion Chromatography (SEC) analysis. The performance evaluation study of synthesized POMA on the flow properties of crude oil were investigated rheometrically. The SEC results show that the number average molecular weight ( $M_n$ ) of the synthesized POMA increases linearly with conversion. The RAFT polymerization produces polymers with much narrow MWDs (1.19-1.35) as compared to that in conventional radical polymerization ( $MWD > 2$ ). Under the optimum condition, the prepared polymer, POMA, reduced the apparent viscosity of the crude to approximately 50% at temperature 5°C. Also, in the temperature range 5-20°C, the crude oil shows shear thinning behaviour, i.e. the apparent viscosity decreases with increase in shear rate. Thus, the reduction in the apparent viscosity signifies that synthesized POMA act as effective polymeric additive for crude oil at low temperature.

**Keywords:** Apparent viscosity; Flow improver; Pour point depressant; POMA; RAFT

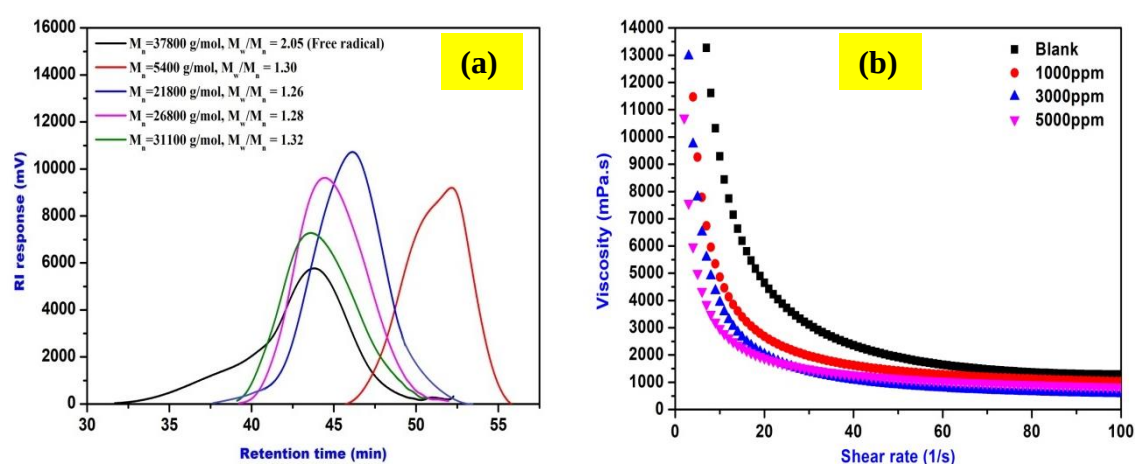


Fig. a) SEC traces of synthesized POMA and b) Effect of POMA on viscosity of waxy crude

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## Poly(eicosyl methacrylate) *via* reverse ATRP and their Evaluation as a Flow Improver for Model crude oil

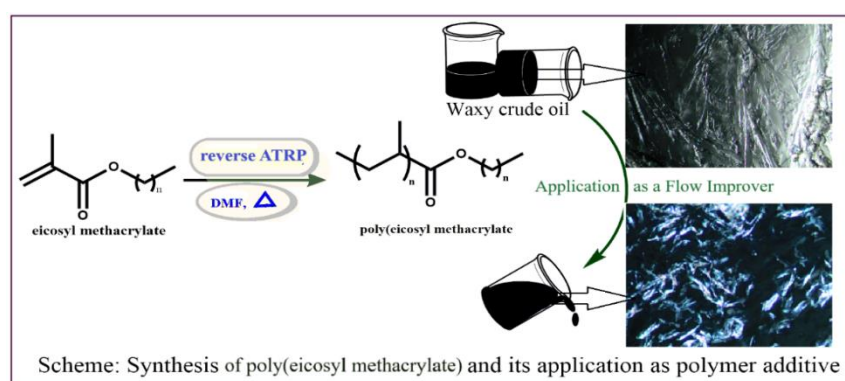
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### Abstract

Escalating energy demand and diminishing petroleum reserves have drew attention to the exploration of cost-effective techniques to efficiently transport high-viscosity, high-pour-point crude oil, addressing challenges like pipeline transport in low temperatures and associated wax depositions. For this purpose, controlled polymerization of comb-type polymer eicosyl methacrylate (EMA) was carried out *via* reverse ATRP using 2,2'-azobisisobutyronitrile (AIBN)/FeCl<sub>3</sub>/2,2'-bipyridine (bpy) as initiating system in N, N-dimethylformamide (DMF). The number average molecular weight ( $M_n$ ) of the synthesized poly(eicosyl methacrylate) (PEMA) shows a linear increase with monomer conversion with much narrow molecular weight distribution ( $M_w/M_n$ ) values in the range 1.20-1.55. Spectroscopic techniques such as FT-IR, NMR studies confirmed the formation of PEMA while the X-ray diffraction analysis confirmed the amorphous behavior of PEMA. The synthesized PEMA was evaluated as flow improver on model crude oil through rheological analysis and wax crystal morphological study. The results indicates that the addition of PEMA improved flowability of the model oil as well as effectively modulated the wax crystal morphology. From the rheological analysis, the addition of PEMA reduces yield stress and viscosity by more than 70 %. On the otherhand, apparent viscosity decreases with increase in shear rate at lower temperatue range. The wax crystal morphological observation by polarized optical microscopy shows that PEMA can strongly crystallize with wax molecule and tigger the formation of compact regular platelet like wax crystal, which greatly improve the rheological properties of model crude oil.



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## DLP 3D Printing demonstrated using Modified PEEK Polymer

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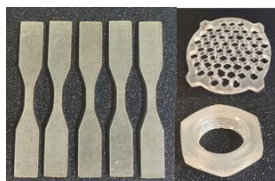
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### Abstract

Polyether ether ketone (PEEK) belongs to a family of high performance engineering thermoplastics, that finds wide application in automotive and aerospace industries. With the advances in Additive Manufacturing or 3D printing technology, increasing efforts are directed towards utilization of high-performance polymers like PEEK for 3D printing. The most common reports of 3D printing PEEK are based on melting and fusion based approaches.<sup>1,2</sup> PEEK being a high melting polymer, this approach is highly energy intensive and 3D printers have to be specifically designed for this. On the other hand, light based 3D printing technologies like the Digital Light Processing (DLP) are not so energy intensive and are easy to use. For the material to be used in a light based 3D printing technology, it should have polymerizable groups or functional groups that can be activated using light. Here we report our efforts at designing modified PEEK monomers that are end functionalized with urethane acrylate moieties. Photocurable formulations comprising of the modified PEEK oligomer together with reactive acrylate diluents formed a flowable resin that could be printed using a DLP 3D printer. The structural properties of the PEEK polymers were characterized by NMR spectroscopy and the curing kinetics of the resin formulations were studied by photoDSC. The final 3D printed part exhibited excellent thermal properties with high glass transition temperature around 140 °C and 10 % degradation temperature around 400 °C. The 3D printed parts demonstrated high strength, resolution and are promising for applications in different fields like dentistry, automobile, and robotics.



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## Polymers as corrosion inhibitors for mild steel corrosion prevention

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### Abstract

Metal and alloy structures are integrated parts of refineries and chemical industries. During the service, the corrosion of the metal substrate and alloys is accelerated by the severe corrosive environment comprising various operating and atmospheric variables in addition to process chemicals.<sup>1</sup> These unavoidable conditions lead to service-equipment failure resulting in economic and human life losses. Globally, 3-5 percent of GDP is spent yearly on corrosion-related failure and maintenance.<sup>2</sup> There are various corrosion control measures to enhance service equipment's life. Recent literature indicates that corrosion mitigation can be achieved by using polymeric corrosion inhibitors.<sup>3</sup> Present research work highlights the synthesis of pentadecyl phenol functionalized polypyrroles as a corrosion inhibitor. These polymers are synthesized by cross-coupling methodology and characterized using NMR, and IR. For corrosion studies, the synthesized polymers were evaluated for corrosion mitigation under an HCl-corrosive environment. While carrying out performance evaluation studies, results indicate the better anticorrosion performance of synthesized polymers compared to standard polypyrrole polymers.

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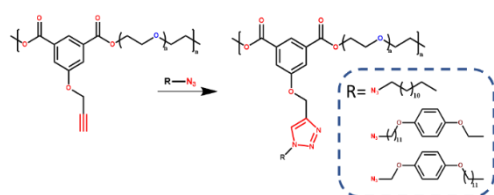
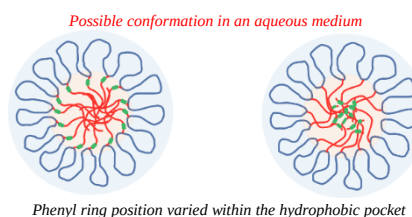
## Probing Chain Collapse in Periodically Grafted Amphiphilic Polymers

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### Abstract

A series of periodically grafted amphiphilic polymers (PGAPs), where hydrophobic segments were grafted at a regular interval was prepared; these carried hydrophilic polyoxyethylene (PEG) segments in the backbone and long alkyl chains as the hydrophobic pendant segments. Using a modular strategy, wherein propargyl units were located at periodic intervals along the polyester backbone, different types of alkyl segments were installed by azide-alkyne reactions, resulting in PGAPs carrying one alkyl segment per repeating unit. The purpose of the study was to examine the solution properties of such PGAPs both in water and nonpolar solvents, wherein they would adopt distinctly different conformations.



We had earlier observed that the proton NMR spectra of phenyl ring containing surfactants, in D<sub>2</sub>O, varied significantly depending on the exact location of the phenyl ring within the alkyl segment,<sup>1</sup> which suggested that the phenyl ring appeared to be sensing water penetration in micellar aggregates. In the present study, we extend this approach to examine the nature of the hydrophobic domains formed during the chain collapse induced by increasing solvent polarity; to do so two different systems – one where the phenyl ring is close to the tail end and the other where it is close to the polymer backbone were prepared. Likewise, alternate strategies to probe deeper within the hydrophobic pocket using covalently linked fluorophores will also be discussed, thus revealing the process of chain collapse in such amphiphilic polymeric systems. In another design a dipolar chromophore was introduced into the alkyl pendant segment of the PGAP, such that their collocation within the core region would cause net cancellation of the second harmonic light scattering (SHLS) signal; thus a measurement of the SHLS signal as a function of solvent composition can reveal the collapse transition in such PGAPs. The presentation will discuss the study of collapse transition in PGAPs using a variety of these techniques.

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## Synthesis of Well defined Soluble Coil-like Polypyridyl Appended Polymers to access Functional Side-chain Metallopolymer by Controlled Radical Polymerization

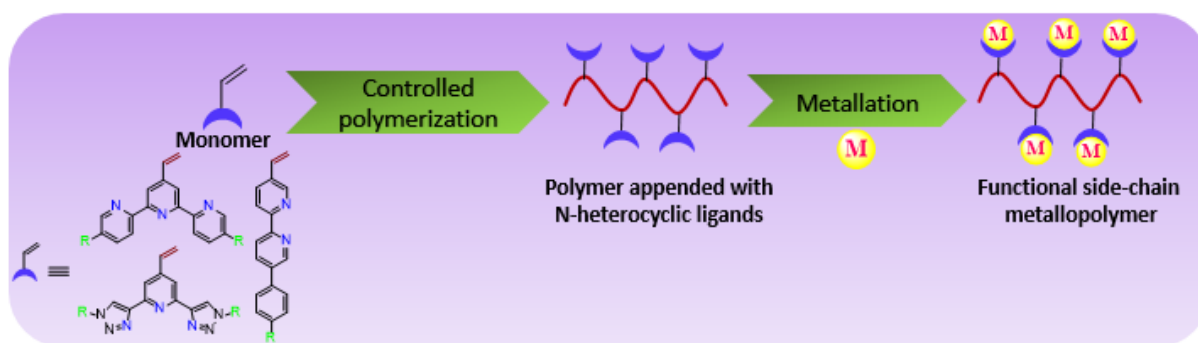
Chhanda Mondal<sup>a</sup>, Chinmoy Kumar Behera<sup>a</sup> and Sanjib K. Patra<sup>\*a</sup>

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### Abstract

Functional polymers appended with chelating sites to access soluble and processable side-chain metallo-polymers are emerging class of easily processable materials for its smart applications such as macromolecular catalysis, photovoltaics, organic light-emitting diodes, lithography, patterned array of metal nanoparticles and data storage, stimuli-responsive and self-healing materials.<sup>1,2</sup> Facinated by the emerging opprtunity of the metallopolymers, our work focuses on the developemnt of soluble side-chain metallopolymers with targeted applications. We have designed and developed functionalized N-heterocyclic based polymerizable monomers. Controlled radical polymerization (NMP and RAFT) succefully provides soluble and flexible coil-like homo/copolymers with pendant N-heterocyclic chelating units. For solubilizing in common organic solvents, a alkyl/alkoxy chain either C-alkylation or N-alkylation to monomers have been introduced. The well-defined polymers have been characterized by multinuclear NMR and tetradetector GPC with a expected average molecular weight and a narrow molecular weight distribution as manifested by the excellent PDI values demonstrating good control of the polymerization. The macromolecular complexation with suitable transition metal precursors will offer various interesting stimuli-responsive applications such as self-healing, shape-memory and self-assembly. Our preliminary attempt on design, synthesis and exploring properties will be presented.



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## Design and synthesis of fluorene based zirconocene catalysts for ethylene polymerization

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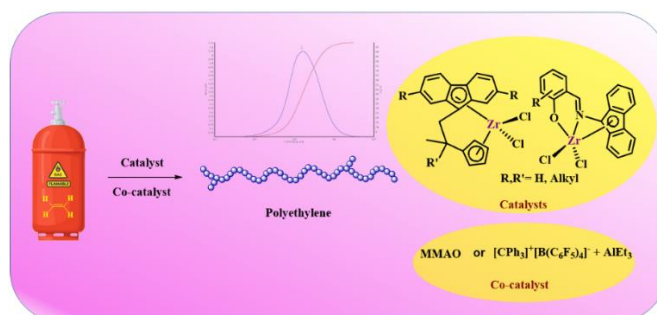
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### Abstract

Discovery of group 4 metallocene olefin polymerization catalyst introduced a new era in polymerization industry and showed significant advancement in this field accompanied by increasing number of catalyst commercializations.<sup>1</sup> Substantial efforts have been devoted on the development of novel catalyst systems by modifying the catalyst structures addressing steady growth in the demand for tailor-made metallocene grade polymers.<sup>2,3</sup> In this work, we have developed indegeous Zr(IV) catalyst systems containing fluorene moiety. The ethylidene-bridged zirconocene catalysts were synthesized with varying bridging atom substitutions, altering steric and electronic factors to influence catalytic behaviour and polymer properties, using a series of stepwise reactions starting from fluorene.<sup>4</sup> While, another set of half-metallocene complexes of phenoxy-imine ligands were designed with a focus on achieving efficient and cost-effective catalysts for ethylene homo and co-polymerization. Both the catalyst systems showed high to moderate catalytic activity in ethylene polymerization on activation with suitable activator like MMAO or trityl borate/aluminium alkyl under low ethylene pressure and produced polymers with molecular weight in the order of  $10^5$  g.mol<sup>-1</sup> and monomodal molecular weight distribution. The polyethylen samples were characterized with high temperature GPC and differential scanning calorimetry (DSC). The preliminary results of design, synthesis and catalytic performance of those indigenous catalyst systems will be presented.



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## Thermal and rheological analysis of *Cassia fistula*-based hydrogels

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### Abstract

In recent decades, plant-derived polymers have gained significant interest within the realm of hydrogels, influencing their physicochemical, biological, and mechanical properties. *Cassia fistula* is renowned for its abundant polymer content, presenting an opportunity for the development of hydrogels with tailored properties. This study deals with the synthesis of hydrogels based on *Cassia fistula* (CA-AA) by incorporating a chemically crosslinked poly-acrylic acid backbone. Subsequently, we conducted a thorough analysis of CA-AA thermal and rheological properties utilizing state-of-the-art techniques such as Perkin Elmer's Thermogravimetric Analyzer (TGA 4000) and Anton Paar's Modular Compact Rheometer (MCR 302). The TGA analysis is primarily conducted to elucidate phase transitions and degradation temperatures, under inert atmospheric conditions. It showed that CA-AA exhibited a substantial mass percentage, approximately 67%, up to 450°C, surpassing both the control hydrogel (CA-C) and pure *Cassia fistula*, which were recorded around 60% and 50%, respectively. Furthermore, at 800°C, CA-AA displayed an impressive residual mass of over 38% in contrast to the 19% and 30% observed for *Cassia fistula* and CA-C. Additionally, an amplitude sweep test on CA-AA revealed that the elastic behavior( $G'$ ) dominates its viscous behavior ( $G''$ ) across the entire shear strain range. This finding Supports a high swelling index of hydrogel and improved elastomeric properties. <sup>12345</sup>

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## Norbornene Conjugated Small Molecular Probe-based Organogel for Removal of $\text{Cu}^{2+}$ Ions from Aqueous Media

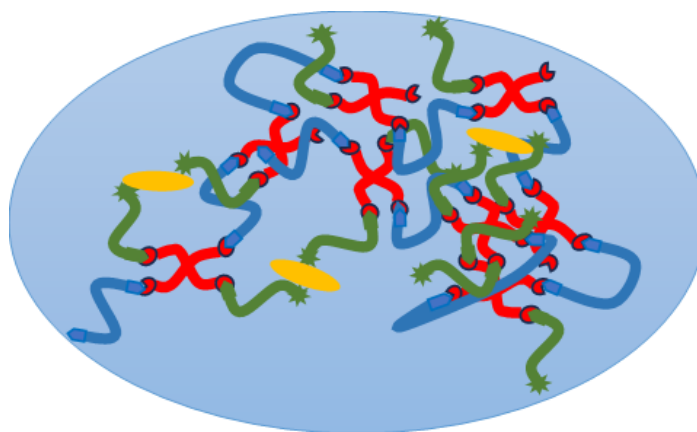
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### Abstract

Ground-water contamination is a growing concern owing to rapid industrialisation. Development of novel techniques for detection and removal of toxic chemicals and metals from water is crucial to maintain sustainable drinking water. Most common heavy metals found in fresh-water are arsenic, cadmium, chromium, copper, iron, zinc, lead and mercury.<sup>1</sup> Copper is both essential and toxic to living systems. Being an essential micronutrient and a coenzyme, it plays several key roles within the body. Copper excess/deficiency disrupt healthy metabolic function by creating mineral imbalance. Accumulation of copper in the body occurs from ingestion, inhalation and absorption; food and water being the primitive source. As per the WHO, maximum permissible limit of copper in drinking water is  $\sim 1.5$  ppm.<sup>2</sup> Also, patients with excess copper accumulation in their body tend to have abnormal copper concentration in their serum and urine. Thus, quantitative detection of copper from aqueous samples (water supply as well as biological samples) is crucial and can provide a preliminary and cheap detection of such illnesses.<sup>3</sup> Existing probes for copper detection provide low sensitivity, long synthetic protocols, need for organic solvents, etc. Additionally, not many designs are available to safely remove the metal from water without leaching of other toxicities.<sup>4,5</sup> Thus, a norbornene-based colorimetric probe was designed, that binds with  $\text{Cu}^{2+}$  ions in 2:1 ratio, providing naked-eye detection of copper from aqueous media. Furthermore, the probe, when incorporated into a macromolecular network via thiol-ene click reaction; can absorb copper from aqueous media and might be useful in water treatment and purification.



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## Fine tuning of polyfluorene backbone in molecular and aggregated level: A new strategy for HSA detection.

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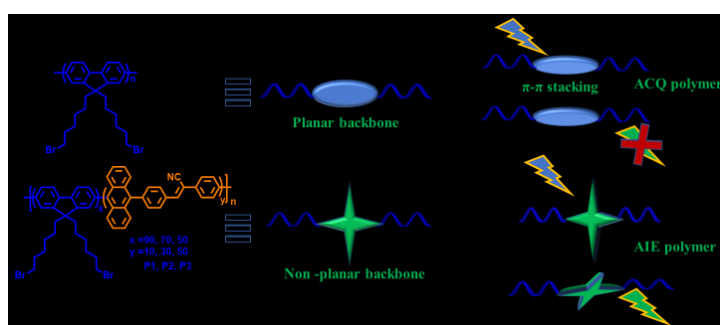
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### Abstract

Molecular movements are key features of matter and play crucial roles in their structures and behaviours. However, due to the diversity and complexity of structures and behaviours, studying motion-structure-property correlations remains a problem, particularly at all levels of structural hierarchy, from molecules to macro-objects. A series of Conjugated polymer (CPs) P1, P2 and P3 were developed by incorporating different mole fraction of AIE monomer into the polyfluorene backbone in order to unravel the correlation between photophysical property and their structure-property relationships at the molecule and aggregate levels. By changing the mole fraction of AIE monomer the photophysical properties of the resulting copolymers are highly tuned which are quite useful for various types of application. Further, the PFAN polymer is utilized for the light up detection of HSA. The method of detection is direct and ratiometric and can be utilized for the real analysis of various disorder in our body.

**Keywords:** Conjugated polymer, molecular wire effect, ACQ, AIE, light up, ratiometric



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## Study of poly(ether-imide)s post introducing Triptycene moiety

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### Abstract

Aromatic polyimides are well known as high performance polymers because of their outstanding thermal stability, high mechanical strength and modulus, and superior chemical resistance. Triptycene is a rigid, bulky, three-dimensional molecular unit consisting of three benzene blades protruding from a single hinge. Because of the unique structural feature of triptycene, synthesizing and charactering new polymers bearing triptycene moieties in the backbone are interesting enough to be investigated further. We have synthesized five poly(ether-imides)s namely PI 1 to PI 5. These polymers were synthesized by reacting 1, 4-bis (4-aminophenoxy)-2, 3-benzotriptycene (BAPB) monomer with commercially available five different aromatic dianhydrides in two steps. First step involved the formation of poly(ether-amic acid)s, and second was thermal dehydration of poly(ether-amic acid)s to yield poly(ether-imide)s. After synthesis of poly(ether-imide)s these polymers were characterized by Differential Scanning Colorimetry to determine its Glass transition temperature which found in range of 227-276°C., Thermal Gravimetric Analysis to determine its thermal behavior which found in between 566°C to 636°C, and X-Ray diffraction to study its morphology indicating its amorphous nature. The incorporation of 3D triptycene moiety, and multiple ether linkages increased gap between Tg and Td of poly(ether-imide)s offering them a enough processing margins and thus, the opportunities for melt processability.

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## Evaluation and Optimization of Mechanical properties of bio-polyol based Polyurethane Films.

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### Abstract

Polyurethane is a polymer material that is widely used in various applications due to its versatility and durability. It is commonly used in manufacturing foam insulation and flexible foam products, such as cushions and mattresses, as well as in coatings, adhesives, and sealants. Bio Based polyurethane synthesis involves the reaction of a diisocyanate with a renewable source of polyol, followed by a curing process. Biobased polyurethane is a renewable and sustainable material that can replace traditional petroleum-based plastics in many applications, and that can be made from materials such as plants oils, soybeans, or algae, while recycled polyurethane can be produced from post-consumer or post-industrial waste. Biobased polyols improve the energy efficiency of the production process and can reduce the carbon footprint of polyurethane manufacturing [1, 2] Properties of the Polyurethane synthesised either by bio-polyol or by recycled Polyurethane can be studied by thin films. This study focuses on the mechanical properties of the polyurethane films casting onto a flat surface of a spin coater. The polyurethane is then cured and removed from the surface to create the film [3]. The resulting films can be studied for their strength, flexibility, and chemical resistance. The mechanical properties of polyurethane, including its stress-strain behaviour and Young's modulus, depends on its molecular structure and the amount and type of additives included during synthesis [4]. This work provides insight to further optimization of Polyurethane properties by developing new biobased materials and adjusting the manufacturing process.

**Keywords:** - Biobased polyol, Sustainability, Polyurethane, Mechanical Properties.

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## Transparent Superhydrophobic Coatings of Silica Nanoparticles Using Functionalized Polyurethanes

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### Abstract

For certain materials, superhydrophobic coatings are essential to repel water on the surfaces, self-cleaning in nature, etc. Most often, silica nano-materials are immobilized on different surfaces to imparting super-hydrophobicity.<sup>[1]</sup> Merely coating silica nanoparticles on surfaces leaches out under different environments. To sort this out, we have explored a way to facilitate the strong binding of silica nanoparticles onto the desired surfaces using functionalized polymeric interactions. In general, the triazole has the ability for the hydrogen-bond-accepting and hydrogen-bond-donating ability arises out of presence of nitrogen atoms in the 2- or 3-positions and presence of hydrogen atom in the 5-position respectively.<sup>[2]</sup> Due to this ability, incorporating triazole moiety into the polymeric chain induces the inter-chain interaction and enhances the mechanical strength of the polymer to the greater extend. Here we have incorporated the phenyl triazole into the polymeric chain (i.e. polyurethane) through the end functionalization using copper(I)-catalyzed alkyne-azide cycloaddition (CuAAC) click chemistry. The synthesized alkyne terminal polyurethane and phenyl functionalized polyurethane were further characterized by <sup>1</sup>H and <sup>13</sup>C nuclear magnetic resonance (NMR), and <sup>1</sup>H spin-lattice relaxation times (T<sub>1</sub>s). Interestingly, we found that after functionalization, there is an increase in glass transition temperature (T<sub>g</sub>)<sup>[3]</sup> due to enhanced interchain interactions evident from T<sub>1</sub>s experiment. Further, T<sub>1</sub>s and spin-spin relaxation (T<sub>2</sub>s)<sup>[4]</sup> NMR experiments reveals that the spatial interactions between various protons of functionalized silica nanoparticles and those of phenyl triazole functionalized polyurethanes, indicating a strong binding. After coating functionalized silica nanoparticles to leather surface using functionalized polyurethanes, the surface exhibits superhydrophobic character, whereby having the contact angle value of more than 157 degrees with transparency.<sup>[5]</sup> We anticipate the results to help design varieties of materials with super-hydrophobicity where the structural integrity of the surfaces is retained.

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## Synergistic Enhancement of Polyethylene Characteristics through Graphene Incorporation using Catalyst-Driven Polymerization

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### Abstract

In the realm of polymer science, graphene has emerged as a pivotal additive for enhancing various properties of polyethylene (PE). Even minute quantities of graphene introduced during the extrusion process can significantly augment PE performance characteristics <sup>(1)</sup>. In this study, graphene was incorporated in-situ during the preparation of Ziegler Natta-type catalysts, featuring TiCl<sub>4</sub> immobilized on a MgCl<sub>2</sub> support. These catalysts were employed for high-pressure slurry polymerization of ethylene in hexane, utilizing triethylaluminium as a co-catalyst. The resulting polymer underwent rigorous evaluation of its rheological, thermal, and mechanical properties <sup>(2)</sup>. To draw meaningful comparisons, we also introduced graphene via a conventional melt mixing process. This finding strongly suggests that the presence of graphene via catalyst preparation promotes superior packing of polymer chains. Furthermore, similar trends were observed in the thermal and mechanical properties of the polymer. This study sheds light on a promising avenue for optimizing polyethylene properties through graphene integration and highlights the pronounced benefits of incorporating graphene via catalyst-assisted polymerization <sup>(3)</sup>.

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## Fabrication of Chitosan based Microgel Enzyme Bioconjugates and Study their Catalytic Application

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### Abstract

Microgels are a new class of "ideal" enzyme carriers causing their high enzyme loading capacity, chemical and process stability, biocompatibility and stability during manufacturing processes. In this work, we have synthesized a new crosslinked microgel platform for polymer-urease bioconjugates. The microgel enzyme bioconjugates(MBCs) have been synthesized using a specific crosslinker NHMA, as well as the naturally occurring, non-toxic monomer chitosan with styrene, and DMA with the aid of a VA044 initiator. Three different grades have been prepared by varying the amount of urease enzyme to achieve pH and thermo-responsive properties without affecting the urease enzyme activity. MBCs were well characterized by FT-IR, Powder XRD, SEM, TEM, TGA and UV-Vis. Spectroscopy. Microgel bioconjugates have well designed to avail thermal stability, pH-stability, longer storage in buffer and active microenvironment for urease enzyme to work on higher temperature and different pH level. Urea hydrolysis have analysed by BCs at 30°C, 40°C and 80°C. MBCs catalytic activity and effect of temperature, pH, crosslinking and time was studied in different parameters.

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## Biopolymer-Cellulose Nanofiber Composite Film: High Strength, Chemical Resistant and Printable Material for Packaging Application

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### Abstract

Biopolymers can be used as an alternative to single-use petroleum material.[1] However, pure biopolymeric films have poor water and chemical resistance, which is a significant barrier to their packaging applications. Thus different chemical modification has been carried out to improve the properties of biopolymer. Sometimes nanomaterial was also incorporated into the biopolymer to enhance the property of biopolymer. Nanomaterials like cellulose nanofiber, and carbon dots have been used widely to improve their properties.[2] During such modifications of the properties of biopolymer, there are harsh toxic chemicals were used. To manage these issues, green approaches are required for a sustainable and eco-friendly environment. In this report, a novel formulation of biopolymer nanocomposite was developed. The fabrication of biopolymer film used a green process to produce a highly robust, chemical-resistant system. Which can be easily colour printed on the biopolymer film for the information of food items being packed. Such high strength and chemical stability biopolymer film was achieved by utilising the electrostatic interaction between two biopolymeric materials owing to their inherent functionality by tuning the pH of the medium. The composite film was obtained by the incorporation of natural cross-linker and cellulose nanofiber, prepared from the natural source by a green fabrication process. Fabricated films show tensile strengths up to ~59 MPa after optimising the composition. The fabricated film shows stability at both an acidic and basic pH as well as resistance to different organic solvents. Thus the optimized formulated biopolymer nanocomposite film can be used as packaging and printable material with a wide scope.

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## Synthesis and Characterization of Polyethylene Furanoate (PEF) using Monomer 2, 5-Furandicarboxylic Acid (FDCA)

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### Abstract

Biomass is one of the renewable sources for obtaining value-added products, energy and fuels due its cost-effectiveness and abundance. 2, 5-furandicarboxylic acid (FDCA) is one of the valuable platform chemicals derived from biomass, having potential of replacing terephthalic acid as a monomer for bio-plastics like PEF. Polyethylene furanoate (PEF) is used for replacement of petroleum-based plastics like PET, PBT etc. as it has higher melting point, glass transition temperature, barrier and tensile strength than its petroleum-based counterpart like polyethylene terephthalate (PET) and helps in reducing greenhouse gas emission, carbon footprint. Generally, FDCA is formed from the catalytic oxidation of 5-hydroxymethyl furfural (HMF). 2, 5-diformyl furan (DFF), 5-hydroxymethyl-2-furancarboxylic acid (HMFCFA) and 5-formyl-2-furancarboxylic acid (FFCA) as intermediates are formed. The present study focuses on preparing non-precious metal oxide catalysts such as cobalt-manganese (Co-Mn) bimetallic oxide synthesized by two step process: 1) co-precipitation method using various bases followed by 2) calcination at 500°C for 4 h. The results of catalytic study revealed that 98.8% of HMF was oxidized to 38.6% FDCA, 35 % FFCA and 0.7% DFF in water. Polymerization reaction of FDCA with Ethylene Glycol is done via esterification polycondensation reaction in presence of Tin (II) octoate as a catalyst at 160-240°C in inert condition. Many studies till now showed that polymerization reaction depend on the concentration of substrates, pressure, temperature, catalyst and inert condition.

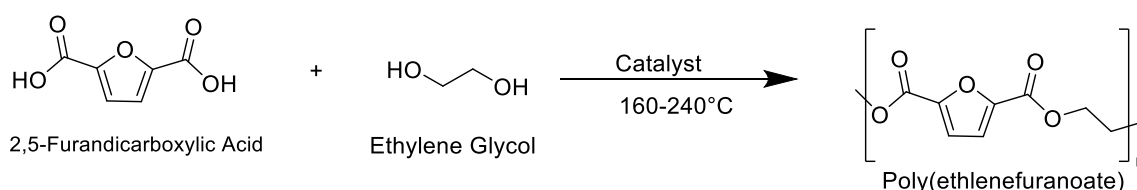


Fig. - Synthesis of Polyethylene furanoate (PEF)

Keywords: polymer synthesis, PEF, FDCA, biomass, catalysis

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## Synthesis and characterization of biobased succinic acid derived Polybutylene Succinate (PBS)

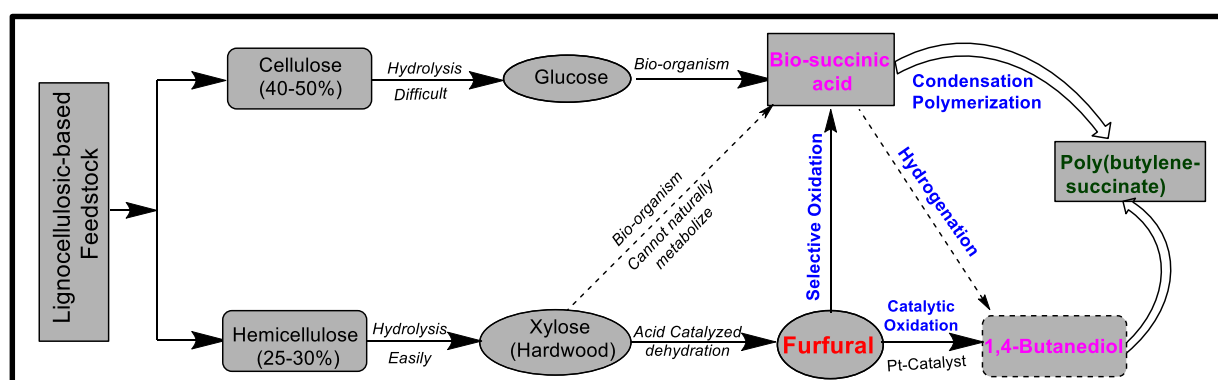
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### Abstract



Polybutylene succinate (PBS), a biodegradable polymer derived from succinic acid offers a unique combination of properties that make it suitable for mulching films, biodegradable bags, nonwoven sheets, clothing, catering supplies and foams where flexibility, good barrier properties, and resistance to moisture and chemicals are desired. It is anticipated that Global PBS production will rise from 4% in 2021 to 16% in 2026.

In this study, direct polymerization of SA and BDO and their characterization is studied in the melt condition. The polymerization consists of two steps: first, the esterification reaction occurs at temperatures from 160 °C to 190 °C under inert atmosphere in the presence of catalyst until all succinic acid is melted. In the second step, the polycondensation is carried out under a high vacuum at a higher temperature (220–240 °C) for a well-established time range.

Keywords: Succinic acid, catalysis, 1,4-butanediol, polymer synthesis, PBS

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## Structure Property Correlation Studies of Homo Polypropylene Grades of Injection Moulding Application

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### Abstract

Polypropylene, a major commodity polymer has seen continuous growth in its production since its inception in market around 1954. The high versatility of this polymer has allowed for process modifications and designing of properties to suit a vast number of applications [1]. In this work, commercially produced homo polypropylene grades applied in injection molding application are structurally characterized in terms of their methyl branching, chain structure & tacticity, crystalline phase, lamellae thickness and morphology. The structural findings are correlated with the property profile to arrive with a rationale. The insights gained through this investigation can help redesigning the polymer targeting newer applications.

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## Melt processed polylactic acid/ polycaprolactone/ sawdust based biocomposites trays with enhanced compostability

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### Abstract

The major drawback associated with petroleum-based polymer products is pollution, leading to environmental hazards. Biodegradable polymers and biocomposites have the potential to play a major role in replacing the conventional polymers in specific applications on a case to case basis. In the current study, sawdust reinforced polylactic acid/ polycaprolactone (PLA/PCL) biocomposites were developed using the melt extrusion technique. Primary processed fine sawdust was reinforced with PLA/PCL blend in a mini twin screw extruder in different weight fractions (10%, 20%, 30%, and 40%). The developed biocomposites were subjected to tensile testing, which indicated that the increased weight percent of sawdust reduced the tensile strength. The materials were further characterized, using sophisticated analytical such as field emission scanning electron microscopy, differential scanning calorimetry and thermogravimetry analysis. The composite containing 30% sawdust concentration presented the best results with tensile strength of 26.5 MPa, tensile strain of 4.4% and onset degradation temperature of 320 °C. The same formulation was successfully scaled up to the pilot level of 5 Kg batch. It was further subjected to secondary processing to produce market ready cutlery items. Biodegradability studies in simulated composting environments revealed that addition of sawdust drastically reduces the lag phase in degradation and total degradation may be obtained in approximately 90 days. Based on the investigation, there is optimism that the PLA/PCL composites, blended with sawdust may ensure commercial application of sustainable polymer blends at affordable prices.

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## Blends of Poly-hydroxybutyrate and Polypyrrole: Rheological and Mechanical properties

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### Abstract

This work highlights the effect of blending on the rheological and mechanical properties of Polyhydroxy-butyrate (PHB). PHB is biodegradable and biocompatible whereas Polypyrrole is electrically conductive and non-toxic. The miscible blends of Polyhydroxy-butyrate (PHB) and Polypyrrole (Ppy) are prepared using chloroform as solvent and Dodecyl benzenesulfonic acid (DBSA) as surfactant. The blend films of ratios 5% to 25% are prepared by the solvent casting method. The detailed rheological and mechanical characterization is carried out by rheometer, melt flow index, and universal testing machine. The melt rheology and viscoelasticity get altered by the addition of polypyrrole to neat PHB. Shear thinning behavior is observed that is influenced by shear rates drastically. Blend shows higher mechanical strength than pure PHB. To guarantee smooth process operation, rheologically optimized blends are a must for applications namely Injection molding, extrusion, blow molding, film blowing, pressure-sensitive adhesives, sensors, optoelectronics, and biomedical engineering.

**Keywords** – PHB (Poly Hydroxy Butyrate), PPy (Polypyrrole), Blend, Rheology.

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## Assessing Rheological Properties and Self-Healing Capabilities of Moringa-Chitosan based Hydrogel for Bioprinting

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### Abstract

Hydrogels have gained significant attention for their versatile applications, particularly in the field of medical 3D printing, or bioprinting and tissue engineering. This research investigates a novel hydrogel composed of Moringa and Chitosan, both natural polysaccharides. Our study focuses on comprehensively characterizing the rheological properties of this hydrogel and exploring its potential as a bioink for medical 3D printing in the medical industry. The hydrogel synthesis utilizes the Schiff's base reaction, imparting self-healing properties to the material, typically within 3 to 8 hours. We aim to deeply understand the rheological behavior of the Moringa and chitosan-based hydrogel under various conditions, including viscoelastic properties, shear thickening, and particularly shear thinning, observed during extensive rheological analysis. This examination establishes a robust foundation for prospective research into its use as a bioink for medical 3D printing. These properties, including self-healing and shear-thinning, enhance the hydrogel's potential for medical 3D printing applications. Additionally, the cross-linking of the Schiff base hydrogel typically occurs within a duration of 4 to 40 minutes. Our study represents a crucial step in realizing the potential of polysaccharide-based functional materials, contributing significantly to the fields of biomaterials and functional materials, and advancing 3D printing technology in the medical sector.

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## Influence of Spin Bath Parameters and Spinning Speed on Mechanical Properties of Viscose Filaments

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### Abstract

To convert Cellulose into usable textile material it must dissolve/derivative and convert it into other form. One of old method is to convert Cellulose by preparing Viscose solution and spun it form Viscose fiber. In this process cellulose derivatization performed of using CS<sub>2</sub> and Cellulose derivative is subsequently dissolved in NaOH. Then it is regenerated in a coagulation bath, of form Cellulose fibers/filaments. In general, the coagulation bath consists of H<sub>2</sub>SO<sub>4</sub>, ZnSO<sub>4</sub> & Na<sub>2</sub>SO<sub>4</sub> wherein H<sub>2</sub>SO<sub>4</sub> & Na<sub>2</sub>SO<sub>4</sub> plays the role of converting cellulose xanthate solution into regenerated cellulose. The ZnSO<sub>4</sub> retards the reaction to slower down the regeneration process and play critical role in fiber/filament structure formation. In this study different concentration of acid and zinc were studied along with varying spinning speed and its effect on the physical and mechanical properties of the yarn was evaluated. The yarn morphology and cross section was studied using Scanning Electron Microscopy (SEM), the orientation of cellulose in yarn was studied using Birefringence & X-ray Diffraction (XRD). From this study it was observed that with lower ZnSO<sub>4</sub> concentration tenacity of yarn increased by ~9% with the increase of ~35% H<sub>2</sub>SO<sub>4</sub> concentration in coagulation bath. Whereas at higher ZnSO<sub>4</sub> concentration the opposite trend was observed with tenacity decreasing by ~21% with similar increase bin acid concentration. In this study the effect of spinning speed was also studied, and it was observed with decreasing the speed by ~31% the average tenacity decreased by ~6.5%.

## Effect of Alumina Addition on The Gelation Behaviour Of Pluronic F127

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### Abstract

Pluronic F-127 hydrogel is a tri-block co-polymer. It becomes a solution below room temperature and converts to gel upon heating beyond room temperature [1]. Pluronic F-127 hydrogels with 14 wt.%, 18 wt.%, 22 wt.%, and 26 wt.% were studied for gelation behaviour and the transition temperatures. From the visual observation, it is found that the hydrogel below 18 wt.% shows liquid at room temperature above 18 wt.% Pluronic F-127 hydrogel becomes solid gel at room temperature. For 14 wt.% of Pluronic F-127 hydrogel no gelation transition temperature was observed. For 18 wt.% hydrogel, the gelation temperature was observed to be 26.1 °C, for 22 wt.% hydrogel, the gelation temperature was 22.1 °C and for 26 wt.% showed the gelation of 16.1 °C. The gelation temperature decreased with increase in wt. % of Pluronic-F127. Subsequently, when 65 wt.% alumina was added to this hydrogel, drastic changes in gelation temperature were observed for all the samples. 14 wt.% hydrogel with alumina shows a gelation temperature of about 22.8 °C, which was not observed in the pure hydrogel. The gelation transition temperature of 65 wt.% alumina loaded 18 wt.% hydrogel was 19.1 °C, for 22 wt.% hydrogel with 65 wt.% alumina it was 13.8 °C, and for 26 wt.% hydrogel with 65 wt.% alumina shows gelation temperature of about 9.8 °C. Therefore, with the addition of alumina to the Pluronic F-127 hydrogel, 14 wt % hydrogel showed initiation of gelation which was not observed for pure hydrogel solution. For 18, 22, and 26 wt.% the gelation temperature decreased by 7 °C, 8.3 °C and 6.3 °C. This shows significant influence of alumina addition on the decrease of gelation temperature.

**Keywords:** Pluronic F-127, Hydrogel, Gelation, Alumina

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## Concerted effect of boron and porosity on shear thickening behavior of hybrid mesoporous silica dispersions

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### Abstract

In the present work, the influence of porosity and boron on shear thickening behavior of hybrid mesoporous silica has been studied. Three different levels of boron modification were performed by varying the molar composition of boric acid viz., 1.5 mmol, 2.5 mmol, and 3.5 mmol in a co-condensation approach. The incorporation of boron in mesoporous silica network was confirmed by various techniques such as Fourier transform infra-red (FTIR), and <sup>11</sup>B solid- state nuclear magnetic resonance (NMR) spectroscopy. The morphology and particle size were confirmed by using scanning and transmission electron microscopy. To evaluate the effect of boron and porosity on the shear thickening behavior, dispersions were prepared from mesoporous boron- modified silica (MSiB), control mesoporous silica (MSi), non-porous boron-modified silica (SiB), and control non-porous silica (Si) in polyethylene glycol. The shear thickening behavior was studied using steady shear rheology. The dispersion prepared from different loadings of synthesized MSiB containing 1.5 mmol boron showed more than 16 times increase in viscosity (657.7 Pa.s) compared to that of MSi (39.2 Pa.s) at a fairly low volume fraction ( $\phi = 0.15$ ) of silica. It is expected that the highly ordered mesoporous architecture of hybrid silica has improved the interaction between the particle and the dispersing medium through hydrogen bonding. The porous morphology of the hybrid mesoporous silica as well as the incorporation of boron in the silica network favors the formation of a frictional contact network, and a transition from continuous shear thickening (CST) to discontinuous shear thickening (DST) behavior was observed.

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## An experimental study on lubricating behaviour of pectin-based gel by rheological and tribological measurements

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### Abstract

The utilization of biopolymer-based lubricants has garnered increasing attention due to their biodegradability, safety, and potential applications in various industries. Pectin, a water-soluble polysaccharide found in the cell walls and intercellular tissues of certain plants, is well known for its gelling ability, thickening and stabilizing properties. Depending on degrees of acetylation, methylation and contents of galacturonic acid in it, pectins demonstrate gelling properties and can form complexes with divalent cations like  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$ . Although several other gels have found a large number of applications as a lubricant in every day medical, food products and cosmetics industries, but lubrication behaviour of pectin-based gel is still not understood. This study focuses on characterizing the lubrication properties of a pectin-based gel lubricant through a combination of rheological and tribological measurements. The rheological properties of the pectin-based gels were investigated using steady shear, large amplitude oscillatory shear (LAOS), small amplitude oscillatory shear (SAOS), measurement of stress and normal stress difference as a function of shear rate and complex modulus over the time at low and high shear strain. Tribology measurements were carried out in order to examine the coefficient of friction of the gels in dependence of the concentration. Rheological insights provided a comprehensive understanding of the gel's mechanical behaviour, while tribological measurements underscored its potential in reducing friction and wear. The findings can contribute to the development of sustainable lubrication alternatives and open avenues for further exploration in various industries.

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## Rheological Characteristics of Methylcellulose based TiO<sub>2</sub> Inks

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### Abstract

Methylcellulose (MC) based TiO<sub>2</sub> inks were prepared by mixing 2 wt.% of MC solution with 35 wt.%, 50 wt.% and 65 wt.% of solid loading of TiO<sub>2</sub> powder to obtain Mc-TiO<sub>2</sub> inks. The prepared inks were characterized for rheological behavior. Significant effect of solid loading and temperature was observed on the viscosity of the MC-TiO<sub>2</sub> inks. The viscosity was observed to increase with solid loading of TiO<sub>2</sub> from 35 to 50 wt.%. The gelation temperature for 35 wt.% and 50 wt.% MC-TiO<sub>2</sub> inks was 52 and 44 °C respectively. However, for 65 wt.% of MC-TiO<sub>2</sub> ink the gelation temperature was observed to be initiated at 28 °C. The viscosity vs shear rate for MC-TiO<sub>2</sub> inks was measured at constant temperature of 23, 35, and 50 °C. At 23 °C, the initial viscosity of the inks increases with increase in solid loading of TiO<sub>2</sub> from 32000 m.Pa.s (35 wt.% TiO<sub>2</sub>) to 295550 m.Pa.s (65 wt.% TiO<sub>2</sub>), and at 35 °C the initial viscosity of the inks was observed to increase from 44763 m.Pa.s to 275340 m.Pa.s. At 50 °C, initial viscosity value increased from 58438 m.Pa.s to 413720 m.Pa.s. The viscosity of MC-TiO<sub>2</sub> inks decreased with increasing shear rate which shows shear thinning behavior. The yield stress was found to increase with increasing TiO<sub>2</sub> content at 23 °C from 94 Pa to 100 Pa, at 35 °C from 354 Pa to 365 Pa, and at 50 °C from 692 to 699 Pa, from 35 wt.% to 65 wt.% TiO<sub>2</sub> respectively.

## Effect of chirality on the ferroelectricity of hydrogen-bonded supramolecular assemblies of ambipolar systems

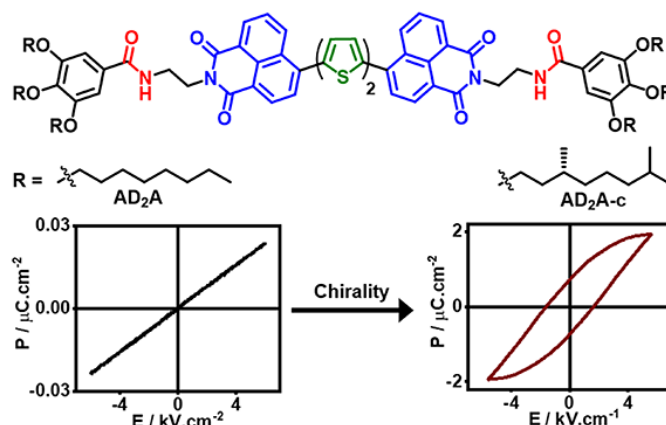
Aritri Pal<sup>1</sup>, Shubhankar Barman<sup>1</sup>, Anurag Mukherjee<sup>1</sup>, Suhrit Ghosh<sup>\*1</sup>, Anuja Datta<sup>\*1</sup>

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### Abstract

In the recent publication of our group, a series of acceptor-donor-acceptor conjugated ambipolar  $\pi$  systems have been introduced as a new organic ferroelectric material having the acceptor and donor moieties in the same molecule to achieve the desired intra-molecular charge-separation.<sup>1</sup> Now taking into consideration that chirality has an influence on FE-polarization,<sup>2</sup> we have compared ferroelectricity of achiral molecule (AD<sub>2</sub>A) and the chiral analogue (AD<sub>2</sub>A-c). In both systems the same ambipolar chromophore is connected symmetrically with two benzamide units along with peripheral hydrophobic groups with either chiral (AD<sub>2</sub>A-c) or achiral (AD<sub>2</sub>A) alkyl chains. Though both are showing similar entangled fibrillar morphology for their supramolecular polymer in hydrocarbon solvent, AD<sub>2</sub>A-c exhibits stable ferroelectricity with a Curie temperature of 361 K and a saturation polarization of  $\sim 2 \mu\text{C cm}^{-2}$ , while no such effect is realized in achiral system (AD<sub>2</sub>A) due to the absence of any chiral wedge (scheme 1). Furthermore, mixing of the chiral and achiral components gives rise to co-assembled structures with chiral induction by Sergeant and soldiers effect, which again showed ferroelectricity with the magnitude of polarization depending on the relative amounts of the chiral and achiral components in the mixture. Recent results from our group<sup>3</sup> in this area will be discussed in this poster presentation.



**Scheme 1:** Schematic representation of molecular structures of AD<sub>2</sub>A and AD<sub>2</sub>A-c and their ferroelectric response.

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## Study the effect of constituent components of PANI/PVA Conductive Hydrogels for Sensing Applications

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### Abstract

The tunability of flexible electro-conductive polymer hydrogel by retaining the gel-ness and swelling nature with significant electrical conductivity remains a challenging problem. Conductive hydrogel (CH) should exhibit gel-like behavior with an appreciable conductivity. The combined property of gel and conductivity depends on the relative proportion of the constituent components. Herein, we present the detailed investigation on the effect of composition of polyvinyl alcohol (PVA) and polyaniline (PANI) on the structure and properties of PANI/PVA conducting hydrogels. We have prepared a series of hydrogel by varying the ratio of PANI and PVA. We have observed that the property of the PANI/PVA hydrogel significantly depends on the PANI content in the hydrogel. The detailed analysis based on XRD reveals that the peak intensity at  $2\theta = 19.3^\circ$  has been decreased and the bandwidth has been increased with increasing PANI content, implying a decrease in the degree of crystallinity and enhancing amorphous nature. The interaction between PANI and PVA is also evident from the change in FTIR spectra of OH group. Detailed morphological analysis shows the formation of well-interpenetrated structure of PANI and PVA. Swelling study and current-voltage measurement in DI water and artificial tear fluid show composition dependent gel and conducting behavior, respectively. Tuning the composition of PVA and PANI results the blend to possess adequate “gel” with improved flexibility and “conducting” nature, required for a conducting hydrogel (CH). We have presented the viability of CH as an enzymatic glucose biosensor, with a significant LOD ( $\sim 0.001 \mu\text{M}$ ).

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# Synergetic H-bonding and C-T Interaction Mediated Hierarchical Assemblies Results in Room Temperature Ferroelectrics Exhibiting Piezo- and Pyroelectric Energy Conversion

Deepak<sup>1</sup>, Z. Mallick<sup>2</sup>, Dipankar Mandal<sup>\*2</sup> and Raj Kumar Roy<sup>\*1</sup>

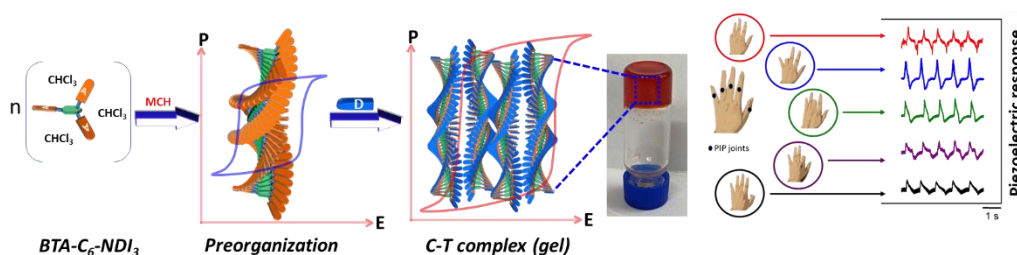
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## Abstract

The development of soft ferroelectrics as a new class of piezo- and pyroelectric materials is due to increasing demand for flexible and wearable electronic devices.<sup>1,2</sup> In this work, we demonstrated the 1,3,5 Benzenetricarboxamide (BTA) derivatives, comprised of an electron-deficient naphthalene diimide (NDI) at the periphery of three arms of the BTA core. The self-assemblies of these scaffolds are mainly driven synergistically by H-bonding, pi-pi stacking, and charge transfer interactions. Three NDI molecules are covalently linked to the periphery of the BTA core with different hydrocarbon lengths (C<sub>2</sub>, C<sub>4</sub>, C<sub>6</sub>, and C<sub>8</sub>) and abbreviated as (BTA-C<sub>n</sub>-NDI<sub>3</sub>, where n is no of carbon). In nonpolar solvents, the supramolecular scaffold self-assembled into a 1-D columnar structure with three electron-deficient naphthalene diimide (NDI) arms at the periphery and BTA as the middle core. Various photophysical and gelation studies found C<sub>6</sub> has an optimum length for the effective establishment of H-bonding (BTA core) and *pi-pi* (NDI periphery) interactions synergistically, which results in very low critical gelation concentration in comparison to C<sub>4</sub> and C<sub>8</sub>. Further, pyrene (donor) was intercalated to the pre-organized state of BTA-C<sub>6</sub>-NDI<sub>3</sub> resulting in gelation at a very low concentration in comparison to without donor, which proved that C-T complexation works synergistically with H-bonding results in the formation of hierarchical self-assembly exhibiting ferroelectric ( $T_c \sim 47^\circ\text{C}$ ) properties at room temperature due to directional polar amide bonds.<sup>3</sup> The piezoelectric and pyroelectric responses observed in the organogel network suggest potential mechanical and thermal energy harvesting applications.



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## A Bioinspired Nanoengineered Hydrogel for Versatile Applications

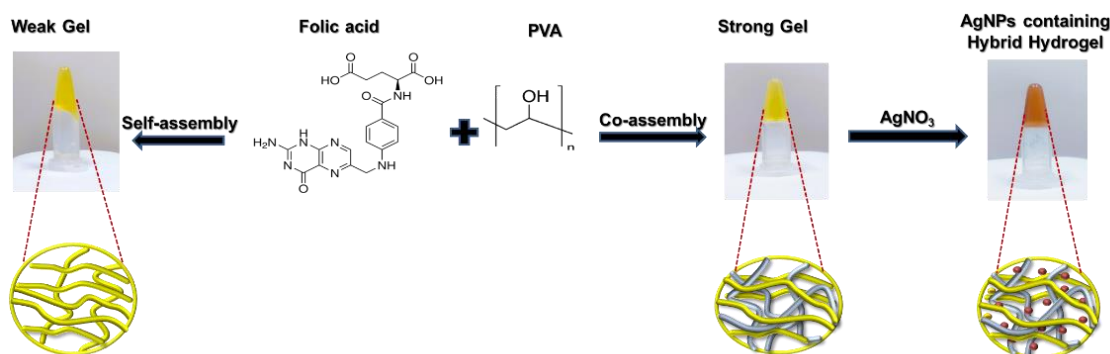
Ipsita Sahu and Priyadarshi Chakraborty\*

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### Abstract

Skin, the largest organ of the body, plays an important role in protecting us from thermal and physical damage and invading pathogens. Consequently, it is essential to accelerate the healing of skin injuries and avoid bacterial infections. Hydrogels can act as novel antimicrobial wound dressings due to their drug-delivery abilities. Self-assembled supramolecular hydrogels offer appealing advantages over prevalent chemically crosslinked polymeric hydrogels in terms of reversibility, stimuli-responsiveness, dynamic nature, and tunability. Furthermore, supramolecular systems allow the introduction of various physical properties and possess simpler syntheses. Folic acid (F), (vitamin B<sub>9</sub>) is an important biomolecule that forms a self-assembled hydrogel in 1:1 dimethyl sulfoxide (DMSO)–water mixture (v/v) having a critical gelation concentration of 0.2% w/v.<sup>1</sup> However unimolecular F gel is mechanically weak which restricts its practical applications. Co-assembly of F with 10% polyvinyl alcohol (P) increases its mechanical properties by 1000 times. FP hydrogel exhibits thixotropic behaviour which is an important parameter for the injectable nature of the gels. Ag nanoparticles were synthesized in the FP hydrogel in the presence of diffused sunlight without the addition of any reducing and stabilizing agent. Since Ag nanoparticles exhibit antimicrobial<sup>2</sup> and catalytic activities<sup>3</sup>, this research may pave the way for the development of novel materials with therapeutic and catalytic applications.



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# Enhancement of electrochemical performance of a cathodically coloured organic electrochromic material through the formation of hydrogen bonded supramolecular polymer assembly

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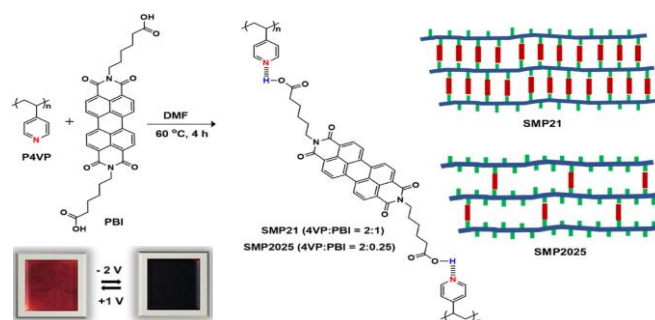
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## Abstract

Electrochromic materials (ECM) can be used to create smart windows, anti-glare rearview mirrors, and electrochromic sensors as they can reversibly alter their colour shade when a voltage is applied.<sup>1</sup> Organic ECMs are desirable because of EC endurance, high coloration efficiency, and band gap tunability, providing a broad and vibrant colour spectrum.<sup>2</sup> PBI-based moieties show multicolor EC activity on applied potentials, making them promising in electrochromism.<sup>3</sup>

Herein, we have developed an H-bonded network polymer architecture with improved crystallinity and photophysical properties through a supramolecular interaction between carboxylic acid-containing perylenebisimide (PBI) cross-linker and poly(4-vinyl pyridine) (P4VP) polymer chains. The electrochromic (EC) measurements have shown reversible EC colour change of the PBI and SMP films from pristine red to deep violet (with vis-to-NIR electrochromism) on potential sweeping along with the significant improvement of the EC parameters in SMP films compared to pristine PBI film. The colouring time (red to deep violet) is improved by 63%, while the bleaching time (deep violet to red) is speeded up by 51% along with the increment in colouration efficiency by 50%. Therefore, this work is very advantageous to deliver a simple and viable strategy for the enhancement of the EC parameters of organic electrochromes through the generation of ordered H-bonded polymer network formation.



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## Dynamic metal-coordinated and hydrophobically associated mechanically robust hydrogel for multifunctional applications

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### Abstract

Recent advances in mechanically robust and flexible multifunctional materials have focused on polymer hydrogels with dynamically crosslinked networks structures. Because of their versatility and reversibility, metal-ligand interactions and hydrophobic associations are frequently used to build dynamic crosslinked networks. Combining the synergistic benefits of reversible metal-ligand cross-linking and hydrophobic association along with small chemical cross-linking, we have developed a mechanically robust and stretchable hydrogel by micellar copolymerization of acrylamide (AM), maleic acid (MA), and butyl acrylate (BA) monomer. BA unit provides hydrophobic association and after subjecting to Fe<sup>3+</sup> solution, hydrogel forms a strong coordination complex with the dicarboxylate unit of maleic acid, which serves as secondary physical cross linker. Due to this chemical and physical crosslinking, hydrogel exhibited high strength (>3 MPa), stretchability (> 600%), and superior self-recovery and antifatigue properties. This hydrogel is highly pH-sensitive and utilised for shape memory applications. Hydrogel is significantly conductive and the conductivity is highly strain-sensitive. So this hydrogel was utilised as strain sensor. A thermoresponsive Poly(N-isopropylacrylamide) layer was added to the hydrogel to create a bilayer hydrogel that can sense temperature changes through its actuation mechanism. Hydrogel was employed as solid electrolyte in flexible supercapacitors due to its strong ionic conductivity. Specific capacitance (~173 Fg<sup>-1</sup>) Energy density (8.65 Wh/kg) and power density (6 kW/kg) are also higher than many other solid electrolytes<sup>[1-3]</sup>. This supercapacitor can last 1000 electrochemical cycles without electrolyte damage. Overall this hydrogel has exceptional properties for a wide range of multifunctional applications.

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## Freeze-thaw induced, metal-co-ordinated, stimuli-responsive, mechanically robust hydrogel for multi-functional applications

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### Abstract

Soft-wet nature of hydrogel makes it resemblance with bio-logical tissue but lack of robust mechanical properties limited its application in various fields like bio-medical field<sup>[1]</sup>, flexible devices<sup>[2]</sup>, drug delivery<sup>[3]</sup> etc. Additionally conventional hydrogels suffer from poor fracture energy ( $\sim 10 \text{ J m}^{-2}$ )<sup>[4]</sup>, susceptible to brittleness after swelling and lack of suitable combination among mutually exclusive properties. We have synthesised a physically cross-linked, mechanically robust double network hydrogel, incorporating hydrogen bonding interaction and metal-ligand interaction along with small amount of chemical cross-linker. This was accomplished through thermal initiated free radical co-polymerization followed by freeze-thaw technique. Owing to dynamic non-covalent interactions and micro-crystalline domain, optimized gel achieved very high tensile strength in MPa range without compromising with fracture strain. Because of its great toughness, this hydrogel demonstrated good puncture resistance, high fracture energy, and high tearing energy. The inclusion of dynamic non-covalent interactions, provide significant amounts of dissipative energy, rapid self-recovery and exceptional fatigue resistance. Furthermore, this gel exhibited long-term swelling stability and pH responsive mechanical properties. The results showed that freeze-thaw approach effectively regulates microstructure and crystallinity, which greatly affect hydrogel's mechanical characteristics. This hydrogel demonstrated multi-functional application in resistive sensor, stimuli-responsive actuator and as an electrolyte for flexible supercapacitor.

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## Liquid-Liquid Phase Separation as Metastable Process for Kinetically Controlled Synthesis of Supramolecular Polymers

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### Abstract

Chemists often derive inspiration from biological systems to engineer sophisticated supramolecular structures using biomimetic methodologies. The process of amyloid fibrillogenesis has proven to be a critical foundation for governing supramolecular polymerization. It has been observed that misfolded or intrinsically disordered proteins (IDPs) goes to amyloid fibril via metastable membrane-less organelles (MLOs,<sup>1</sup> a particular class of dynamic compartments in cells) following a liquid-liquid phase separation (LLPS).<sup>2</sup> Although, LLPS, also known as coacervation, has emerged as a synthetic mimic to realize the formation of MLOs, however, investigation of MLOs transforming from LLPS into fibers in a synthetic system are seldom reported.<sup>3</sup> Here, we endeavored to harness the potential of liquid-liquid phase separation (LLPS) as a metastable process in order to regulate the length and dispersity of supramolecular fibers. Initially, we aimed to construct LLPS based on small molecules through electrostatic interactions. The temporal formation and characterization of metastable LLPS are investigated through a comprehensive array of spectroscopic and microscopic techniques. Furthermore, we observed the gradual transformation of the LLPS into a thermodynamically stable fiber state that bears a striking resemblance to the formation of biological amyloid fibrils. Next, by employing a biomimetic seeding strategy, we were able to precisely regulate the length, dispersity, and growth kinetics of the resulting fiber state. Finally, by fine-tuning the supramolecular interactions once again, we successfully visualized the dynamic disassembly of the kinetically grown fibers into monomers in real-time. This observation provides valuable insights into the reversible nature of the system.

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## Emission Enhanced Supramolecular Polymers in Aqueous Medium

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### Abstract

Nature inspires researchers with its complex hierarchical structures and functionalities, which lead to many interesting scientific discoveries, including supramolecular polymers. Supramolecular polymers have expanded the scope of polymer science by developing stimuli-responsive and dynamic materials in virtue of their directional and reversible noncovalent interactions.<sup>[1,2]</sup> Combining the properties of two or more components can generate supramolecular copolymers with new functionalities.<sup>[3]</sup> However, the conventional metal-ligand and H-bonding interaction can curtail the applications of copolymers in aqueous solutions. Cucurbit[8]uril (CB[8])-based Host-Guest supramolecular polymers are considered some of the best aqueous supramolecular polymers owing to their high solubility in water and strong and highly specific host-guest interactions of the CB[8] molecule.<sup>[4]</sup> These interactions are also utilized to develop multicomponent systems with donor-acceptor pairs and ternary systems with interlinked polymer chains in aqueous media.<sup>[1,5]</sup> If we could tackle the poor fluorescence intensity of supramolecular polymers in water, caused by the free rotor effect of  $\pi$ -conjugated organic guest molecules, they can be utilized for many applications. Herein, we report the design, synthesis, and characterization of a linear  $\pi$ -system based on biphenyl backbone and 1-methylpyridinium moiety, that not only shows good solubility in water and strong interaction with CB[8] but also enhanced emission (5 fold) with a possible J-type aggregate formation.

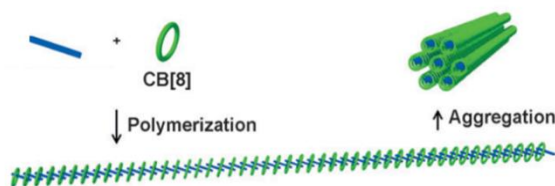


Figure 1. Representation of supramolecular formation via host-guest interaction.<sup>[4]</sup>

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## Fidelity of self-sorting and mixed co-block supramolecular polymerization in peptides as minimal structural preturbation for eventual functional response

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### Abstract

Despite recent strides in supramolecular polymerization, controlling spatial distribution and order in self-assembled systems remains challenging. Multi-component systems with minimal structural variation are crucial for designing complex materials with orthogonal functions.<sup>1</sup> Investigating structural fidelity in multiple peptide amphiphiles offers insights into self-assembly scenarios like random co-assembly, self-sorting and mixed co-block nanofibers. Herein, we have designed four peptide amphiphiles with varying methylene spacer lengths between bis-urea motifs. The  $\beta$ -sheet forming amyloid-inspired peptide sequence VFFAK is tethered to these motifs. Spacer length (three to six carbons) drives the fidelity towards self-sorting or co-assembly, studied through Cy3/Cy5 FRET and super-resolution microscopy. Designed peptides of different spacer sizes form randomly co-assembled and orthogonal networks. Co-assembly yields random monomer sequences due to intermolecular H-bonding between urea units with matching spacers. Conversely, non-matching spacer lengths lead to self-sorted homomeric nanofibers. Self-sorting fidelity also depends on odd or even carbon counts between bis-urea motifs. Peptide amphiphile with odd number of carbon atoms preferable self-sort in case of even number of methylene spacer units. Utilizing these self-sorted and co-assembled nanofibers results in distinct piezoresponse behaviors.<sup>2</sup> Ultimately, supramolecular block co-polymers are achieved via seed-mediated supramolecular polymerization using fiber seeds and matching spacer length monomers.

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## Stereocomplex Formation of Polylactides in Gels and Aerogels: Studies on the Influence of Molecular Weight and Composition of Homopolymers

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### Abstract

The demand for biodegradable aerogels with superior properties has escalated in various fields of application, such as packaging, tissue engineering, thermal insulation, acoustic insulation, and environmental remediation. In the present work, we systematically investigated the role of polymer chain length and number density of enantiomeric polylactides in the gel state stereocomplex formation and the corresponding effect on the structure and morphology of aerogels. Poly(L-lactide) (PLLA) and poly(D-lactide) (PDLA) with large molecular weight differences are blended in the solution state and subjected to thermoreversible gelation. The obtained gels are solvent exchanged with water and freeze-dried to obtain the corresponding aerogels. On gelation, the equimolar blend gels of PLLA<sub>100k</sub>/PDLA<sub>15</sub> (1:1) have crystallized predominantly into stereocomplex (SC) and this structure remains even after the thermal annealing and cooling of the gel. In contrast, the non-equimolar blends of PLLA<sub>100k</sub>/PDLA<sub>15k</sub> (1:4) and PLLA<sub>100k</sub>/PDLA<sub>15k</sub> (1:7) crystallize into almost equal fractions of SC and  $\epsilon$ -form. This structure on heating transforms to complete SC through the  $\alpha$  crystalline phase. But unlike the equimolar gel, pure crystalline SC is not obtained by cooling the annealed gel to room temperature. Instead, a mixture of  $\alpha$  and SC phases is obtained due to the independent crystallization of the excess enantiomeric chains. Thus, we have proved that the composition of PLLA and PDLA in the blend is critical in obtaining crystalline pure SC gels and aerogels.

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## Rapid Adsorption of Molecular Iodine by Tripodal Receptor Cross-linked Polymer

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### Abstract

One of the major concerns worldwide is the treatment of effluents from nuclear reactors. Nuclear reactors are a major energy source that produces the most harmful radioactive isotopes like <sup>129</sup>I and <sup>131</sup>I. These isotopes have high volatility and a long half-life period, which causes health issues for humans and the environment. Hence, such isotopes have to be eliminated unharmed, particularly for the treating effluents from nuclear reactors. The tripodal-based receptor cross-linked polymer was synthesized through Friedel-Crafts polymerization and has shown high iodine vapor adsorption capacity and efficiency. The synthesized polymer was characterized using CP-MAS, FT-IR, BET and SEM analysis. UV-visible spectroscopy evidences the adsorption of iodine from the solution phase. It was found that iodine vapor capture ability of ~2.5 g g<sup>-1</sup> through gravimetric studies. One of the important properties of a polymer is its recyclability. The polymer showed high iodine adsorption without significant loss in iodine adsorption up to five times. Due to its cost-effective synthesis and high iodine adsorption capability provide significant application of this polymer for water remediation, specifically for nuclear reactor waste effluents.

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## Synthesis of “Orthogonal Hetero-Structures” through Stereo-selective Surface-Catalyzed Nucleation

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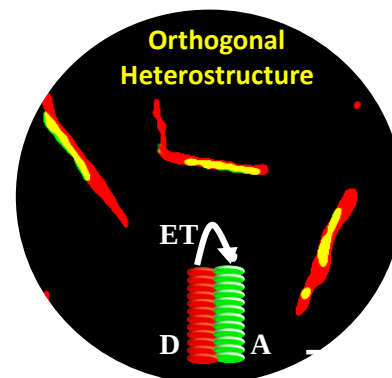
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### Abstract

In the realm of supramolecular polymerization, a pressing challenge has emerged: how to revolutionize the field by devising novel strategies that can yield a wide array of topologies in supramolecular polymers, rivaling the versatility of classical covalent polymers, and thus unlocking their unique and captivating applications.<sup>[1]</sup> Recent developments in the surface-catalyzed nucleation-elongation process have ushered in a new era in supramolecular polymer science, which enabled the creation of an extensive range of supramolecular polymeric structures, including Archimedean spirals, non-covalent catenanes, and branched architectures.<sup>[2]</sup> Nevertheless, the precise manipulation of these pathways to achieve finer monomer discrimination within linear supramolecular polymer chains, especially for the creation of orthogonal heterostructures, remains an unmet aspiration. Orthogonal heterostructures hold immense promise in the fields of optoelectronics, photovoltaics, and spintronics, but their attainment with precise control remains an elusive goal.<sup>[1]</sup>

In response to this challenge, we have devised a novel approach: engineering surface-catalyzed nucleation to stabilize the growth of secondary chains on top of the primary chain, while leveraging specifically designed sites on the parent chains, allowing us to achieve precise control over orthogonal heterostructure formation. Utilizing the cue of chirality,<sup>[3]</sup> this approach enables controlling of surface-catalyzed nucleation events over the primary nucleation-elongation, thereby achieving unprecedented controlled growth of orthogonal heterostructures. Moreover, the efficient energy transfer between the interconnected strands opens up a realm of possibilities for harnessing these heterostructures in a myriad of cutting-edge applications.



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## Octaazacryptand-Crosslinked Polymer for Efficient Iodine Vapor Capture and Water Remediation

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### Abstract

The fission reaction yields hazardous radionuclides, including  $^{129}\text{I}$  and  $^{131}\text{I}$ , which find applications as adsorbents.  $^{124}\text{I}$ , utilized in thyroid research and cancer treatment, serves as a vital radioactive isotope for thyroid disease imaging. Notably,  $^{129}\text{I}$ 's extraordinarily long half-life ( $1.57 \times 10^7$  years) and cost-effective synthesis have garnered significant interest, particularly in nuclear medicine. However, its eventual release into the environment poses serious risks. Therefore, the quest for stable and eco-friendly sources of radioactive iodine is of paramount importance for nuclear safety.

Various solid absorbents, such as alkali/alkaline earth metal exchange zeolite and activated carbon, have been developed for capturing radioactive iodine. Among them, materials structurally similar to crown ethers have demonstrated promising applications. The Cryptand-Based Cross-Linked Polymer was synthesized from Cryptand as a monomer and Mesitylene Tribromide as a cross-linker, employing anhydrous  $\text{FeCl}_3$  as a catalyst via Friedel-Craft alkylation, over a three-days at  $80^\circ\text{C}$ . Characterization was performed through FT-IR, CP-MAS, SEM, and BET analysis, revealing an Iodine vapor capture ability of  $3.72\text{g g}^{-1}$ . This polymer, with its well-established guest recognition properties, has been incorporated onto polymers, ushering in a novel class of supramolecular porous polymer adsorbents for micropollutant removal.

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## **Pillararene-based 3D-Cross-linked Polymer for Fast and Efficient Iodine Removal from Water**

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### **Abstract**

The presence of iodine in natural ocean environments is a common occurrence, but when it is detected in wastewater, it poses a significant environmental concern as it is considered a form of pollution. Therefore, finding effective methods to recover iodine from wastewater is of paramount importance to mitigate its environmental impact.

In the realm of supramolecular chemistry, pillar[n]arenes have emerged as versatile macromolecules with a wide range of applications.[1] These applications span fields such as drug delivery, transportation, and heterogeneous catalysis, showcasing the pivotal role they play in addressing contemporary challenges in science and technology.[2] To address the issue of iodine recovery from wastewater, we embarked on a research endeavor. Our approach involved the design and synthesis of a novel 3D cross-linked polymer using pillar[5]arene and hexakis (bromomethyl) benzene as cross-linker via Friedel-Crafts polymerization reaction. Various analytical techniques were employed, to assess the properties and potential applications of the synthesized polymer including CP-MAS NMR spectroscopy, FT-IR spectroscopy, UV-Vis spectroscopy, surface area analysis, SEM imaging, and gravimetric studies. These analyses provided valuable insights into the polymer's structural, spectroscopic, surface, and morphological properties. It was found that the synthesized polymer could be recycled up to five times without significant loss of its iodine recovery capabilities. This finding enhances the sustainability of our approach and underscores its potential for practical application in wastewater treatment and iodine resource recovery.

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## **Development and characterization of hybrid recycled polymer composite reinforced with naturally sourced basalt fiber and groundnut shell powder**

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### **Abstract**

Eco-friendly and naturally existing basalt fibers (BFs) have received attention in the composite industry due to their exceptional mechanical, thermal, and chemical stability properties. Because of their great commercial value, BFs have a wide range of uses in the automotive, construction, and polymer composite sectors. BFs-reinforced polymeric composites have become the most fascinating topic for scientists due to the resemblance of the BFs with glass fiber. On the contrary, poor adhesion and interaction of the fiber-matrix interface, crucial for polymer composites, is still challenging. The polymeric matrix and BFs must adhere to each other for a successful load transfer and improve the composite's mechanical properties. Furthermore, to make BFs-reinforced polymeric composites more sustainable, a mixture of waste plastics was used as a matrix using the melt blend process. The current work aims to prepare composite with minimal use of chemicals that can be biodegradable, environmentally friendly, and recyclable using mixed recycled plastic, rubber, basalt fiber, and groundnut shell powder (GSP) as a filler. Mixed recycled plastics were used as polymeric matrix, BFs as reinforcing short fiber, and GSP as microparticulate reinforcement to reduce the interfacial gap between BFs and waste plastics matrix.

## Structure-Property Study of Bio-based Vitrimer Composites

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### Abstract

Recently, there has been an increase in demand for Glass Fiber Reinforced Polymer (GFRP) composites in heavy-duty applications due to their high strength-to-weight ratio characteristics. Epoxy resins are one of the extensively used thermosetting resins in composites. However, due to their permanent crosslinked networks, traditional epoxy resins cannot be reprocessed or recycled. However, reversibility of such composites can be achieved using covalent adaptable networks (CANs), which contain a number of reversible covalent bonds to enable the crosslinked network to alter its topology in response to an external stimulus. Such materials are called vitrimers. They are covalently crosslinked polymer materials that can be directly reprocessed above the Topology freezing transition temperature ( $T_v$ ) without depolymerization through an associative mechanism. This results in a constant crosslink density during network rearrangement.<sup>1,2</sup> This study focuses on vitrimers and glass fiber-reinforced polymer (GFRP) properties. The GFRPs were prepared by vacuum bagging process using uni-directional fabric. The tensile properties of vitrimer-thermosets and composites were analyzed and tabulated. The cure kinetics of the commercial epoxy resin (DGEBA) with Vanillin-based hardener was established through DSC tests. The cured epoxy thermoset demonstrated high  $T_g$ , Tensile strength, Young's modulus, and excellent heat stability. This thermoset demonstrated typical vitrimer behavior and it completely dissolved in acetic acid/water mixture.

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## Presence of volatile organic compounds and odorous compounds in recycled plastics

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### Abstract

Nowadays, packaging materials used in food, cosmetic and pharmaceutical industries are single use plastic [1]. 50 % of worldwide debris is currently from this kind of litter in marine ecosystem. While advancements have been made in waste management and the plastics recycling industry is expanding, there remains an opportunity for further improvement in safeguarding the environment against plastic pollution. Currently, recycled materials produced through mechanical recycling face challenges in matching the quality of virgin polymers, making it more challenging to achieve a closed-loop system for plastic production [2]. One contributing factor is the presence of contaminants or unwanted substances in recycled polymers, which can emit strong odors, volatile organic compounds (VOCs) thereby compromising the resin's quality. Consequently, the use of recycled polymers is often limited to applications of lower quality compared to the source material. This study aims to assess the disparity in VOCs and odor between virgin and post-industrial recycled polymers [3]–[5]. To accomplish this goal, both sensory and chemical instruments have been employed to quantify odor emissions in plastic materials. These VOCs and odorous compounds are identified and quantified by solid phase microextraction (SPME) and Gas chromatography-Mass spectrometry (GC-MS). The aim of this research is identification and quantification of the VOCs and odorous compounds and then making remediation strategies to reduce these compounds without compromising mechanical, thermal, and rheological properties. Mechanical recycling process will reduce the waste from the environment and will contribute to sustainability and circular economy by using recycled materials for high value applications.

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## Landfill-Mined Soil-Like Fractions has polymer composting potential: A study using precision metagenomics and geo-environmental characterization

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### Abstract

ASTM-D5338 mandates a compostable bioplastic to be degraded more than 90% within 180 days at 60°C in simulated composting conditions. However, the compost, which is used as the bulk matrix in the degradation process, is already an application-ready product for the agricultural sector. Thus, an alternative matrix needs to be used which can efficiently replace compost while also increasing the rate of degradation of the biopolymers. The potential for landfill-mined soil-like fractions has been tested for its polymer degradation potential with PET/PETase system as a model. Genes coding for PET degrading enzymes PETase/MHETase along with their probable host, were screened from a landfill-mined soil-like material using high-precision Whole Genome Metagenomics (WGM). Landfill soil under a freshly deposited waste dump was taken as the control. The abundance and taxonomic distribution of PETase and MHETase enzymes in the samples, when co-related with the FTIR spectra of the samples using OpenSpecy (software for spectral matching analysis of polymeric residues) indicated that PET residues might have degraded to MHET under natural conditions. Natural extremophilic conditions of the landfill hosts many plastic degrading bacteria, which is promising for the future of plastic/bioplastic waste management. However, one of the major obstacles in fully exploiting their utility is the incapability of reproducing ambient growth environments for the microbes in laboratory experiments. Thus, thorough geoenvironmental characterization of the samples were performed to facilitate microcosm-based experiments with the goal of development of easily implementable plastic degradation technology.

## Impact Analysis of the Forward Osmosis Process Combined with Ultrafiltration Pretreatment in Coconut Water Concentration

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### Abstract

Coconut water is one of the most popular drinks worldwide due to the nutritional benefits offered by it<sup>1</sup>. The demand for packaged coconut water is increasing day by day. Several Membrane technologies are utilized to process the coconut water before packaging. Few of these processes are used for clarification, whereas Reverse Osmosis (RO) and Forward Osmosis (FO) are used for concentration. Due to Lower energy requirements during processing and lower transportation costs associated with the concentrated product of coconut water, the FO process offers superiority over other membrane processes. However, flux during the process is difficult to maintain throughout the FO process, which limits its application in Industrial products<sup>3</sup>. In this study, an attempt has been made to increase the flux by using Ultrafiltration (UF) hollow fibre membrane for the pretreatment step before the FO process, and in retentate of UF process has been added again in the concentrated product of the FO process. It is observed that pretreatment results in increased water flux for all three draw solutions (i.e., 1M NaCl, 2M NaCl, and 4 M NaCl) used in our study. Also, this two-step treatment process can achieve higher concentration factors while utilizing retentate as the first step for nutritional preservation. Thus it can be concluded that pretreated coconut water has higher flux in the FO membrane process, and with the addition of UF retentate, nutritional values of coconut water are also preserved.

**Keywords:** Membrane process, Forward osmosis, Concentration, Pretreatment, Flux enhancement

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## **Plastic Waste Recycling by Utilizing Advanced 3D Printing Approach**

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### **Abstract**

Single-use plastics have become a global problem because of their extensive use, persistent nature, and detrimental environmental impacts [1]. So, efforts are being made to combat the issue of single-use plastic by 3D printing technology [2]. This mushrooming technology, 3D printing, can serve as an innovative and sustainable approach to deal with the issue of plastic waste. Sorting, cleaning, pre-processing, and extrusion of plastic waste are necessary steps, which can be done beforehand in order to convert it into 3D printing filament. Sorting of wastes is important as different plastics have different properties. This technology has gained popularity because a variety of materials can be used to make complicated geometries. The recycled plastic filament is used as the raw material for 3D printing which is obtained by shredding and extruding of plastic waste. In this work, the recycling demonstration of locally available plastic waste which contains PET, PP, ABS, and PVC is done by the use of advanced 3D printing technology [3]. These wastes are collected from different industrial sectors including the packaging, beverage, tire, and construction industries. Further, the characterization of 3D printed filament is performed by utilizing techniques such as TGA, DSC, SEM, XRD, tensile and compression analysis. This 3D filament can be used to make a variety of products like are made of it.

**Keywords:** Recycling, 3D Printing filament, Sustainable, Waste polymer, Sorting.

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## Vitrimeric Chemistry as a Tool for Combating the Issue of Plastic Waste Recycling.

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### Abstract

Plastic waste refers to the accumulations of plastic products of different grades, which are discarded by the consumer after their usage [1]. Plastic waste is a global problem and each and every country is running on the same road to deal with this issue by some upcycling methods. The conventional recycling methods include plastic incineration, pyrolysis, mechanical recycling, chemical recycling and composite formation etc. but all the mentioned methods have their own pros and cons. Plastic waste includes both thermoplastic and thermoset [2]. Out of which, thermoplastics are more recyclable upto an extent than the thermosets. The reason behind this, is the crosslinked-architecture of thermosets [3]. To address these issues vitrimeric chemistry may play an important, sustainable and innovative role. Vitrimers are new class of polymers which possess properties of both thermoplastic and thermosets [4]. They are the materials which can go through reversible bond exchange reactions enabling them to be reshaped, reprocessed, and repaired multiple times without significant degradation. This characteristic may make polymers more readily recyclable and reusable, which would lessen the demand for single-use plastics and increase the useful life of plastic products. For this purpose, many dynamic crosslinker like disulfide crosslinker, boronic ester crosslinker, polyols, hydrazone crosslinker and thiol-ene crosslinkers are used [5]. Which allows the formation of temporary and reversible crosslinked networks in the polymer. In this work, different vitrimers of PE, PP and PET are mentioned.

**Keywords:** Vitrimer, CAN (covalently adaptable network or reversible covalent bonds), Plastic waste, Thermoplastic and Thermoset polymers.

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## Study of the effect of pH on the thermal properties of the various compositions of polymer Thermosets with Cleavable Bonds for Hydrogen Storage

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### Abstract

pH plays an important role when cleavable bonds like disulphide is present in the back bone of any polymer chain. Lots of material development work is directed towards the reuse of expensive carbon and glass fibres in hydrogen storage tank. Incorporating dynamic covalent bonds in the back bone of relatively inexpensive thermoset polymers solves both the purpose. These modified thermosets are economically viable and can easily be dissolved by an aqueous solution containing glutathione or dithiothreitol. Three different compositions of polymer thermosets were prepared by varying cross-linker composition in 0.9, 1.0 and 1.1 molar ratio. Effect of pH on the thermal properties of the polymer thermosets prepared with cleavable bonds is studied using thermal techniques like thermogravimetric analyzer and the Differential scanning calorimeter. pH solutions in the range of pH 2.5 to 8 were prepared. Polymer thermoset samples were kept submerged for 24, 90 and 144 hrs to study the effect of pH solutions on the thermal properties of the samples.

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## Poly (lactic acid)/ Vitamin D3 based composites for active food packaging application

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### Abstract

Recently, there has been a growing interest in the usage of food supplements as fillers in poly (lactic acid) (PLA) to ensure safer contact with food materials and provide a functional role. PLA based active packaging composites were developed by incorporating cholecalciferol (Vitamin D3) (CC) with varying concentrations (1, 3, 5, 10 wt%). The films were prepared by solvent casting method and their performance was analyzed in terms of food packaging applications through optical, oxygen barrier, anti-bacterial, anti-oxidant studies. Physico-chemical characterizations like FT-IR and XRD were performed to understand the interaction between PLA & CC and the surface morphology was studied using FE-SEM analysis. The PLA/CC-5 composite films exhibited complete blockage of UV-B light at 320 nm with UPF value above 50. These films (PLA/CC-5) also showed ~2-fold enhancement in the elongation-at-break (%) and 52 % reduction in OTR compared to PLA. The composite films were effective in inhibiting the growth of food borne bacterial (*E. coli* and *S. aureus*). PLA/CC-5 composite films recorded ~8-fold improvement in DPPH scavenging activity hence giving improved anti-oxidant property than PLA. Thermal analysis demonstrated that the addition of CC lowers PLA crystallization rate due to the slow diffusion of PLA chains to the surface. The migration and release of CC from the composite films were analyzed based on EU regulations, and the PLA/CC-5 composite films showed values below the regulatory limit.

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## **Amine functionalized green mesoporous silica reinforced polylactic acid based composite films for active food packaging**

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### **Abstract**

This study presents a novel approach to the development of environmentally friendly bio-composite films for potential application in food packaging. The primary focus of this research is on utilizing poly(lactic acid) (PLA) as a biopolymer matrix and incorporating amine-functionalized green mesoporous silica (MS) using solution casting method. The objective is to explore the impact of MS on the physio-chemical and active food packaging properties of PLA-based films. The incorporation of amine-functionalized MS into the PLA matrix significantly enhances the ductility of PLA/MS composite films, making them more flexible and suitable for various packaging applications. Furthermore, these composite films exhibit promising improvements in their performance attributes. Oxygen transmittance rate is notably reduced, making them efficient barriers against oxygen infiltration, and they display potent antibacterial properties, particularly against the pathogen *S. aureus*. One of the notable findings is the antioxidant activity exhibited by PLA/MS composite films, with an efficacy of approximately 78% against DPPH. This feature suggests their potential use as scavengers of harmful free radicals in packaged foods, contributing to the preservation of product quality. In summary, environmentally friendly PLA/MS composite formulation demonstrates exceptional strength, flexibility, antioxidant properties, and antibacterial characteristics. These promising outcomes highlight the potential of these bio-composite films for use in food packaging, offering a sustainable and effective solution for enhancing the shelf life and safety of packaged products while reducing environmental impact.

## Chitosan-Guar gum-Tannic acid Based Composite Films for Active Packaging Applications

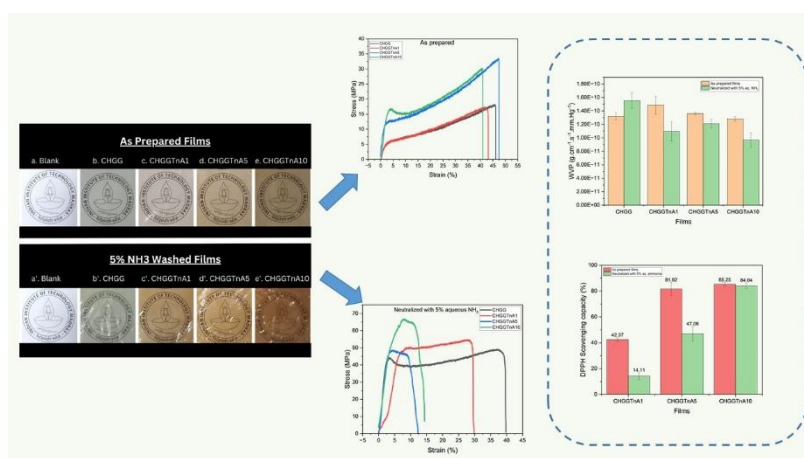
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### Abstract

Composite films based on chitosan, guar gum and tannic acid were prepared using solution cast method. 1, 5 and 10 % (w % with respect to chitosan) of tannic acid was used to crosslink the chitosan-guar gum films. The dried films were then neutralized using 5 % aqueous  $\text{NH}_3$  to obtain the films, whose property was investigated in detail. All the films were studied for physiochemical properties like moisture content, swelling and solubility in water, water contact angle, water vapor permeability, optical property like opacity, mechanical property and antioxidant activity. Upon the addition of guar gum and tannic acid to the chitosan matrix the physiochemical and mechanical properties of films of chitosan changed significantly. The addition of guar gum<sup>1,2</sup> decreased the intrinsic brittleness of chitosan film while tannic acid<sup>3</sup> was used to incorporate the antioxidant property. The results from the detailed study suggested that the films based on chitosan, guar gum and tannic acid can be used in active packaging applications.



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## **Tailoring Curcumin Migration in PLA-Based Active Films by Cellulose Nanocrystals and its Application as Secondary Packaging**

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### **Abstract**

This study presents the development of PLA-based bio-nanocomposite films incorporating algal cellulose nanocrystals (CNC) and curcumin (CUR) using a customized solution casting machine, where CUR serves as a bioactive agent. Two different types of bio-composites were fabricated one with CUR and one without, aiming to investigate the impact of varying CNC concentrations (0, 0.5, 1, and 2 wt.%) while maintaining a constant CUR concentration of 2 wt.%. The overall and specific migration (OM & SM) study was performed using aqueous food simulants. PLA films containing CNC/CUR were tested for SM, whereas those containing only CNC were tested for OM. Through a comprehensive analysis, it was observed that the inclusion of CNC increased the OM rate of the composite films, but remained below the permissible limits. Notably, during storage at 40 °C, the CUR-incorporated active films demonstrated an accelerated CUR migration compared to neat PLA films, with migration kinetics fitting best to the Korsemeyer-Peppas model. As attributed CUR-incorporated active films exhibited superior UV-light blocking, antioxidant, and antimicrobial properties. The physical and chemical properties of developed bio-composites were characterized by TGA, FTIR, XRD, WVTR, and WCA. The nanocomposite films displayed their potential as secondary packaging for cut potatoes, highlighting their potential for advanced sustainable packaging solutions.



## Predicting polymer properties using graph-based multi headed attention transformers with hierarchical aggregation

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### Abstract

The development of new materials, especially polymers, is crucial to meet the demands of evolving technological applications. Traditionally, material discovery has heavily relied on time-consuming and costly experimental approaches rooted in the structure-property relationship. In contrast, computational methods such as Density Functional Theory (DFT) and Molecular Dynamics (MD) have limitations, particularly in handling the intricate multi-scale nature of polymers. In recent years, deep learning (DL) has emerged as a promising avenue for efficient and accurate material property prediction. In this work, we introduce graph-based techniques to predict the glass transition temperature (T<sub>g</sub>) demonstrated over a comprehensive dataset comprising of 7174 monomer SMILES (simplified molecular input line entry system) strings spanning the entire polymer space. Our approach is based on a graph-based transformer model with a trainable multi-headed attention block that transforms the graph representation using hierarchical aggregation and top-K pooling. The monomer depicted by SMILES strings, a popular Molecular representation scheme, is initially converted into a graph data structure, with node and edge embeddings representing atom and bond properties, respectively. After multiple training iterations, the node features of the final layers capture aggregated information from neighboring nodes and connected edges, weighted by trained attention weights. Consequently, the new representation space of the graph transformer effectively captures the relationships between the structure and the property, extracting crucial features such as backbone rigidity/flexibility important for T<sub>g</sub> prediction. Through rigorous evaluation, our model demonstrates a commendable R<sup>2</sup> value of 0.83 in the regression task for T<sub>g</sub> prediction, underscoring its efficacy in capturing essential information from the SMILES representations with a reduced inference time. The study further reveals that graph-based transformer representations for polymers yield predictive performance comparable to the widely adopted extended-connectivity circular fingerprint (ECFP) representation, such as Morgan fingerprints, for T<sub>g</sub> prediction.

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## QSPR and Density functional theory study for estimating the mechanical properties of Polymers

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### Abstract

The ability to predict polymer properties accurately and efficiently is of paramount importance for tailoring the polymeric materials to meet specific application requirements. Polymer informatics, in-particular quantitative structure property relationship (QSPR) approach,<sup>1,2</sup> has the ability to predict the mechanical properties of polymers on the basis of polymer molecular structure. The present investigation deals with a combined approach involving density functional theory (DFT) and quantitative structure property relationship (QSPR) to estimate the intrinsic viscosities of polymers in different solvents.<sup>3,4</sup> The results predicted by QSPR models are in very good agreement with the experimental values. The extension of the present dataset with additional polymers to estimate other properties viz glass transition temperature ( $T_g$ ) and refractive index of polymers is underway in our group. To validate the developed QSPR models, a diverse dataset comprising a wide range of polymer classes and properties is employed. The reliability of the QSPR models is demonstrated through the rigorous evaluation through cross-validation and external validation approaches.

**Keywords:** QSPR, Polymer database, Intrinsic viscosity, density functional theory

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## Polymer Membrane Fuel Cells: *Ab Initio* Quantum Chemical and Density Functional Theory Perspective

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### Abstract

The practical implementation of fuel cells in the hydrogen economy can be reached only through the reduction of the production cost and significant improvement of the electrocatalytic characteristics of the electrodes. This warrants the judicious designing of novel materials including polymer membrane,<sup>0</sup> that can facilitate an understanding of the electrocatalysis-mechanism at the molecular level. Computational simulations within the premise of *ab initio* quantum chemistry and density functional theory enables this understanding quite accurately. An account of computational investigation of degradation mechanism of modelled membrane oligomers, for the reactivity,<sup>0</sup> thermodynamics, as well as hydrophilic and hydrophilic effects will be presented.

**Keywords:** Polymer membrane, fuel cells, *ab initio* quantum chemistry, density functional theory

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## In vitro and in silico approach towards biocidal and antioxidant behaviour of water soluble chitosan dialdehyde biopolymers

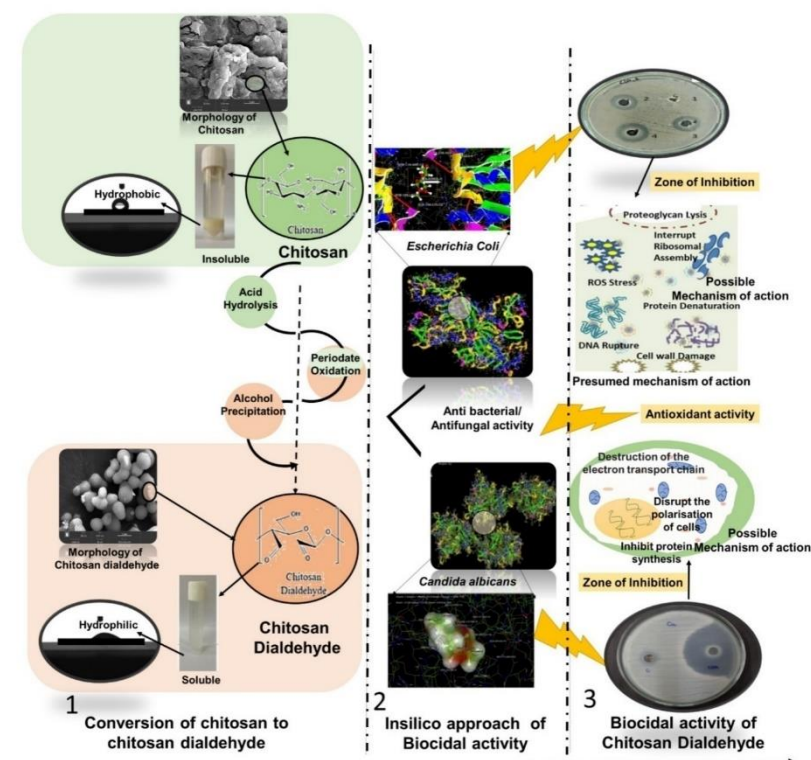
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### Abstract

Chitosan dialdehyde (ChDA) was prepared from a three-step process initiated by thermal organic acid hydrolysis, periodate oxidation, and precipitation from native chitosan (NCh). The developed ChDA resulted in an aldehydic content of about 82% with increased solubility (89%) and maximum yield (97%). The aldehydic (-CHO) group functional alteration in ChDA was established using vibrational stretching at  $1744\text{ cm}^{-1}$ . The increase in the zone of inhibition of ChDA than NCh has confirmed the inherent antimicrobial effect against bacterial and fungal species. The novel *insilico* predictions of the ChDA's biocidal activity were confirmed through molecular docking studies. The amino acid moiety such as ARG 110 (A), ASN 206 (A), SER 208 (A), THR 117 (B), ASN 118 (B), and LYS 198 (B) residues of 7B53 peptide from *E. coli* represents the binding pockets responsible for interaction with aldehyde group of ChDA. Whereas, PHE 115 (E), ALA 127 (H), TYR 119 (C), GLN 125 (H), ASN 175 (E), ARG 116 (E), LYS 101 (H), and LYS 129 (H) of 1IYL A peptide from *Candida albicans* makes possible for binding with ChDA. The current study has escalated to the next level of establishing that the water-soluble biopolymer ChDA, is a carrier for delivering complex drugs by studying the *insilico* molecular docking studies. Hence, the synergistic effect of ChDA, as a biocidal compound finds a plausible use in the drug delivery system for therapeutic applications.



## A Molecular Simulation Study of Barrier Properties of PLA-PBAT Blends with Cellulose Nanocrystals

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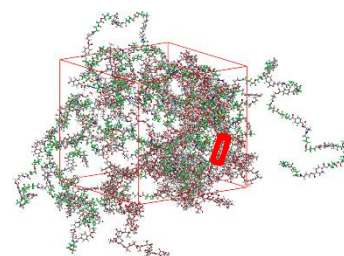
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### Abstract

Nanofillers in polymer blends have attracted considerable attention due to their potential for enhancing mechanical, thermal, and barrier properties. In this study, we focus on incorporating cellulose nanocrystals (CNC) as a sustainable and economically viable nanofiller in blends of polylactic acid (PLA) and polybutylene adipate-co-terephthalate (PBAT). We employed molecular simulations to investigate CNC's influence on the polymer matrix's overall properties. First, we generated realistic molecular models of pure PLA, pure PBAT, and their blends with CNC filler by utilizing Materials Studio 7.0 for modeling the amorphous polymer structures and the LAMMPS software package with the CVFF force field for equilibrating the system<sup>1</sup>. Next, we conduct molecular dynamics simulations to examine the transport of oxygen, water, and carbon dioxide within the modeled polymers and blends. The simulations demonstrate that increasing the CNC content in the blends leads to a decrease in the mean-square displacements and self-diffusion coefficients of the gases. Furthermore, the radial distribution function (RDF) and trajectories of different gases in the polymer matrix provide insights into the interactions between the polymer components and the CNC filler in blends. These findings enhance our understanding of gas transport behavior in CNC-filled PLA-PBAT nanocomposites and may aid in optimizing the design and performance of nanofiller polymer materials.



**Keywords:** Simulation, filler, PLA-PBAT blends

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## Formulation and Modeling of Polyol based crosslinking systems

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### Abstract

Polymer curing and polymer crosslinking are processes used to transform liquid/ malleable polymers into solid materials with desirable mechanical strength, stiffness and thermal stability. During polymer curing, typically initiated by heat/radiation, monomers undergo a polymerization reaction that forms a 3D network of interlinked polymer chains [1]. The applications of these processes are diverse, ranging from coatings and adhesives to automotive parts, medical devices, and extended to military and aerospace applications. Polyol refers to a group of chemicals that contain multiple hydroxyl functional groups, and is commonly used to make products, such as polyesters, polyurethanes, alkylamines and more. Polyols can be derived from various sources including natural fats & oils, carbohydrates & biodiesel, making them a renewable & sustainable alternative to synthetic alternatives [2]. There are a variety of polyols, including polyether polyols, polycarbonate polyols, and hybrid polyols. Polyester polyols are made by reacting diols with dicarboxylic acids or their derivatives, while polyether polyols are synthesized by reacting epoxides with an initiator and an acid catalyst [3]. Trihydroxyethyl-isocyanurate (THIEC) is a polyol used in the coating industry for heat resistant wire enamels, electrical insulators, alkyd resins, urethanes, water-soluble stoving enamels and polyesters [3] [4]. It is used as an intermediate for the synthesis of dyes, agrochemicals, pharmaceuticals and plasticizers [5]. This work aims to study the electron beam curing mechanism of THIEC based crosslinking systems for creating effective curing formulations. We also study the effect of -CH<sub>2</sub>- spacer in crosslinking density of THIEC based systems.

**Keywords-** *Ab-initio* Calculations, Polymer curing, Polyol, crosslinking density

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## Non-linear Rheology of Polymer Grafted Nanoparticle Solutions

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### Abstract

Polymer-grafted nanoparticles have gained significant attention due to their unique properties and potential applications in various fields, including nanomedicine, nanocomposites, and adhesives [1]. The collective structure of polymer-grafted nanoparticles (GNP) solution can be tuned by adjusting the grafting concentration, polymer length and nanoparticle loading. This enables control over parameters like stability, compatibility, and rheology [2]. However, the composition-structure-property correlation is not fully understood. Here, we combine experiment and computer simulation and report a aggregation to dispersion transition of a GNP solution. We further establish a connection between the rheology of the materials and morphological transition. At a threshold value of GNP concentration there is a significant increase in the viscosity of the composite due to the dispersion of GNP in the matrix. This transition is further tuned by the grafting concentration of polymer chains in a nanoparticle surface as shown in Figure 1. High grafting enhances the miscibility and solubility of NPs in the solvent. It imparts mechanical strength to the material, making it stiffer and more resistant to deformation. The transition from aggregation to dispersion determines the point at which the material transits from a liquid-like behavior to a gel-like behavior. Overall, the aggregation to dispersion transitions leads to a non-monotonic change in the rheology of the material.

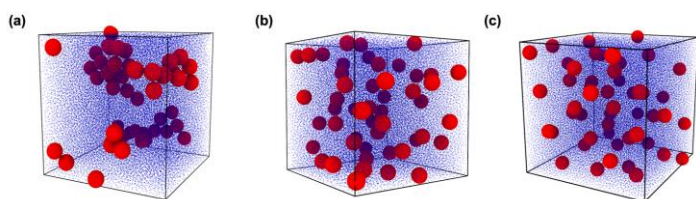


Figure 1: CGMD simulation of GNP solution. The MD snapshots for grafting density 0.12, 0.35 and 0.62 are shown in (a), (b) and (c), respectively.

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## Post-consumer Recycling of High-Density Polyethylene Lubricant Bottles

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### Abstract

The Plastic solid waste from synthetic polymers are creating new challenges, which in today's scenario are major research concerns. The concept of Post-Consumer Recycling (PCR) of High-Density Polyethylene (HDPE) can be achieved by recycling the consumer goods produced using virgin HDPE. In the present work, we have carried out the recycling of waste HDPE lube bottles obtained from the market. These HDPE bottles were cleaned, shredded, and made into granules in a twin screw extruder. These granules were injection molded into standard ASTM test specimens and made into blow-molded PCR HDPE bottles. All these samples were characterized for their MFI, thermal (DSC, TGA), Mechanical (Tensile strength, Modules & % elongation), Rheological, Molecular characteristics, and Color. Accelerated weathering, ESCR & IR studies carried to know the thermal stability of these products. The results indicated that there is no change in the mechanical, thermal, and rheological properties of our 100 % PCR HDPE bottles made from waste HDPE lube bottles. These properties obtained are comparable with commercial PCR HDPE having 30 % virgin HDPE material which was also extruded and molded under identical conditions. The HPGRDC Produced recycled HDPE can be used in the manufacturing of blow-molded bottles and small containers.

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## **Development of a Micro-Raman spectroscopic system for visualization and identification of micro-plastics from environmental samples**

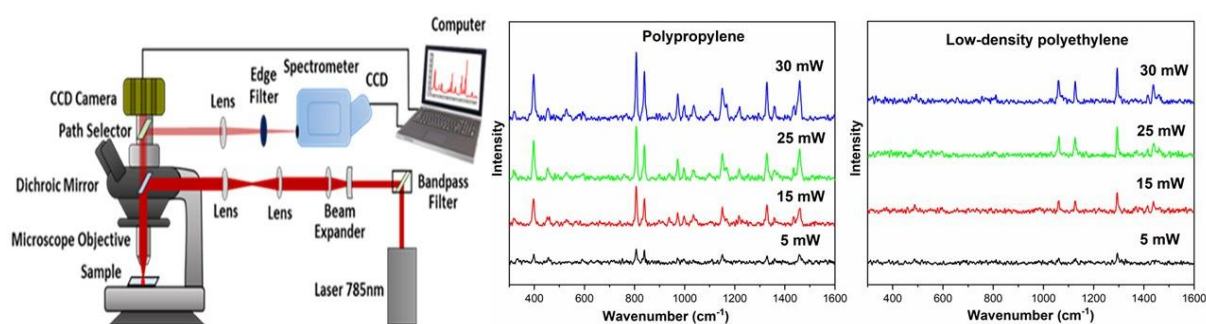
**Megha Sunil, Meril Charles, Mithun N, Santhosh Chidangil, Satheesh Kumar M.K and Jijo Lukose\***

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### **Abstract**

The steady and significant growth in the manufacturing and use of plastics in recent years has raised global awareness of plastic wastes and plastic waste management<sup>1</sup>. Microplastics, with size ranging from 1  $\mu\text{m}$  to 5 mm, are tiny fragments of degrading plastic that are mostly produced as a result of environmental conditions<sup>2</sup>. Conventional microplastic detection techniques have flaws in the accurate identification of polymers and are also destructive, restricting the sample availability for any further research and resulting in poor sample quality for later identification and analysis of microplastics<sup>3</sup>. Micro-Raman spectroscopy, a non-destructive spectroscopic technique that does not necessitate extensive sample pre-processing, can be used to determine the chemical composition of polymer materials. The method is highly promising for identifying microplastics especially from waterbodies due to its sensitivity and minimal interference from watery samples<sup>4</sup>. Most of microplastic research are carried out utilising expensive commercial Raman platforms, which demands the requirement of indigenous instruments. In the present study, a lab-based micro-Raman spectroscopy setup was developed, which enable microplastic visualization, identification as well as size measurement.. To get high-quality Raman spectra, the experimental parameters such as laser power, exposure time, and acquisition were optimised. The effectiveness of the Micro-Raman setup has been evident from the identification of microplastics dervied from Polystyrene (PS), Polyethylene Terephthalate (PET), High Density Polyethylene (HDPE), Low Density Polyethylene (LDPE), and other routinely used plastic materials.



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## Application of Vitrimeric Chemistry for the Upcycling of Commodity Polymer Poly-Vinyl Chloride (PVC)

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### Abstract

PVC is a thermoplastic versatile vinyl polymer, with resin code 3 [1]. It is used to manufacture a variety of products including pipes, fittings, cable insulation, flooring, roofing, etc. having short and long lifespans. Plastic waste, including PVC, is nowadays causing serious concern. The challenges associated with PVC recycling include the release of toxic Cl-based compounds, posing environmental and health issues. Additionally, recycling techniques that are specifically customized to deal with PVC are limited unlike PET, HDPE, etc. polymers [2]. Moreover, the demand for recycled PVC is lower than other polymers, making it less economically advantageous. Hence, it is necessary to develop a more sustainable alternative to PVC and valorization of post-recycling products [3]. In this work, an attempt is made to deal with this issue by converting the irreversible bonds into dynamically reversible bonds via the application of vitrimeric chemistry. For this purpose, a dynamic cross-linker and radical initiator are used. The role of a dynamic crosslinker is to form reversible covalent bonds. Further, characterization was performed by DSC, TGA, FTIR, DMA, and SAXS [4]. In this manner, PVCs can be converted into PVC CANs which increases the potential applications of PVC and effectively addresses the difficulties of recycling and reprocessing.

**Keywords:** Vitrimer, CAN (covalently adaptable network), PET (polyethylene terephthalate), PVC (polyvinyl chloride), Dynamic Cross-linker.

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## Upcycling of Fast-Moving Consumer Goods Waste Through Catalytic Pyrolysis for Fuel Oil Production: A Strategy for Multi-Layer Plastic Management

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### Abstract

Fast-Moving Consumer Goods (FMCG) are packed of multilayered plastic (MLP) as they provide better functionality for packaging films. There is a barrier to their recycling because of significant additives used to achieve improved performance's inherent mechanical and barrier properties. The present study illustrates an integrated refinery strategy for producing fuel oil (FO) by pyrolyzing MLP. The thermal investigation illustrates the three-stage degradation using the KAS, Starink, and FWO methods, with average activation energies of 182.99 KJmol<sup>-1</sup>, 183.47 KJmol<sup>-1</sup>, and 185.30 KJmol<sup>-1</sup> respectively. Pyrolysis follows the diffusion model (D1-4) control mechanism, relying on the Popescu method and master plots. Valorization of MLP under inert conditions at various temperatures produced an average oil yield of 36% and char 11% with the highest yield of oil at 550°C. The obtained oil is upgraded by hydro-processing using a catalyst, resulting clear and stable oil with reduction in density from 0.796 g/cm<sup>3</sup> to 0.783 g/cm<sup>3</sup>. The content of paraffinic and aromatic compounds is increased by hydro-processing with a catalyst, determined by GCMS and NMR analysis, which makes the oil as a potential fuel. FO blended fuels results low emissions, leads a better life style by minimizing the greenhouse effect based on engine performance and combustion characteristics.

**Key Words:** Multi-Layer Plastic Waste, Pyrolysis, Fuel Oil, Kinetic Triplets, Hydro-processing

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## Redox-Responsive Two-Dimensional Assemblies from a Chromophore-Appended Crystallizable Poly(L-lactide): Effect of Variation of Chain Length on Highly Efficient Energy Transfer

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### Abstract

Functional  $\pi$ -conjugated systems primarily tend to form supramolecular assemblies that are predominantly spherical or one-dimensional (1D) in nature. There are relatively few instances of these systems adopting two-dimensional (2D) structures. A promising method for creating various hierarchical and anisotropic structures, particularly in 2D arrangements, involves the use of crystallization-driven self-assembly (CDSA) of semicrystalline block copolymers (BCPs). Previously, our group explored precise diamond-shaped 2D platelets in isopropanol under suitable condition, causing the terminally attached chromophores to assemble into 2D array on the platelet surface by either dipole-dipole interactions for dipolar chromophores: naphthalene monoimide (NMI) and merocyanine (MC) or aromatic stacking for nonpolar pyrene (PY). Now we are diversifying the chromophoric effect and have introduced a highly emissive, redox-sensitive dipolar phenothiazine (PTZ) dye, to enable colloidal stability to the 2D platelets. Co-crystallization (1:1) between PTZ- and PY-functionalized PLLAs (DP = 100) with comparable chain length yielded two-component co-platelets of similar shape with highly efficient Förster Resonance Energy Transfer (FRET) from the donor (PY) to the acceptor (PTZ) with remarkable efficiency (~90%) on the 2D surface. Again co-crystallization (1:1) of PTZ-PLLA with PY-functionalized PLLAs (DP = 245 and 550) of greater chain length reduces the FRET efficiency (~70%). Like never before, we see chain length dependency on the FRET properties exhibited by the 2D platelets. Further, we introduced the PTZ-PLLA system in 80% water-IPA medium where morphologically similar luminescent 2D platelets could be generated that could change the emission colour from orange (reduced form) to cyan (oxidised form) via white-light emissive pathway keeping their size and shape intact. This redox process is assisted by NaOCl and H<sub>2</sub>O<sub>2</sub> which are very important Reactive Oxygen Species (ROS). Therefore, this phenothiazine containing 2D platelets can act as a potential sensor of ROS.

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## Enzyme Mediated Disintegration of a Polymeric Scaffold: Noncovalent Drug Encapsulation and Targeted Chemotherapeutic Applications

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### Abstract

Supramolecular materials that respond to external triggers are being extensively utilized in developing spatiotemporal control in biomedical applications ranging from drug delivery to diagnostics.<sup>1</sup> DT-diaphorase, a cytosolic flavoenzyme widely distributed in tissues of animal species, catalyzes two-electron reduction of various quinones to their corresponding hydroquinones using (NADH) or (NADPH) as a coenzyme.<sup>2</sup> More importantly, DT-diaphorase levels are strongly elevated in a number of tumor types, including lung carcinoma, breast carcinomas, liver cancers and colorectal carcinoma, as compared with normal tissue.<sup>3</sup> In the present work, we described the self-assembly of main-chain azobenzene based polyurethane into nano aggregates in water. Microscopic and spectroscopic analyses confirmed the formation of supramolecular aggregates with a dimension of 165-170 nm. The azobenzene moiety undergoes reduction to form amine in presence of azoreductase enzyme and NADPH coenzyme. The characteristic absorbance peak of this azo ( $-N=N-$ ) moiety comes at 365 nm, which got diminished in the presence of azoreductase enzyme due to degradation of azo bonds. Furthermore, we demonstrated the cell viability experiment to investigate the cytotoxicity of the polymer towards two types of cell lines using MTT assays. The drug loaded nanoaggregate shows strong cytotoxicity towards DT-diaphorase overexpressed A549 cells as compared to non-DT-diaphorase overexpressed H9C2 cells. To get better insight into the cellular uptake, the fluorescence response in (A549 and H9C2) were employed for cell imaging. The A549 cells shows strong fluorescence intensity upon incubation with the drug loaded nanoaggregate. On the other hand, the H9C2 cells exhibit undetectable fluorescence under the same treatment. Synthesis, characterization, self-assembly, drug encapsulation, enzyme triggered release and biological evaluation will be the topic of this poster presentation.

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## Highly efficient and well-controlled ring-opening polymerization and copolymerization of cyclic esters using a cesium complex

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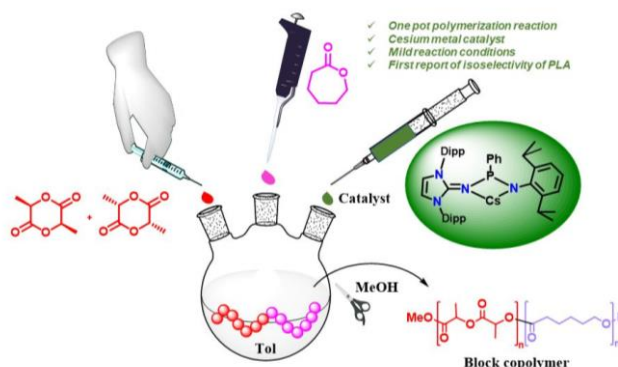
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### Abstract

An imino-phosphanamidinate-supported cesium complex,  $[\{NHI^{Dipp}P(Ph)NDipp\}Cs]$  was utilized as a catalyst in a highly competent and well-controlled ring-opening polymerization/copolymerization of *rac*-LA and/or  $\epsilon$ -caprolactone to form a homopolymer ( $P_i = 0.81$ ) and di-block PLA-*b*-PCL copolymers. The block copolymers of *rac*- lactide (LA) and  $\epsilon$ - caprolactone (CL) have improved degradability, elasticity, mechanical strength, and permeability over the PLA and PCL homopolymers. The cesium complex was highly competent towards *rac*-LA and  $\epsilon$ -CL copolymerization, allowing for good control over the molecular weights and characteristics in a one-pot reaction to selectively produce diblock copolymers. The polymer samples were thoroughly characterized by  $^1H$ ,  $^{13}C$  NMR, DSC, POM, AFM, and SEM. The influence of different comonomer contents on thermal, optical and morphological properties of different PLA-*b*-PCL copolymers are explicitly discussed.



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## Binuclear and Mononuclear Aluminum Complexes as Quick and Controlled Initiators of Well-ordered ROP of Cyclic Esters

Shweta Sagar,<sup>1</sup> Priyanku Nath,<sup>1</sup> Kulsum Bano,<sup>1</sup> Himadri Karmakar,<sup>1</sup> Jyoti Sharma,<sup>1</sup>  
Alok Sarkar\*<sup>2</sup> and Tarun K. Panda\*<sup>1</sup>

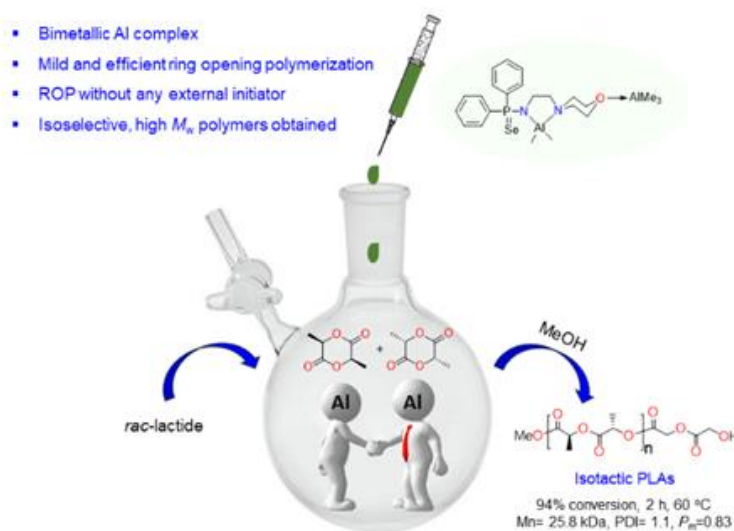
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### Abstract

An efficient ring-opening polymerization (ROP) of *rac*-lactide and  $\epsilon$ -caprolactone ( $\epsilon$ -CL) using novel bimetallic and monometallic aluminum complexes supported by functionalized P–N ligands. All the aluminum complexes were seen to be active catalysts in the ROP of both *rac*-lactide and  $\epsilon$ -CL in toluene at 60 °C. Bimetallic aluminum complex, [Al(Me)<sub>2</sub>{Ph<sub>2</sub>P–(Se)N(CH<sub>2</sub>)<sub>2</sub>N–(CH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>O}(AlMe<sub>3</sub>)] containing an uncoordinated selenium atom and an auxiliary Al ion within the proximity of another central Al cation was observed to exhibit the highest catalytic activity among all the catalysts studied. Kinetic experiments, comparing bimetallic and related monometallic complexes revealed that bimetallic cooperativity among the two metallic centers in the Al complex plays an essential role in driving such superior reactivity. We synthesized several isoselective polylactides (PLAs) and polycaprolactones (PCLs) with controlled molecular weights and narrow molecular weight distributions and characterized by <sup>1</sup>H, <sup>13</sup>C NMR, DSC, and TGA.



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## A Versatile Transesterification Approach for Functional Degradable Polyesters from an Activated diester Monomer

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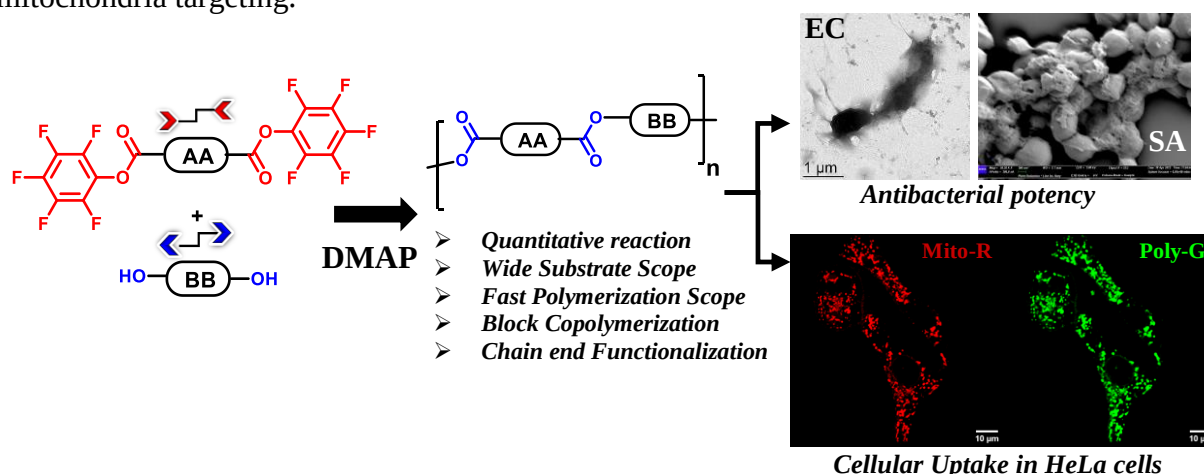
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### Abstract

The work describes a versatile and efficient condensation polymerization route to synthesize functional aliphatic polyesters<sup>[1]</sup> through organo-catalyzed (4-dimethylaminopyridine) transesterification<sup>[2]</sup> reactions between an activated pentafluorophenyl-diester of adipic acid and structurally different diols, ranging from simple linear and cyclic to quarternized naphthalene monoimide (NMI) moieties. By introduction of the "monofunctional impurity" or "stoichiometric imbalance," this methodology is able to generate well-defined end-functionalized polyesters with predictable molecular weights and narrow dispersity under mild conditions without the need for the removal of any byproduct to accelerate the polymerization reaction, which has been a major challenge in conventional polyester synthesis with non-activated diesters. Polymerization kinetics studied in both presence and absence of the catalyst, showing differential conversion rates within 24 hours, thereby providing an idea of the mechanistic pathway of the reaction course. Block copolymer synthesis by chain extension following either controlled radical polymerization or ring-opening polymerization has also been effectively achieved. Following this methodology, quarternized and fluorescent aromatic pendant moieties with variation in hydrophobic chain lengths were incorporated to synthesize enzymatically degradable water soluble polyesters with differential molecular weights, which show great potential as broad spectrum antibacterial agents. Furthermore, these polyesters were found to exhibit excellent cellular uptake through endocytosis pathway with prospective mitochondria targeting.



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## Stereoselective Ring-Opening Polymerization of Racemic Lactide by Racemic Organo-catalyst at Room Temperature: Direct Access to Stereocomplex Poly lactides

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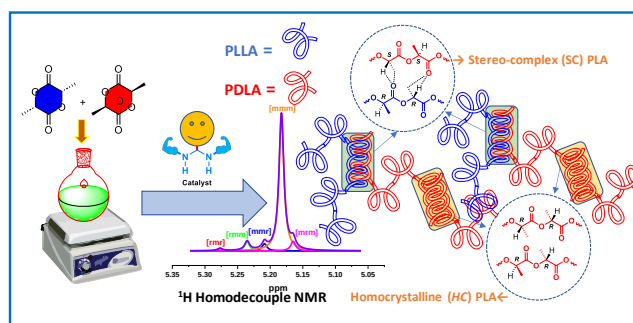
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### Abstract

Poly(lactic acid) (PLA), derived from renewable sources, stands as a biodegradable alternative to petrochemical-derived materials.<sup>[1,2]</sup> Its production primarily involves ring-opening polymerization (ROP) of lactide, the cyclic dimer of lactic acid (LA).<sup>[3]</sup> In PLA polymerization, metal-based inorganic catalysts are crucial for precise stereocontrol. Catalyst choice varies with properties and applications, favoring organic catalysts for biomedical compatibility. Stereocontrol significantly impacts PLA, including the notable thermal properties of the PLA stereocomplex. Chiral organic catalysts<sup>[4]</sup> enhance PLA structure control, while exploration of easily synthesizable racemic organo-catalysts with similar efficiency is limited. Two stereocontrol mechanisms for PLA are enantiomeric-site and chain-end control. The former yields isotactic polymers with improved thermal traits, needing additional isotactic polymers for stereocomplexes. The latter forms stereoblock copolymers with D and L-lactides in one chain, facilitating intra/intermolecular stereocomplexes.

In this context, binary organo-catalysts combining diverse bases and chiral/achiral thio-ureas were investigated for stereo-controlled ROP of racemic lactide (rac-LA) under mild conditions. Notably, DMCHA base displayed high activity (98% conversion in 48 hours) and impressive stereoselectivity ( $P_m = 0.89$ ) at room temperature, producing a stereo-block PLA with well-defined characteristics: predictable molar mass, narrow distribution ( $\mathcal{D} = 1.10$ -1.20), and notably high melting temperature ( $T_m = 201^\circ\text{C}$ ). In-situ NMR analysis explored interactions between various bases and the initiator, revealing DMCHA leads to loose ion pair formation with benzyl alcohol (BnOH). This phenomenon accounted for the simultaneous achievement of high activity and stereoselectivity. Kinetic studies involving different LA monomers at room temperature suggested chain end control as the mechanism in stereo-controlled ROP.



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## TEMPO-Oxidized Nanofibrillated Cellulose as a potential drug carrier for sustained delivery of Triclosan

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### Abstract

There is an upsurge of interest for the development of novel techniques to combat bacterial infection, which has been intensified over decades and are gaining enormous attention. A suitable nanocarrier that can effectively deliver antimicrobials in sustained manner will render the microbial spread can tackle this threat. Triclosan is a broad-spectrum biocide *efficacious* against both gram-positive and gram-negative. However, its poor solubility, low entrapment efficiency and undesirable release profile limits its applicability. Moreover, it remains a challenge to develop a simple, cost-effective support for anchoring this antimicrobial drug beneficial for real field applications. In this study, we exploit a simple straight forward strategy to synthesize carboxylated Nanocellulose fibers. Resulting nanocellulose fiber owes abundant carboxyl groups, better dispersibility as well higher surface/pore-volume ratio to facile the drug adsorption and release process. In addition to this, this system successfully allocates higher percentage of drug (~92%) in their matrix and manifests a sustained release of drug over a period of 8 days. Release kinetics analysis revealed that the synergistic effect of a primary burst release stage and a secondary slow sustained release stage is crucial for the practical applicability. Assessments of antibacterial activity of the triclosan loaded system were carried out against *Escherichia coli* and *Staphylococcus*; significant sustained inhibition of bacterial growth was observed for a period of 8 days, thus making them a promising candidate for the potential applications that demands sustained antibacterial activities.

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## Enhancing the Mechanical Stability of Carboxymethylcellulose Hydrogels through Dual Crosslinking: A Comparative Study

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### Abstract

Carboxymethylcellulose (CMC) is a cellulose ether derivative that is highly soluble in water making it a very good material for hydrogel applications. Water uptake and mechanical strength of these hydrogels can be moderated by crosslinkers. Biobased non-toxic crosslinkers such as citric acid (CA) are desired for hydrogels in healthcare applications. It has widely been used with CMC to crosslink at high temperatures ( $> 60^{\circ}\text{C}$ ). In recent years, crosslinking of carboxymethyl cellulose nanofibers (CMCF) with CA under subambient temperatures has been demonstrated. However, this approach is not possible with CMC. We have developed an approach to introduce dual crosslinking in CMC, which helps to enhance the strength of the hydrogels significantly and tune the water uptake. The effect of crosslinker concentration and other parameters has been systematically investigated through small amplitude oscillatory shear (SAOS) experiments and microstructure of the gels has been examined by scanning electron microscopy (SEM). There exists an optimum concentration of CA beyond which the mechanical strength of the hydrogels is compromised.

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## **Tuning the hydrophobicity of cellulose through controlled esterification with various fatty acids**

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### **Abstract**

Cellulose is converted to its organic esters in the laboratory and commercially, for two reasons. First, cellulose is poorly soluble in common solvents and is not melt-processable because it decomposes before it undergoes melt flow. Conversion of cellulose to its esters affords materials that are processable into various useful forms, such as three-dimensional objects, fibers, and solutions to be used for coating or casting (of films or membranes, for example). When homogeneous esterification was used, the acyl chloride method was the most effective esterification method and cellulose esters prepared using this method have the highest degree of substitution (DS). We have conducted a systematic investigation on esterification of cellulose using THF and pyridine in different ratios, viz, 90:10, 80:20, 70:30, 60:40, 50:50 with three different types of fatty acid chlorides (stearyl, palmityl and myristyl). The degree of substitution and melting characteristics of the cellulose esters were determined. Good free-standing films of various degree of hydrophobicity were obtained and some of the cellulose esters were melt processable into films.

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## Single-Step Synthesis of Tailored Biodegradable Core-Shell Microparticles for Controlled Herbicide Release in Sustainable Agriculture

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### Abstract

In the pursuit of efficient and sustainable agricultural solutions, the development of precise agrochemical delivery systems is paramount. Contemporary agricultural practices are tasked with addressing the escalating demands for food production while mitigating the ecological footprint. This study introduces an innovative approach, employing a single-step solvent evaporation method, to craft customized biodegradable core-shell microparticles for controlled and extended herbicide release. The method enables the fabrication of PLA-based microparticles with adjustable diameter, shell thickness, and surface morphologies through parameter tuning. The core-shell architecture achieves remarkable encapsulation efficiency for atrazine and 2,4-dichlorophenoxyacetic acid herbicides. By utilizing specialized PLA grades, controlled in vitro release assays demonstrate sustained release profiles programmable from a few days to several weeks. This adaptability underscores the system's efficacy for precise agrochemical delivery. This methodology marks a significant stride in modern agriculture, empowering practitioners with meticulous control over agrochemical administration. It not only mitigates ecological risks but also optimizes resource utilization. The prolonged-release properties also hold the potential to reduce herbicide application frequency, leading to economic gains and heightened ecological sustainability. Furthermore, the demonstrated capacity for extended herbicide release allows tailored crop management, accommodating variables such as crop types, soil compositions, and environmental factors. As agriculture embraces eco-conscious strategies, this innovation introduces a strategic breakthrough in effective, targeted, and environmentally responsible crop protection.

**Keywords:** Biodegradable polymers, core-shell microparticles, polylactic acid, single-step solvent evaporation, controlled release, agricultural applications, herbicides.

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## Property optimization of melt processed starch: An experimental and computational study

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### Abstract

Starch based polymeric materials using water and glycerol as plasticizing systems have earlier been developed using solvent casting method which inspite of its competitive properties presented serious roadblocks towards scalability. The current study deals with optimization of glycerine content in the formulations (15, 20, and 25 wt.%) and processing temperature (80 °C, 100 °C, 120 °C and 140 °C) to be used during melt processing of native starch, without the use of secondary fillers and additives. The polymer developed through the optimized settings was subjected to mechanical (tensile experiments), thermal (TGA, DSC), wettability, morphological (FESEM), interaction (FTIR) and degradation analysis. From the results, it was identified that the starch-based system containing 15% glycerin processed at 120 °C showed best results for mechanical (tensile strength: 21 MPa, Young's modulus: 392 MPa, and the elongation in break: 9%) and wettability (contact angle ~ 93.8°) properties compared to other formulations. Another observation was that the increase in plasticizer concentration decreased thermal stability. However, the optimized formulation was more stable than native starch up to 270 °C, with gelatinization temperature around 51 °C. Typical soil burial degradation analysis revealed, at the end of 35 days, the samples underwent 90% degradation (weight loss) under compost soil and 35% under typical agricultural soil. Molecular Dynamics simulation was also performed using Materials Studio software for the same formulations and similar trends of mechanical properties were observed. The results obtained from this investigation showed that the optimization of process parameters could help to enhance the properties of the starch formulation without the need for costly additives.

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## Effect of Ionic Liquid Combined Hygrothermal Pretreatment on Porosity, Chemical Composition and Cellulose Crystalline Structure of Poplar Wood Cell Walls

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### Abstract

In this study, we investigate the effects of two ionic liquid (IL)-based pretreatment methods, 1-ethyl-3-methylimidazolium acetate/dimethyl sulfoxide (EMIMAc/DMSO) and 1-Ethylpyridinium bromide/dimethyl sulfoxide [EtPy][Br]/DMSO, on the poplar wood cell wall characteristics. EMIMAc is an imidazolium-based IL, while [EtPy][Br] is a pyridinium-based IL. The wood samples were subjected to the hygrothermal treatment, followed by EMIMAc/DMSO and [EtPy][Br]/DMSO pretreatment under controlled conditions, and detailed characterization. Porosity changes were assessed using scanning electron microscopy (SEM) and nitrogen adsorption-desorption isotherms. Chemical composition alterations were determined using Fourier-transform infrared spectroscopy (FTIR) and solid state <sup>13</sup>C NMR spectroscopy. The cellulose crystalline structure modifications were analyzed using X-ray diffraction (XRD). Our findings reveal that both EMIMAc/DMSO and [EtPy][Br]/DMSO pretreatments significantly affect the wood cell wall properties. EMIMAc/DMSO leads to dissolution of cellulose chains, while [EtPy][Br]/DMSO treatment partially or negligibly affect the cellulose chains. Pore volume and pore diameter increased with an increase in IL concentrations. Morphological study showed heavy destruction of wood cell wall in the case of EMIMAc/DMSO, while the cell wall remains intact in [EtPy][Br]/DMSO treatment. These treatments lead to increased porosity, facilitating better access to the wood's internal structures. Furthermore, chemical composition analysis indicates changes in lignin and hemicellulose content, which could impact wood's reactivity and suitability for downstream processes. Notably, the cellulose crystalline structure undergoes substantial alterations, specially decrease in microfibril angle (MFA), which may enhance the enzymatic digestibility and saccharification potential of wood for biofuel production. A reusability study revealed that [EtPy][Br]/DMSO was efficient and reusable for up to three cycles.

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## Development of active coatings based on carnauba wax and neem oil nanoemulsion for prolonging postharvest shelf-life of citrus fruits

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### Abstract

Citrus fruits undergo transformations in their physiology, biochemistry, and molecular responses during postharvest life, subjected to different abiotic stress conditions<sup>1</sup>. Originating from subtropical regions, numerous citrus types are highly vulnerable to chilling injury symptoms on their peels, which significantly impact the fruits' quality and marketability<sup>2</sup>. Thus, this research focuses on the development of active coating formulations from carnauba wax (CW), along with neem oil nanoemulsion (NONE), their characterization, and application for extending postharvest shelf life of sweet lemon and Khasi mandarin fruits. NONE was prepared by ultrasonic method, which showed strong antibacterial and antifungal activities. The developed coating formulations were applied by dip-coating methods, which decreased weight loss, sustained titratable acidity and total soluble solids, and decelerate deterioration under ambient storage condition. As compared to the uncoated fruits, composite coatings containing 5% NONE (CW/NONE-5) and 10% NONE (CW/NONE10) minimized decay in coated citrus fruits and prolonged their shelf-life by minimum of 3 weeks. The composite coatings developed in this study hold the potential to act as feasible substitutes to synthetic wax-based coatings for enhancing the shelf-life of citrus fruits. This innovation can offer growers and distributors a sustainable approach to mitigating postharvest losses.

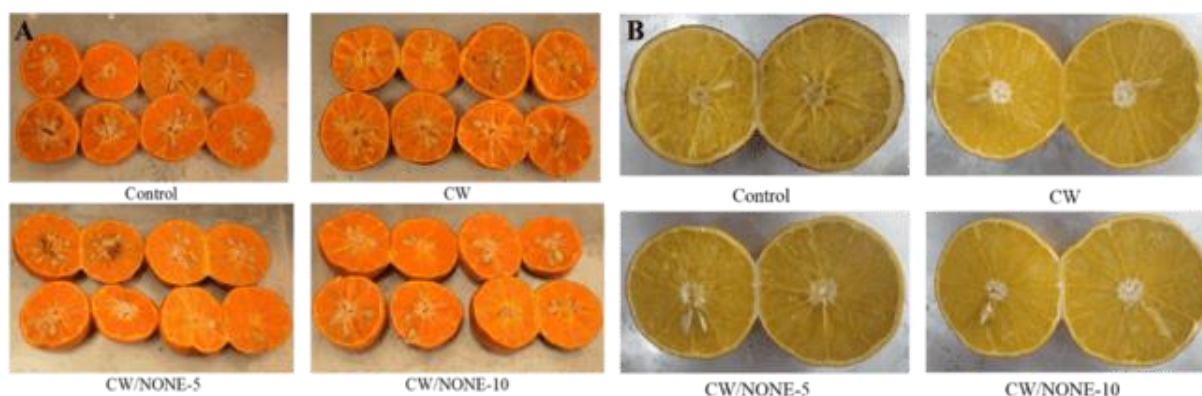


**Figure 1.** Effect of edible coatings on the internal tissue damage and deterioration of Khasi mandarin (A) and sweet lemon (B) after 28 days at ambient temperature

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## Amino acid derived polyhydroxyurethanes as drug carrier and cell adhesive scaffolds

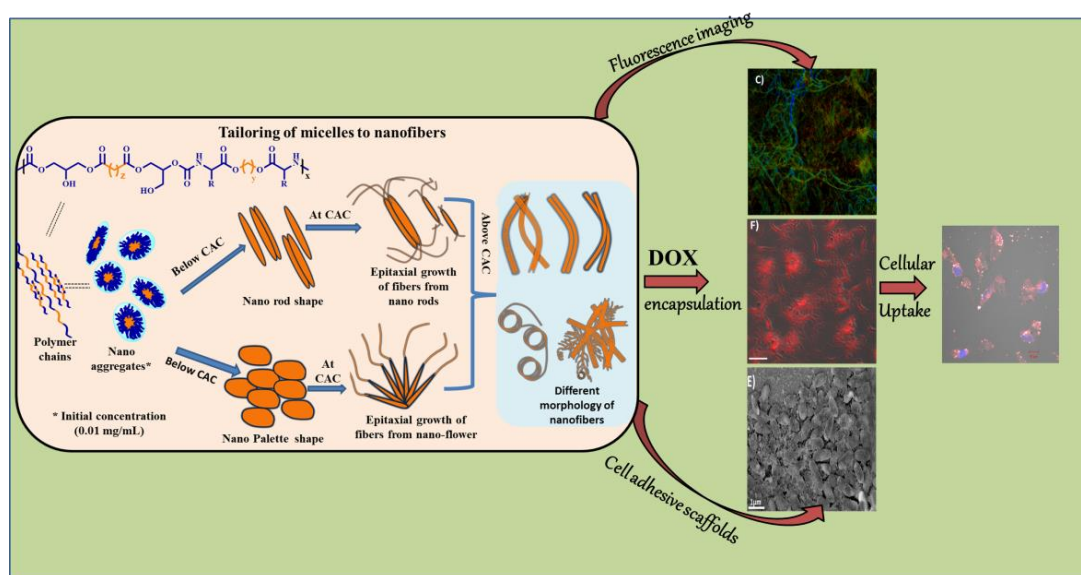
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### Abstract

Development of non-toxic, biodegradable and biocompatible materials are essential for the tissue engineering applications and implantable devices. In this work, we designed amino acid derived polyhydroxyurethanes (PHUs) as biomaterial, by using renewable aliphatic amino acid based diamines and biscyclocarbonates. The presence of carbonyl urethane, ester and hydroxyl groups in the PHU backbone favours the intermolecular hydrogen bonding that elevated these PHUs to be fluorescent active polymer that can be used as biomarker on cell lines. The presence of hydrophilic and hydrophobic segments in these PHUs, promoted the formation of nanofiber like self-assemblies in THF-Water (1:1). The morphology studies demonstrated the evolution of nanofibers proceeds in three steps -1. formation of self-seeded micelles, below Critical aggregation Concentration (CAC), 2. epitaxial growth of these micelles at CAC, and massive growth of the fibers, above CAC. These nanofibers were utilized for the effective Doxorubicin drug delivery studies. Interestingly, we observed that 75% of DOX was released at mild acidic environment i.e. the physiological conditions of cancer cells. These nanofibers can also be used as effective cell adhesive scaffolds for the tissue engineering applications.



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## Green Bio-nanocomposite Prepared Using Polylactic acid and Plant-Based Nano-Particles: A Review

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### Abstract

The excessive consumption of disposable plastic materials and its harmful impact on the environment demands a sustainable material that can degrade without releasing any toxic substance in the ecosystem[1]. Replacing conventional plastic by bio-based biodegradable plastic is the possible solution to the ongoing issue related to the generation of waste plastics and its harmful effect. Polylactic acid (PLA), a non-toxic polymer derived from natural resources, is biodegradable. The added advantage of PLA is moderate mechanical strength, thermal properties, rheological behavior, and toughness compared to conventional packaging plastics[2]. Lower melt strength, high permeability of water and air, poor thermal stability, and high cost of PLA restrict its mass application in the packaging sector. Incorporation of nano-particles derived from natural resources such as starch, cellulose, chitin, and protein in PLA matrix can help to overcome these limitations. In this study we have listed different nano-particles extracted from plant-based resources and how their addition to the PLA matrix positively influences the characteristics of PLA bio-nanocomposite. Method used to synthesize nano-particle have a great influence on the properties of bio-nanocomposite and its overall cost. We have summarized, eco-friendly and economically viable techniques for preparing nano-particles and fabricating composite. The objective of this study to present a sustainable alternative of fossil-based packaging material by listing the various method to prepare green bio-nanocomposite of PLA for packaging application which follow the cycle represented in the diagram.

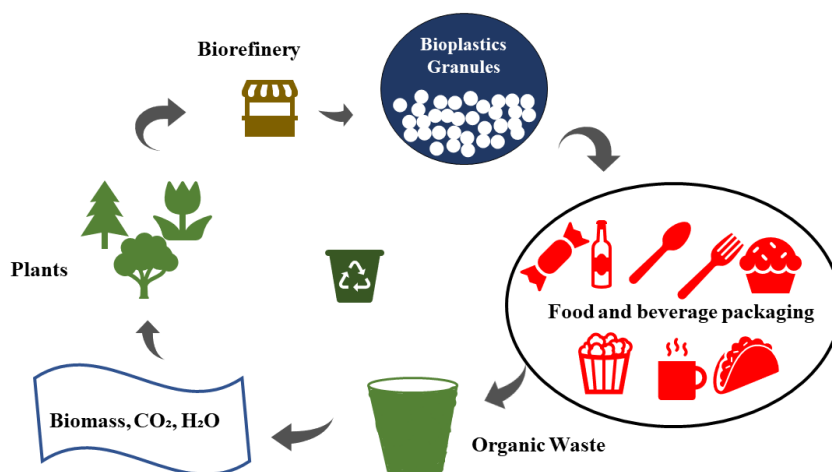


Figure: Schematic representation of lifecycle of bio-based packaging material following circular economy

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## Biodegradable Polymers and the Use of Bamboo Foliage in Plaster Reinforcement: Ancient Knowledge and Sustainable Applications – A review

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### Abstract

During ancient times, biodegradable polymers were commonly used for construction purposes. These biodegradable natural polymers were preferred for their strength, durability, and insulation properties. Bamboo was highly valued for its versatility and strength, and its abundance, fast growth, and eco-friendly characteristics made it a sustainable choice for various applications. Bamboo fiber is undoubtedly one of the most eco-friendly and sustainable cellulosic fibers available, with exceptional features such as rapid growth rate, lightweight, incredible strength, and complete biodegradability. Silica bodies, stomata, long cells, and short cells can help identify bamboo foliage. Silica is an essential component in providing strength and binding properties to plaster. Solapur Fort in the 16th century extensively utilized bamboo foliage as an organic additive in their lime plaster. The discovery of bamboo foliage in plasterworks is a truly groundbreaking moment, marking a new era in the world of art and design. As rice cultivation was scarce in the dry climate of Solapur, bamboo foliage, which contains high silica, was likely used as a substitute to enhance the plaster's strength. Ancient artisans in Solapur had a unique knowledge of the beneficial properties of biodegradable polymers for plaster reinforcement. The use of bamboo culm in construction is a common practice. However, the presence of bamboo foliage found in the plasterworks of Solapur Fort is an exceptional discovery. This finding suggests that the artisans in Solapur had a specific understanding of the usage of biodegradable polymers for plaster reinforcement.

**Keywords:** Bamboo; Biodegradable natural polymer

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## Pullulan: A Comprehensive Review on its Properties, Production and Multifaceted Applications

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### Abstract

Pullulan, a non-ionic exopolysaccharide of fungal origin obtained through the fermentation process of *Aureobasidium pullulans*, has gained considerable attention in the food, pharmaceutical, cosmetic, biomedical and various sectors due to its outstanding versatility. The unique chemical linkage of  $\alpha$  (1  $\rightarrow$  4) and  $\alpha$  (1  $\rightarrow$  6) in Pullulan contributes to its distinct physical properties, including adhesion and the ability to form fibers. Alongside its biodegradability, Pullulan boasts several other favourable attributes, such as non-toxicity, non-immunogenicity, non-carcinogenicity, and non-mutagenicity. Furthermore, it exhibits remarkable attributes, being soluble in water, safe for consumption, lacking any discernible taste, and devoid of any odour. Its derivatives exhibit notable resistance to heat and display a broad range of viscosity and solubility. Consequently, the industrial demand for pullulan is on the rise, as its chemical, biochemical, and physical properties make it highly versatile and well-suited for numerous applications. This extensive range of uses has motivated researchers worldwide to explore and enhance its capabilities further. This review article provides a historical perspective, highlights its structure, properties, production and explores its recent advancements and versatile applications in food, cosmetics, pharmaceuticals and biomedicine.

**Keywords:** Pullulan, exopolysaccharide, fermentation, *Aureobasidium pullulans*

## Silk sericin: A promising biomaterial for the fruit preservation

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### Abstract

The current research seeks to recover and utilize silk sericin, a natural bio polymer obtained during the degumming of silk cocoons, as a promising material for fruit preservation. Sericin has been recognized as one of the most recent therapies for a variety of human ailments due to its antimicrobial, antioxidant, anti-inflammatory, and other functional properties, making it popular to find applications in a variety of fields ranging from the cosmetic industry to the biomedical field and pharmaceuticals<sup>[1]</sup>. The current study focuses on using these unique properties of sericin for fruit preservation using the dip coating technique, followed by performing various studies such as the effect of sunlight, fruit shelf life, aerial oxidation test, load-bearing test, weight loss, acidity test, and microbial resistance properties<sup>[2]</sup>. Additionally, the material was thoroughly investigated using various characterization techniques such as UV-Visible spectrophotometer, FTIR, and Scanning Electron Microscopy to better correlate material properties with the fruit preservation and shelf-life extension. Further, sericin is non-toxic to humans as well as the environment at the concentrations necessary for food preservation and packaging purposes, and it can be seen as a long-term alternative to synthetic chemical-based preservatives, antioxidants, and antibacterial agents. In summary, this study shows sericin recovery and its application as a potential material for preservation of highly perishable fruits on a laboratory scale, as well as providing a pathway for greener, cost-effective, and easily adaptable materials and processes that can slow down the fruit softening and ripening process.

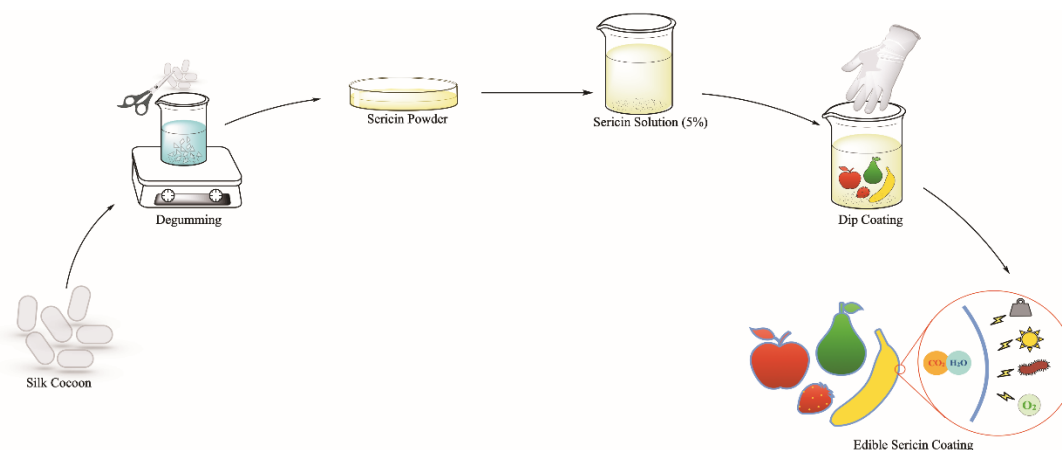


**Figure:** A schematic depicting the sericin recovery followed by fruit coating and preservation.

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Note: The aforementioned abstract work had been submitted to Journal of Food Science and Technology and is currently under review.

## A review of 4D printing: Advanced shape memory polymers in biomedical engineering

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### Abstract

Shape memory polymers represent intelligent materials capable of undergoing shape alterations when subjected to external stimuli. The concept of four-dimensional (4D) printing stems from the fusion of deformable materials and the principles of three-dimensional (3D) printing technology. Presently, 4D printed shape memory polymers and dynamic structures have found widespread applications across various domains, with a notable emphasis on the realm of biomedical science. This innovative 4D printing technology has shattered the boundaries of conventional medical practices, ushering in a new era of personalized customization within the biomedical field. This review provides an overview of recent advancements in shape memory polymers, 3D printing technology, and their amalgamation into 4D printed shape memory polymers and dynamic structures within the biomedical sphere. Additionally, it highlights exemplary use cases and applications of these 4D printed materials in biomedical contexts. Capitalizing on 4D printing capabilities and responsive to diverse conditions, 3D printing techniques enable the fabrication of biomedical components, including cell scaffolds, vascular stents, bone scaffolds, tracheal stents, and cardiac stents. Finally, this review concludes by outlining the potential applications, existing technological constraints, and future development trajectories of 4D printed shape memory polymers and their dynamic structures within the expansive field of biomedicine.

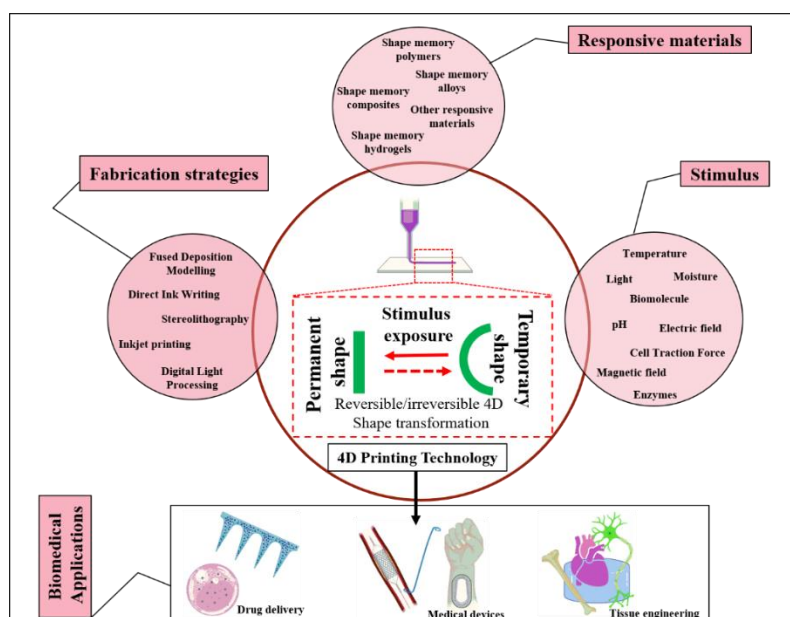


Fig. 1. A graphical abstract for 4D printing for biomedical applications

## Structural Characterization of *Gajal* Soot Obtained from Vegetable Oil

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### Abstract

Nanophased carbon was obtained from the *Gajal* soot generated by burning mustard oil in an open environment using various substrates and vegetable oils. The sample underwent characterization through a combination of analytical techniques, including energy-dispersive X-ray (EDX) analysis, ultraviolet-visible spectroscopy (UV-Vis), Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). These analyses revealed the presence of carbon as a primary element having a C-C double bond with disordered form with some graphitic structure. The surface morphology of the sample observed by SEM exhibited an agglomerated structure with particle sizes ranging from 40-60 nm (see Fig. 1).

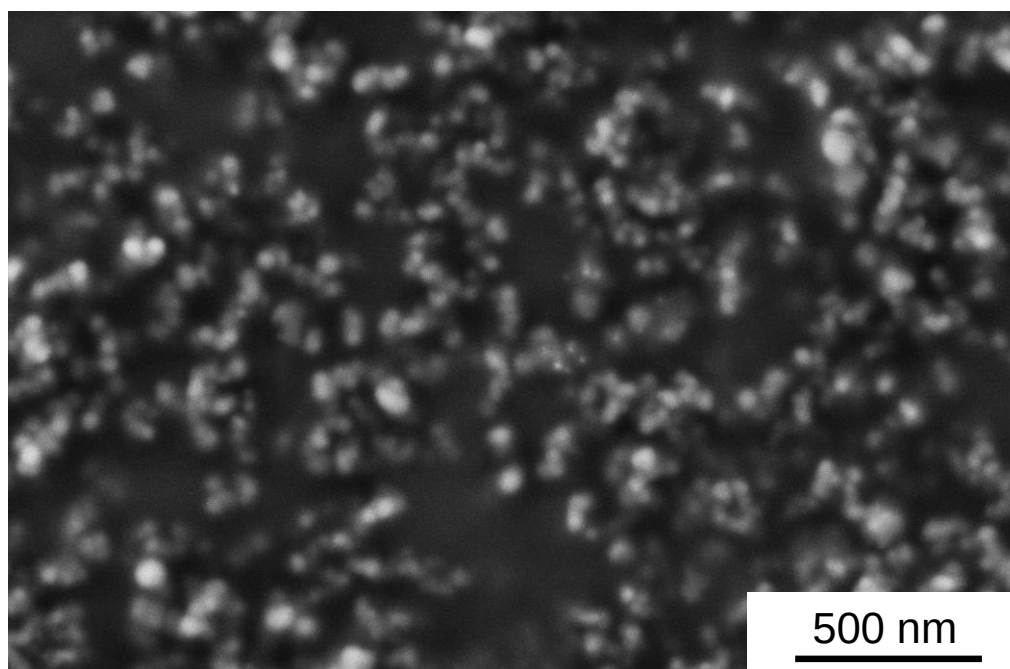


**Figure 1.** Scanning electron micrograph of *Gajal* soot obtained by combustion of mustard oil dipped with a muslin cloth

**Keywords:** *Gajal* soot, SEM, morphology, XRD, graphite structure

**Acknowledgments:** We gratefully acknowledge the support of Mr. Dhanbir Lingden and Prof. Keith J. Stine (Department of Chemistry and Biochemistry, University of Missouri - St. Louis, USA for the SEM analysis of the samples.



## Developing New Composite Material by Blending Waste Commodity Plastics with Natural Fibers

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### Abstract

In response to the escalating environmental concerns arising from plastic waste, particularly the pervasive pollution caused by commonly used polyethylene packaging materials, our project focuses on innovating composite materials. Our objective is to tackle the environmental concerns arising from plastic waste by implementing a solution that involves combining discarded polyethylene with natural fibers. Specifically, we intend to use fibers obtained from sawdust and the bast fibers of certain plants. To enhance the properties of these materials, we plan to subject them to thorough physicochemical treatments. This approach signifies a deliberate effort to transform waste polyethylene into a more environmentally friendly composite material, promoting sustainability and minimizing the negative impact of plastic pollution. The project investigates the influence of various fibers on the mechanical and structural properties of the resulting composites. Using a specially designed molding device, we conducted melt mixing to prepare composite plaques. Our choice of natural fibers includes sawdust (from Pine and Utis), *Daphne bholua*, *Edgeworthia gardneri*, and rice husk, combined with both pure and recycled polypropylene grains. The fiber composition ranged from 10-40 wt.-%, with optimal results observed at 20 wt.-% filler content. Additionally, selected composites were employed in molding prototypes of flower pots, key rings, tea mats, and blocks for furniture. Microscopic examination showcased effective dispersion of filler particles in the polymer matrix, indicating potential enhancements in composite properties through the use of Compatibilizers.

**Keywords:** Waste plastics, recycled polypropylene, natural fibers, reinforcement, *Daphne bholua*, *Edgeworthia gardneri*, rice husk, polymer composites

**Acknowledgments:** We gratefully acknowledge the Ministry of Education, Science and Technology for supporting this Project.

## An overview on alkaline hydrolysis of PBAT: Current Insights and Future Prospects

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### Abstract

Poly (butylene adipate-co-terephthalate) (PBAT) stands out as a promising biopolymer, and its alkaline hydrolysis is a topic of growing significance within the scientific community. This review provides a focused overview on the current understanding of PBAT hydrolysis specifically under alkaline conditions, emphasizing key insights into the underlying mechanisms, influential factors, and methods to achieve accelerated degradation of PBAT. Furthermore, the review addresses the challenges associated with alkaline degradation, including the potential formation of byproducts and the influence of alkaline conditions on the final breakdown products. The interplay between alkaline hydrolysis and other factors, such as temperature and moisture, is also examined to provide a holistic understanding of the process.

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## Melt processed polylactic acid/ polycaprolactone/ sawdust based biocomposites trays with enhanced compostability

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### Abstract

The major drawback associated with petroleum-based polymer products is pollution, leading to environmental hazards. Biodegradable polymers and biocomposites have the potential to play a major role in replacing the conventional polymers in specific applications on a case to case basis. In the current study, sawdust reinforced polylactic acid/ polycaprolactone (PLA/PCL) biocomposites were developed using the melt extrusion technique. Primary processed fine sawdust was reinforced with PLA/PCL blend in a mini twin screw extruder in different weight fractions (10%, 20%, 30%, and 40%). The developed biocomposites were subjected to tensile testing, which indicated that the increased weight percent of sawdust reduced the tensile strength. The materials were further characterized, using sophisticated analytical such as field emission scanning electron microscopy, differential scanning calorimetry and thermogravimetry analysis. The composite containing 30% sawdust concentration presented the best results with tensile strength of 26.5 MPa, tensile strain of 4.4% and onset degradation temperature of 320 °C. The same formulation was successfully scaled up to the pilot level of 5 Kg batch. It was further subjected to secondary processing to produce market ready cutlery items. Biodegradability studies in simulated composting environments revealed that addition of sawdust drastically reduces the lag phase in degradation and total degradation may be obtained in approximately 90 days. Based on the investigation, there is optimism that the PLA/PCL composites, blended with sawdust may ensure commercial application of sustainable polymer blends at affordable prices.

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## Magnetic nanoparticles coated synthetic receptors for the specific capture and detection of *Staphylococcus aureus*

Kritika Narula, Soumya Rajpal, Snehasis Bhakta, Senthilguru Kulanthaivel, Prashant Mishra\*<sup>1</sup>

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### Abstract

*Staphylococcus aureus* (*S. aureus*), a Gram-positive bacteria is a common human pathogen. It causes a wide range of illnesses, including skin infections, pneumonia, and bloodstream infections. It is also a leading cause of healthcare-associated infections (HAIs). Its adaptability and potential for antibiotic resistance present significant challenges in healthcare. The rapid and reliable diagnosis of *S. aureus* is critical for limiting the spread of infection and guiding appropriate antibiotic therapy. Several challenges, however, impede successful detection and treatment. One such challenge, is access to reliable, quick, sensitive and specific detection of bacterial infections and contaminations. Modern diagnostic tools, such as molecular testing is limited in many remote settings as well as in low and middle income nations, making it difficult to identify *S. aureus* and its resistant counterparts rapidly. Molecular imprinting (MIP) has emerged as a novel technique for developing advanced diagnostic tools that offers various advantages over traditional methods. The key benefits of MIPs in diagnostics are their excellent selectivity, sensitivity, stability, reusability, low cost of production, and biocompatibility. In this study, a bacterial surface biomarker, Protein A is used as a target for molecularly imprinted polymer, in order to specifically detect *S. aureus* in biological medium. To rationally select the monomer for imprinting, docking studies were performed in between monomers and Protein A. Monomers showing higher number of binding sites in target were selected. Further, binding assay of MIP with Protein A as well as *S. aureus* were performed. The imprint showed three times higher binding to Protein A as compared to non-specific targets with the imprinting factor of 3. In addition, imprint showed specificity towards *S. aureus* by showing higher binding than *E.coli* and *B. subtilis*.

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## **Survey and Studies of Microplastic on Shorelines of Rivers: A Review**

**A. Gole, S. Nangia, A. Banerjee, S. Behare and Vimal Katiyar\*<sup>1</sup>**

<sup>1</sup>*Indian Institute of Technology- Guwahati, India.*

*\*Corresponding author's E-mail: vkatiyar@iitg.ac.in*

### **Abstract**

Microplastic contamination is a pressing global environmental concern, necessitating a systematic approach involving meticulous sample collection, advanced characterization techniques, and stringent study design for a comprehensive assessment of microplastic abundance. This review focuses on samples collected from diverse global river locations, strategically chosen to represent varying anthropogenic and geographical contexts, from rural to densely populated urban areas. A robust framework and meticulous sampling procedures ensure the generation of representative and comparable data across diverse river environments, considering dynamic environmental factors influencing microplastic dispersion.

Utilizing established methods like chemical digestion, density separation, and filtration, the review identifies studies that successfully isolates microplastics from environmental matrix materials. Method optimization enhances recovery efficiency while minimizing contamination risks, ensuring the accuracy of the collected data. Characterization of isolated microplastics through multimodal techniques is critical for its management through physico-chemical or biological remediation.

Acknowledging the inherent limitations, including challenges associated with local variations impacting sample representativeness, the dynamic nature of river ecosystems poses difficulties in real-time monitoring of changes in microplastic concentrations. This review contributes valuable insights into the global extent of microplastic pollution in river ecosystems, providing a foundation for targeted mitigation strategies and legislative initiatives. The combined application of consistent sampling, robust isolation, and sophisticated characterization techniques enhances understanding of the intricate microplastic landscape observed in various river habitats.

### **References**

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# **Indo-Nepal Symposium**



| <b>Indo-Nepal Symposium</b><br><b>Venue: Mini Auditorium</b> |                                                                                                                                                                                        |
|--------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                              | Chair: Prof. Shinichi Sakurai, KIT Japan and Prof. Rameshwar Adhikari, TU Nepal                                                                                                        |
| <b>14:15-14:40</b>                                           | Guest Lecture-1: Prof. Jeng- Ywan Jeng, NTUST Taiwan<br>Advancing Additive Manufacturing Through Innovations in Large Area Liquid Crystal Display (LCD) Vat Photopolymerization        |
| <b>14:40-15:05</b>                                           | Guest Lecture-2: Prof. Abhijit Patra, IISER Bhopal<br>Controlling Molecular Self Assembly for Task Specific Nanoporous Organic Polymers                                                |
| <b>15:05-15:25</b>                                           | Special Lecture-1: Prof. Balaji Iyer Vaidyanathan Shantha, IIT Hyderabad<br>Multiscale Modeling and Simulations Particle Polymer Hybrid Materials                                      |
| <b>15:25-15:45</b>                                           | Special Lecture-2: Dr. Jyoti Giri, TU Nepal<br>Characterization of LDPE Plastic Waste Recycled Composites Fabricated with Lantana camara Char and Saw Dust for Various Applications    |
| <b>15:45-16:05</b>                                           | Special Lecture-3: Dr. Rajesh Pandit, TU Nepal<br>Morphological and Mechanical Properties of Bamboo Culms                                                                              |
| <b>16:05-16:15</b>                                           | Young Researcher's Presentation-1: Deepshikha Karki, TU Nepal<br>Investigations into Gajal Soot Obtained from Natural Oil and Fibers                                                   |
| <b>16:15-16:25</b>                                           | Young Researcher's Presentation-1: Paudel Palpa, TU Nepal<br>Zinc Oxide Nanoparticles' Anti-Cancer Activity in Photodynamic Therapy                                                    |
| <b>16:25- 16:35</b>                                          | Young Researcher's Presentation-2: N. K. Parajuli, TU Nepal<br>Fabric Dyeing Using Natural Dyes and Mordants                                                                           |
| <b>16:35- 16:45</b>                                          | Young Researcher's Presentation-3: M. Pasawan, NTUT, Taiwan<br>Development of green ceramic membranes from waste coal fly ash and bottom fly ash waste via stereolithography technique |

## Schedule



| Day 0: Saturday, 9 December, 2023                              |                                                                                                                                                                                        |
|----------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:00- 16:00                                                   | Pre-conference Workshop on Polymer-based Additive Manufacturing<br>(For student participants)                                                                                          |
| 19:00- 21:30                                                   | Inaugural Dinner                                                                                                                                                                       |
| Day-1, Sunday, 10 December 2023                                |                                                                                                                                                                                        |
| Venue: Bhupen Hazarika Auditorium, IIT Guwahati                |                                                                                                                                                                                        |
| 8:00-09:00                                                     | Registration                                                                                                                                                                           |
| 9:00-9:45                                                      | Conference Inauguration                                                                                                                                                                |
| <b>Session-1:</b> Chair: Prof. Anil Kumar, IIT Bombay          |                                                                                                                                                                                        |
| 9:45-10:30                                                     | Dr. S. Sivaram Endowment Lecture:<br>Prof. Stefan Mecking, University of Konstanz, Germany<br>Recyclable and Degradable Polyethylene-Like Material Enabled by Catalytic Methods        |
| 10:30-11:15                                                    | PL-1: Prof. Sanjay Rastogi, KAUST Saudi Arabia<br>Equilibration of Non-Equilibrium Polymer Melt, Implications on Physical and Mechanical Properties                                    |
| 11:15 – 11:45                                                  | Tea Break                                                                                                                                                                              |
| <b>Session-2:</b> Chair: Prof. S. Ramakrishnan, IISc Bangalore |                                                                                                                                                                                        |
| 11:45 – 12:15                                                  | Prof. Santappa Award Lecture 1:<br>Prof. Susanta Banerjee, IIT Kharagpur<br>An Overview of High-performance Polymers for Membrane-Based Applications                                   |
| 12:15 - 12:45                                                  | Prof. Santappa Award Lecture 2:<br>Prof. Suhrit Ghosh, IACS Kolkata<br>Molecular Recognition Driven Controlled Supramolecular Polymerization                                           |
| 12:45 – 13:15                                                  | Dr. K.H. Gharda Industrial Innovation Award Lecture:<br>Dr. Anuya Nisal and Team (Serigen-Mediproducs, Pvt. Ltd.)<br>Natural Silk-Based High-Strength Porous Materials for Bone Repair |

| 13:15 – 14:15                   |                                              |                                                   |                                                    |                                                           |
|---------------------------------|----------------------------------------------|---------------------------------------------------|----------------------------------------------------|-----------------------------------------------------------|
| Lunch                           |                                              |                                                   |                                                    |                                                           |
| Day-1, Sunday, 10 December 2023 |                                              |                                                   |                                                    |                                                           |
| Time                            | Hall-1                                       | Hall-2                                            | Hall-3                                             | Hall-4                                                    |
|                                 | Session-3                                    | Session-4                                         | Session-5                                          | Session-6                                                 |
|                                 | <b>Advanced Polymer Synthesis-I</b>          | <b>Supramolecular Polymers</b>                    | <b>Polymer Nanostructures and Nanocomposites</b>   | <b>Polymers for Biomedical Applications-I</b>             |
|                                 | Chair: Prof. S. Ramakrishnan, IISc Bangalore | Chair: Prof. Veena Choudhary                      | Chair: Prof. Ashok K. Dasmahapatra IIT Guwahati    | Chair: Prof. Sangamesh G. Kumbar UConn Health Center, USA |
| 14:15-14:40                     | KL-1<br>Dr. Samir H. Chikkali, NCL Pune      | KL-2<br>Prof. Nikhil Kumar Singha IIT Kharagpur   | KL-3<br>Dr. Shotaro Yamaguchi Amano Enzymes, Japan | KL-4<br>Prof. Sanjeeva Murthy Rutgers University, USA     |
| 14:40-15:00                     | IL-1<br>Dr. Sanjib Banerjee IIT Bhilai       | IL-2<br>Dr. Goutam Ghosh CeNS, Bangalore          | IL-3<br>Dr. Farsa Ram University of Chicago, USA   | IL-4<br>Prof. Chandra S. Sharma IIT Hyderabad             |
| 15:00-15:20                     | IL-5<br>Prof. Priyadarshi De IISER Kolkata   | IL-6<br>Dr. Priyadarshi Chakraborty IIT Hyderabad | IL-7<br>Dr. Subhash Mandal DMSRDE Kanpur           | IL-8<br>Prof. Raja Shunmugam IISER Kolkata                |
| 15:20-15:30                     | OP-1<br>Bhanendra Sahu                       | OP-2<br>Akshay Thorat                             | OP-3<br>Mini Mol Menamparambath                    | OP-4<br>Sulagna Bhattacharjee                             |

|                                                                                                              |                                                                                                                                                                                     |                        |                        |                              |
|--------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|------------------------|------------------------------|
| 15:30-15:40                                                                                                  | OP-5<br>Parshuram Kambale                                                                                                                                                           | OP-6<br>Vidyalakshmi D | OP-7<br>Santanu Basak  | OP-8<br>Manju Saraswathy     |
| 15:40-15:50                                                                                                  | OP-9<br>Yogesh Patil                                                                                                                                                                | OP-10<br>Neha          | OP-11<br>Rajesh Pandit | OP-12<br>Ibrahim Bargathulla |
| 14:15- 16:45                                                                                                 | Indo- Nepal Symposium                                                                                                                                                               |                        |                        |                              |
| 15:50-17:30                                                                                                  | Poster Session (Poster no. PP-1 - PP-105) and Tea break                                                                                                                             |                        |                        |                              |
| 17:00-17:45                                                                                                  | AGM (SPSI)                                                                                                                                                                          |                        |                        |                              |
| Session-7: Chair: Prof. S. Sivaram, Ex-Director, NCL Pune<br>Venue: Bhupen Hazarika Auditorium, IIT Guwahati |                                                                                                                                                                                     |                        |                        |                              |
| 17:45-19:00                                                                                                  | Panel Discussion: Research Education in Polymer Science – Future Roadmap                                                                                                            |                        |                        |                              |
| 19:00-22:00                                                                                                  | Cultural Programme and Conference Dinner                                                                                                                                            |                        |                        |                              |
| Time                                                                                                         | Indo-Nepal Symposium<br>Venue: Mini Auditorium                                                                                                                                      |                        |                        |                              |
|                                                                                                              | Chair: Prof. Shinichi Sakurai, KIT Japan and Prof. Rameshwar Adhikari, TU Nepal                                                                                                     |                        |                        |                              |
| 14:15-14:40                                                                                                  | Guest Lecture-1: Prof. Jeng- Ywan Jeng, NTUST Taiwan<br>Advancing Additive Manufacturing Through Innovations in Large Area Liquid Crystal Display (LCD) Vat Photopolymerization     |                        |                        |                              |
| 14:40-15:05                                                                                                  | Guest Lecture-2: Prof. Abhijit Patra, IISER Bhopal<br>Controlling Molecular Self Assembly for Task Specific Nanoporous Organic Polymers                                             |                        |                        |                              |
| 15:05-15:25                                                                                                  | Special Lecture-1: Prof. Balaji Iyer Vaidyanathan Shantha, IIT Hyderabad<br>Multiscale Modeling and Simulations Particle Polymer Hybrid Materials                                   |                        |                        |                              |
| 15:25-15:45                                                                                                  | Special Lecture-2: Dr. Jyoti Giri, TU Nepal<br>Characterization of LDPE Plastic Waste Recycled Composites Fabricated with Lantana camara Char and Saw Dust for Various Applications |                        |                        |                              |
| 15:45-16:05                                                                                                  | Special Lecture-3: Dr. Rajesh Pandit, TU Nepal                                                                                                                                      |                        |                        |                              |

|                     |                                                                                                                                                                                        |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                     | Morphological and Mechanical Properties of Bamboo Culms                                                                                                                                |
| <b>16:05-16:15</b>  | Young Researcher's Presentation-1: Deepshikha Karki, TU Nepal<br>Investigations into Gajal Soot Obtained from Natural Oil and Fibers                                                   |
| <b>16:15-16:25</b>  | Young Researcher's Presentation-1: Paudel Palpa, TU Nepal<br>Zinc Oxide Nanoparticles' Anti-Cancer Activity in Photodynamic Therapy                                                    |
| <b>16:25- 16:35</b> | Young Researcher's Presentation-2: N. K. Parajuli, TU Nepal<br>Fabric Dyeing Using Natural Dyes and Mordants                                                                           |
| <b>16:35- 16:45</b> | Young Researcher's Presentation-3: M. Pasawan, NTUT, Taiwan<br>Development of green ceramic membranes from waste coal fly ash and bottom fly ash waste via stereolithography technique |

**Day-2, Monday, 11 December 2023**

Venue: Bhupen Hazarika Auditorium, IIT Guwahati

**Session-8:** Chair: Prof. Anup K. Ghosh, IIT Delhi

|                    |                                                                                                                                                                                     |
|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>9:00-9:45</b>   | <b>PL-2:</b> Prof. Subi Jacob George, JNCASR Bengaluru<br>Structural Control on Supramolecular Polymers                                                                             |
| <b>9:45-10:15</b>  | Prof. Kishore Memorial Award Lecture-1:<br>Prof. Leena Nebhani, IIT Delhi<br>Synthetic Strategies to Attain Polymer Functionalized Particles and Catalytic Porous Polymer Particles |
| <b>10:15-10:45</b> | Prof. Kishore Memorial Award Lecture-2:<br>Prof. Asish Pal, INST Mohali<br>Functional Peptide-Polymer Conjugates towards Strain-stiffening and Chiroptical properties               |
| <b>10:45-11:00</b> | Tea Break                                                                                                                                                                           |



**Day-2, Monday, 11 December 2023**

|                    | <b>Hall-1</b>                                        | <b>Hall-2</b>                                                | <b>Hall-3</b>                                                  | <b>Hall-4</b>                                                            |
|--------------------|------------------------------------------------------|--------------------------------------------------------------|----------------------------------------------------------------|--------------------------------------------------------------------------|
|                    | <b>Session-9</b>                                     | <b>Session-10</b>                                            | <b>Session-11</b>                                              | <b>Session-12</b>                                                        |
| <b>Time</b>        | <b>Advanced Polymer Synthesis-II</b>                 | <b>Polymers in Energy Applications-I</b>                     | <b>Biodegradable Polymers-I</b>                                | <b>Functional and Smart Biomaterials-I</b>                               |
|                    | Chair: Prof. M. Jayakannan<br>IISER Pune             | Chair: Prof. Chyi-How Lay<br>Feng Chia University,<br>Taiwan | Chair: Dr. Asha Syamakumari<br>CSIR-NCL Pune                   | Chair: Prof. Shinichi Sakurai<br>Kyoto Institute of<br>Technology, Japan |
| <b>11:00-11:25</b> | KL-5<br>Prof. Tarun K. Mandal,<br>IACS Kolkata       | KL-6<br>Dr. G. Unnikrishnan<br>NIT Calicut                   | KL-7<br>Dr. Bhoje Gowd E.<br>CSIR-NIIST,<br>Thiruvananthapuram | KL-8<br>Prof. Suryasarathi Bose<br>IISc Bangalore                        |
| <b>11:25-11:45</b> | IL-9<br>Dr. Dario Romano<br>KAUST, Saudi Arabia      | IL-10<br>Prof. Sudip Malik<br>IACS Kolkata                   | IL-11<br>Dr. Vivek Verma<br>IIT Kanpur                         | IL-12<br>Dr. Dibyendu Sekhar Bag<br>DMSRDE, Kanpur                       |
| <b>11:45-12:05</b> | IL-13<br>Dr. Debasis Samanta<br>CSIR-CLRI, Chennai   | IL-14<br>Dr. K. Krishnamoorthy<br>CSIR-NCL Pune              | IL-15<br>Dr. Prodyut Dhar<br>IIT(BHU)                          | IL-16<br>Prof. Kanagaraj S.<br>IIT Guwahati                              |
| <b>12:05-12:25</b> | IL-17<br>Dr. Swapnali Hazarika<br>CSIR-NEIST, Jorhat | IL-18<br>Prof. Tushar Jana<br>University of Hyderabad        | IL-19<br>Prof. Sampa Saha<br>IIT Delhi                         | IL-20<br>Dr. Vikram Singh<br>CSIR-CIMFR, Dhanbad                         |
| <b>12:25-12:35</b> | OP-13<br>Radha Sachan                                | OP-14<br>Anusha Kadimisetti                                  | OP-15<br>Shubham Pant                                          | OP-16<br>Devleena Bose                                                   |

|             |                                                               |                                                                           |                                                                 |                                                |
|-------------|---------------------------------------------------------------|---------------------------------------------------------------------------|-----------------------------------------------------------------|------------------------------------------------|
| 12:35-12:45 | OP-17<br>Gorakh Ghuge                                         | OP-18<br>Dhruba P. Chatterjee                                             | OP-19<br>Akhila N S                                             | OP-20<br>Dipanjana Patra                       |
| 12:45-12:55 | OP-21<br>Uddhab Kalita                                        | OP-22<br>Bhanupriya Das                                                   | OP-23<br>Vishalakshi Badalamoole                                | OP-24<br>Harpreet Singh                        |
| 12:55-13:05 | OP-25<br>Monikangkana Talukdar                                | OP-26<br>Mayuri Srivastava                                                | OP-27<br>Kanagaraj S.                                           | OP-28<br>Jit Sarkar                            |
| 13:05-14:15 | Lunch                                                         |                                                                           |                                                                 |                                                |
| Time        | Hall-1                                                        | Hall-2                                                                    | Hall-3                                                          | Hall-4                                         |
|             | Session-13                                                    | Session-14                                                                | Session-15                                                      | Session-16                                     |
|             | <b>Functional and Smart Biomaterials-II</b>                   | <b>Biodegradable Polymers-II</b>                                          | <b>Polymers for Biomedical Applications-II</b>                  | <b>Advances in Polymers-I</b>                  |
|             | Chair: Prof. Christine Jerome<br>University of Liege, Belgium | Chair: Prof. Pravindra Kumar<br>IIT Roorkee                               | Chair: Prof. Biman B. Mandal<br>IIT Guwahati                    | Chair: Prof. Priyadarshi De<br>IISER Kolkata   |
| 14:15-14:40 | KL-9<br>Prof. Sunil K. Sharma,<br>Delhi University            | KL-10<br>Prof. Vijay Rangari<br>Tuskegee University                       | KL-11<br>Prof. Neil Cameron<br>Monash University, Australia     | KL-12<br>Dr. Asha Syamakumari<br>CSIR-NCL Pune |
| 14:40-15:00 | IL-21<br>Dr. Ashootosh Ambade,<br>CSIR-NCL, Pune              | IL-22<br>Dr. Hironori Marubayashi,<br>Kyoto Institute of Technology Japan | IL-23<br>Prof. Sangamesh G. Kumbar,<br>UConn Health Center, USA | IL-24<br>Prof. Biplap Kuila<br>IIT (BHU)       |
| 15:00-15:20 | IL-25                                                         | IL-26                                                                     | IL-27                                                           | IL-28                                          |

|                    |                                                           |                                                           |                                           |                                                                 |
|--------------------|-----------------------------------------------------------|-----------------------------------------------------------|-------------------------------------------|-----------------------------------------------------------------|
|                    | Prof. Utpal Bora<br>IIT Guwahati                          | Prof. Rameshwar Adhikari<br>Tribhuvan University<br>Nepal | Dr. G. Krishnamoorthy<br>MCAS, Tamil Nadu | Dr. Vijayakumar Chakkooth,<br>CSIR-NIIST,<br>Thiruvananthapuram |
| <b>15:20-15:30</b> | OP-29<br>Paramjeet Yadav                                  | OP-30<br>Sagar Bag                                        | OP-31<br>Sudip Mukherjee                  | OP-32<br>Pankaj Baruah                                          |
| <b>15:30-15:40</b> | OP-33<br>Debasish Nath                                    | OP-34<br>Shibam Pal                                       | OP-35<br>Arbind Prasad                    | OP-36<br>Souradeep Ghosh                                        |
| <b>15:40-15:50</b> | OP-37<br>Deepjyoti Basumatary                             | OP-38<br>Vinothkumar D                                    | OP-39<br>Shahidkhan Pathan                | OP-40<br>Dipanjan Giri                                          |
| <b>15:50-16:00</b> | OP-41<br>Somdatta Rudra                                   | OP-42:<br>Aswathy N R                                     | OP-43<br>Kuhelika Das                     | OP-44<br>Sandeep Kumar Sahoo                                    |
| <b>16:00-16:10</b> | OP-45<br>Tanushri Banerjee                                | OP-46<br>Kartik R                                         | OP-47<br>Athira M                         | OP-48<br>Parthiv Trivedi                                        |
| <b>16:10-16:20</b> | OP-49<br>Jayanta Nanda                                    | OP-50<br>Arunava Dutta                                    | OP-51<br>Atish Nag                        | OP-52<br>Parul Shukla                                           |
| <b>16:20-18:00</b> | Tea Break and Poster Session (Poster no. PP-106 – PP-210) |                                                           |                                           |                                                                 |
| <b>18:00-18:30</b> | Springer Workshop (Hall-2)                                |                                                           |                                           |                                                                 |
| <b>18:30-19:30</b> | Cultural Programme at Bhupen Hazarika Auditorium          |                                                           |                                           |                                                                 |
| <b>19:30-21:30</b> | Conference Dinner                                         |                                                           |                                           |                                                                 |

| Day-3, Tuesday, 12 December 2023                |                                                                                                                                                                         |                                                               |                                                           |                                        |
|-------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------|-----------------------------------------------------------|----------------------------------------|
| Venue: Bhupen Hazarika Auditorium, IIT Guwahati |                                                                                                                                                                         |                                                               |                                                           |                                        |
|                                                 | <b>Session-17:</b> Chair: Dr. S. Sivaram                                                                                                                                |                                                               |                                                           |                                        |
| <b>9:00-9:45</b>                                | Dr. S. R. Palit Memorial Lecture: S. Thayumanavan, University of Massachusetts, Amherst<br>Reactive Self-Assembly of Polymers and Proteins for Therapeutic Applications |                                                               |                                                           |                                        |
| <b>9:45-10:30</b>                               | <b>PL-3:</b> Prof. M. Jayakannan, IISER Pune<br>Biodegradable Macromolecular Architectures for Biomedical Applications                                                  |                                                               |                                                           |                                        |
| <b>10:30-11:15</b>                              | <b>PL-4:</b> Prof. Yves Gnanou, KAUST, Saudi Arabia<br>Polycarbonate based Copolymers as Effective and Attractive Substitutes for Polyolefins                           |                                                               |                                                           |                                        |
| <b>11:15-11:45</b>                              | Tea Break                                                                                                                                                               |                                                               |                                                           |                                        |
| Time                                            | Hall-1                                                                                                                                                                  | Hall-2                                                        | Hall-3                                                    | Hall-4                                 |
|                                                 | Session-18                                                                                                                                                              | Session-19                                                    | Session-20                                                | Session-21                             |
|                                                 | Polymer Modelling and Simulation                                                                                                                                        | Polymer Packaging                                             | Advances in Polymers-II                                   | Polymers in Energy Applications-II     |
|                                                 | Chair: Dr. Amit Kumar<br>IIT Guwahati                                                                                                                                   | Chair: Dr. Bhoje Gowd E.<br>CSIR-NIIST,<br>Thiruvananthapuram | Chair: Prof. Jun-Ichi Horinaka<br>Kyoto University, Japan | Chair: Prof. P. K Iyer<br>IIT Guwahati |



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|                    |                                                                            |                                                                                  |                                                                 |                                                             |
|--------------------|----------------------------------------------------------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------------------------|
| <b>11:45-12:10</b> | <b>KL-13</b><br>Prof. Upendra Natarajan<br>IIT Madras                      | <b>KL-14</b><br>Prof. Hajime Nakajima<br>Kyoto Institute of<br>Technology, Japan | <b>KL-15</b><br>Prof. Pralay Maiti,<br>IIT(BHU)                 | <b>KL-16</b><br>Prof. Arun K. Nandi<br>IACS Kolkata         |
| <b>12:10-12:30</b> | <b>IL-29</b><br>Prof. Balaji Iyer Vaidyanathan<br>Shantha<br>IIT Hyderabad | <b>IL-30</b><br>Dr. Bindu<br>CIFT, Kochi                                         | <b>IL-31</b><br>Dr. Kl Suresh<br>CSIR-NIIST, Thiruvananthapuram | <b>IL-32</b><br>Dr. Joshy Joseph,<br>CSIR-NIIST, Trivandrum |
| <b>12:30-12:50</b> | <b>IL-33</b><br>Prof. Gaurav Manik<br>IIT Roorkee                          | <b>IL-34</b><br>Dr. P. Aruna<br>CSIR-IICT Hyderabad                              | <b>IL-35</b><br>Prof. Dibakar Dhara<br>IIT Kharagpur            | <b>IL-36</b><br>Dr. Sujay Chattopadhyaya<br>IIT Roorkee     |
| <b>12:50-13:00</b> | <b>OP-53</b><br>Laxmi                                                      | <b>OP-54</b><br>Tabli Ghosh                                                      | <b>OP-55</b><br>Ankan Sarkar                                    | <b>OP-56</b><br>Uma Chatterjee                              |
| <b>13:00-13:10</b> | <b>OP-57</b><br>Gangotree Rai                                              | <b>OP-58</b><br>Vikrant Bodana                                                   | <b>OP-59</b><br>Medha Surendranath                              | <b>OP-60</b><br>Lyric F                                     |
| <b>13:10-13:20</b> | <b>OP-61</b><br>Sharanya Alluri                                            | <b>OP-62</b><br>Tuhin Bhattacharjee                                              | <b>OP-63</b><br>Subin Kc                                        | <b>OP-64</b><br>Imran Hussain                               |
| <b>13:20-14:30</b> | Lunch                                                                      |                                                                                  |                                                                 |                                                             |
| <b>Time</b>        | <b>Hall-1</b>                                                              | <b>Hall-2</b>                                                                    | <b>Hall-3</b>                                                   | <b>Hall-4</b>                                               |
|                    | <b>Session-22</b><br><br><b>Polymer Recycling</b>                          | <b>Session-23</b><br><br><b>Polymer Degradation<br/>and Stability</b>            | <b>Session-24</b><br><br><b>Polymer Rheology</b>                | <b>Session-25</b><br><br><b>Polymer Nanostructures</b>      |

|                    |                                                                             |                                                                                |                                                                   |                                                                             |
|--------------------|-----------------------------------------------------------------------------|--------------------------------------------------------------------------------|-------------------------------------------------------------------|-----------------------------------------------------------------------------|
|                    | Chair: Dr. Dibyendu Sekhar Bag<br>DMSRDE, Kanpur                            | Chair: Prof. Rameshwar<br>Adhikari<br>Tribhuvan University,<br>Nepal           | Chair: S. Thayumanavan<br>University of Massachusetts,<br>Amherst | Chair: Prof. Shigeru Okamoto<br>Nagoya Institute of<br>Technology,<br>Japan |
| <b>14:30-14:55</b> | KL-17<br>Dr. Smita Mohanty<br>CIPET Bhubaneswar                             | KL-18<br>Prof. Pravindra Kumar<br>IIT Roorkee                                  | KL-19<br>Prof. Christine Jerome<br>University of Liege, Belgium   | KL-20<br>Prof. Sabu Thomas,<br>Mahatma Gandhi University,<br>Kerala         |
| <b>14:55-15:15</b> | IL-37<br>Dr. Sukanya Satapathy<br>CSIR-IICT, Telangana                      | IL-38<br>Dr. Naba Kumar Kalita<br>KTH Royal Institute of<br>Technology, Sweden | IL-39<br>Prof. Kamendra P. Sharma<br>IIT Bombay                   | IL-40<br>Prof. Sidhharth Sirohi<br>University of Delhi                      |
| <b>15:15-15:35</b> | IL-41<br>Dr. S. B. Idage<br>CSIR-NCL, Pune                                  | IL-42<br>Dr. Ajeet Kumar<br>IIT Guwahati                                       | IL-43<br>Dr. Shib Shankar Banerjee<br>IIT Delhi                   | IL-44<br>Dr. Titash Mondal<br>IIT Kharagpur                                 |
| <b>15:35-15:55</b> | IL-45<br>Dr. Utai Meekum<br>Suranaree University of<br>Technology, Thailand | IL-46<br>Dr. Rathna GVN<br>CSIR-NCL Pune                                       | IL-47<br>Dr. Raj Kumar Roy<br>IISER Mohali                        | IL-48<br>Dr. Sravendra Rana<br>UPES, Dehradun                               |
| <b>15:55-16:05</b> | OP-65<br>Harshad R. Patil                                                   | OP-66<br>Karthikeyan<br>Sathrugnan                                             | OP-67<br>Praveen Karebasannanavar<br>Ramachandrappa               | OP-68<br>Akuleti Saikumar                                                   |



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|             |                                                                                |                             |                             |                               |
|-------------|--------------------------------------------------------------------------------|-----------------------------|-----------------------------|-------------------------------|
| 16:05-16:15 | OP-69<br>Aaditya Pandey                                                        | OP-70<br>Nilanjan Mukherjee | OP-71<br>Moumita Sasmal     | OP-72<br>Banalata Kaibarta    |
| 16:15-16:25 | OP-73<br>Punugupati Neelambaram                                                | OP-74<br>Sachin Kuriachan E | OP-75<br>Gopal Kumar Gautam | OP-76:<br>Govind Kumar Sharma |
| 16:25-16:35 | OP-77<br>Kishore Khopade                                                       | OP-78<br>Smruti B Bhatt     | OP-79<br>Vedant Joshi       | OP-80<br>Abhishek Verma       |
| 16:35-16:45 | OP-81<br>Balendu Shekhar Giri                                                  | OP-82<br>Sambit Roy         | OP-83<br>Anant D. Kulkarni  | OP-84<br>Doli Hazarika        |
| 16:45-16:55 | OP-85<br>Rohit Rai                                                             | OP-86<br>Vaibhav Darekar    | OP-87<br>Shailesh Nagarakar | OP-88<br>Vasi Shaikh          |
| 17:00-18:30 | Tea and Poster Session (Poster no. PP-211 – PP-305) at Conference Centre Lobby |                             |                             |                               |
| 18:30-19:30 | Cultural Programme at Bhupen Hazarika Auditorium                               |                             |                             |                               |
| 19:30-21:30 | Conference Dinner                                                              |                             |                             |                               |

**Day-4, Wednesday, 13 December 2023**

Venue: Bhupen Hazarika Auditorium, IIT Guwahati

| Time        | Session-26: Chair: Prof. Susanta Banerjee, IIT Kharagpur                                                               |            |                                    |            |
|-------------|------------------------------------------------------------------------------------------------------------------------|------------|------------------------------------|------------|
| 9:00-9:45   | PL-5: Prof. Shinichi Sakurai, Kyoto Institute of Technology, Japan<br>Strain-Induced Crystallization on Natural Rubber |            |                                    |            |
| 9:45-10:30  | PL-6: Prof. Kana Sureshan, IISER Thiruvananthapuram<br>Two Structurally Different Polymers from a Monomer              |            |                                    |            |
| 10:30-10:50 | Tea Break                                                                                                              |            |                                    |            |
|             | Hall-1                                                                                                                 | Hall-2     | Hall-3                             | Hall-4     |
| Time        | Session-27<br>Advances in Polymers-III                                                                                 | Session-28 | Session-29<br>Polymer Architecture | Session-30 |



|                    |                                                                   | <b>Polymer Coatings and Surface Functionalization</b>          |                                                          | <b>Advanced Polymer Synthesis-III</b>            |
|--------------------|-------------------------------------------------------------------|----------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------|
|                    | Chair: Prof. Kana Sureshan<br>IISER Thiruvananthapuram            | Chair: Prof. Stefan Mecking<br>University of Konstanz, Germany | Chair: Prof. Pralay Maiti<br>IIT(BHU)                    | Chair: Prof. Gaurav Manik<br>IIT Roorkee         |
| <b>10:50-11:20</b> | KL-21<br>Prof. Anil Kumar<br>IIT Bombay                           | KL-22<br>Prof. S. Ramakrishnan<br>IISc Bangalore               | KL-23<br>Prof. Abhijit Patra<br>IISER Bhopal             | KL-24<br>Prof. Sagar Pal<br>IIT (ISM) Dhanbad    |
| <b>11:20-11:40</b> | IL-49<br>Prof. Bimlesh Lochab<br>Shiv Nadar University            | IL-50<br>Dr. Anindita Das<br>IACS Kolkata                      | IL-51<br>Prof. Parbati Biswas<br>University of Delhi     | IL-52<br>Dr. Ujendra Kumar Komal<br>IIT Guwahati |
| <b>11:40-12:00</b> | IL-53<br>Dr. Hari Sharan Adhikari,<br>Tribhuvan University, Nepal | IL-54<br>Dr. Murugan E.<br>University of Madras                | IL-55<br>Dr. Sushanta Sethi<br>IIT Dharwad               | IL-56<br>Dr. Pavan K. Kancharla<br>IIT Guwahati  |
| <b>12:00-12:20</b> | IL-57<br>Prof. Santanu Chattopadhyay<br>IIT Kharagpur             | IL-58<br>Dr. Suman Kalyan Samanta<br>IIT Kharagpur             | IL-59<br>Dr. Rohidas Arote<br>Jain University, Bangalore | IL-60<br>Dr. Poonam Kumari<br>IIT Guwahati       |
| <b>12:20-12:40</b> | IL-61<br>Prof. Chyi-How Lay<br>Feng Chia University,<br>Taiwan    | IL-62<br>Dr. Ketan Patel<br>CSIR-CSMCRI Bhavnagar              | IL-63<br>Arindam Kundagrami<br>IISER Kolkata             | IL-64<br>Prof. S.T Mhaske<br>ICT Mumbai          |
| <b>12:40-12:50</b> | OP-89                                                             | OP-90                                                          | OP-91                                                    | OP-92                                            |

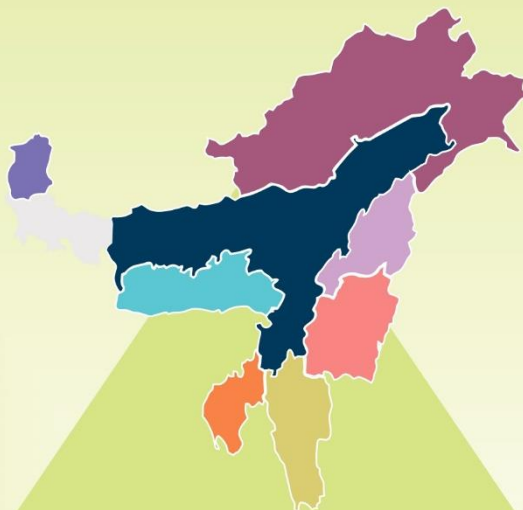
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|--------------------|-------------------------------------------------------|-------------------------------------------------------------------------|-----------------------------------------------------|------------------------------------------------------|
|                    | Srikanth Billa                                        | Rajan Kumar                                                             | Nikhil Dhore                                        | Runa Runa                                            |
| <b>12:50-13:00</b> | OP-93<br>Tonmoi Hazarika                              | OP-94<br>Theerdha V. Nair                                               | OP-95<br>Ujjal Haldar                               | OP-96<br>Ayan Jati                                   |
| <b>13:00-13:10</b> | OP-97<br>Balaji Krishnasamy                           | OP-98<br>Pankaj Kumar                                                   | OP-99<br>Rajkumar Birajdar                          | OP-100<br>Krishna Dan                                |
| <b>13:10-13:20</b> | OP-101<br>Ananda Basak                                | OP-102<br>Ermiya Prasad Paradhakshina                                   | OP-103<br>Nitin Bapurao Basutkar                    | OP-104<br>Bhawna Sharma                              |
| <b>13:20-14:30</b> | Lunch                                                 |                                                                         |                                                     |                                                      |
| <b>Time</b>        | <b>Hall-1</b>                                         | <b>Hall-2</b>                                                           | <b>Hall-3</b>                                       | <b>Hall-4</b>                                        |
|                    | <b>Session-31</b><br><b>Advances in Polymers-IV</b>   | <b>Session-32</b><br><b>Advances in Polymers-V</b>                      | <b>Session-33</b><br><b>Advances in Polymers-VI</b> | <b>Session-34</b><br><b>Advances in Polymers-VII</b> |
|                    | Chair: Prof. Kamendra P. Sharma, IIT Bombaykamendra   | Chair: Prof. Kuruvilla Joseph IIST Thiruvananthapuram                   | Chair: Prof. Nikhil Kumar Singha IIT Kharagpur      | Chair: Dr. Vivek Verma IIT Kanpur                    |
| <b>14:30-14:55</b> | KL-25<br>Prof. Nita Sahai<br>University of Akron, USA | KL-26<br>Prof. Shigeru Okamoto<br>Nagoya Institute of Technology, Japan | KL-27<br>Prof. Biswajit Ray<br>BHU                  | KL-28<br>Prof. Arup Bhattacharyya<br>IIT Bombay      |



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|--------------------|-----------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|------------------------------------------------------|---------------------------------------------------|
| <b>14:55-15:15</b> | IL-65<br>Prof. Niranjana Karak,<br>Tezpur University                                    | IL-66<br>Dr. Jyoti Giri<br>Tribhuvan University, Nepal                         | IL-67<br>Prof. Rabibrata Mukherjee, IIT<br>Kharagpur | IL-68<br>Dr. Arukkani Murugesan<br>SSNCE, Chennai |
| <b>15:15-15:35</b> | IL-69<br>Dr. Senthil Kumar Thangaraj<br>CSIR-Indian Institute of<br>Petroleum, Dehradun | IL-70<br>Prof. A.S Achalkumar<br>IIT Guwahati                                  | IL-71<br>Prof. Kinsuk Naskar<br>IIT Kharagpur        | IL-72:<br>Sanjib Kumar Patra<br>IIT Kharagpur     |
| <b>15:35-15:55</b> | IL-73<br>Prof. Jun-Ichi Horinaka<br>Kyoto University, Japan                             | IL-74<br>Dr. T. Umasankar Patro<br>Defence Institute of Advanced<br>Technology | IL-75<br>Dr. Uttam Manna<br>IIT Guwahati             | IL-76<br>Dr. Uday Shankar<br>NIT Allahabad        |
| <b>15:55-16:15</b> | IL-77:<br>Dr. Rajaram Nagarale,<br>CSIR-CSMCRI, Bhavnagar                               | IL-78:<br>Dr. Santosh Kumar<br>Central Institute of Technology,<br>Kokrajhar   | IL-79<br>Dr. S.N Jaisankar<br>CSIR-CLRI              | IL-80<br>Dr. Amit Kumar<br>IIT Guwahati           |
| <b>16:15-16:25</b> | OP-105<br>Murali Siva Sundar MS                                                         | OP-106<br>Harish Sharma                                                        | OP-107<br>Balaji Krishnasamy                         | OP-108<br>Vijaykumar Ubale                        |
| <b>16:25-16:35</b> | OP-109<br>Balaji Krishnasamy                                                            | OP-110<br>Yub Narayan Thapa                                                    | OP-111<br>Umesh Thapa                                | OP-112<br>Shikha Sharma                           |
| <b>16:35-17:00</b> | Tea Break                                                                               |                                                                                |                                                      |                                                   |
| <b>17:00-17:30</b> | Valedictory session (Bhupen Hazarika Auditorium)                                        |                                                                                |                                                      |                                                   |



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