

# Proceedings of PolyTech – 2012

## International Conference on Advances in Polymeric Materials & Nanotechnology

December 15 – 17, 2012

*Jointly organized by*

*Advanced Research Centre in Pharmaceutical Sciences & Applied Chemistry*

*Poona College of Pharmacy, Bharati Vidyapeeth University, Pune*

*The Society for Polymer Science, India*

*National Chemical Laboratory, Pune*

*C - MET, Pune*

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**PolyTech - 2012, Pune**

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## Message from the Chancellor

**Hon'ble Dr. Patangrao Kadam**  
**Founder and Chancellor, Bharati Vidyapeeth Deemed University, Pune**  
**Minister for Forests, Earthquake Rehabilitation, Rehabilitation and Relief Works,**  
**Government of Maharashtra**

I am glad to know that Bharati Vidyapeeth Deemed University, Poona College of Pharmacy and Advanced Research Centre in Pharmaceutical Sciences & Applied Chemistry, Pune is organizing PolyTech - 2012: International Conference on Advanced Polymeric Materials and Nanotechnology, during December 15-17, 2012. In the present era, India has shown tremendous growth in Advanced Materials, Nano-materials and Pharmaceutical business. As per my knowledge, India is the prominent country in Materials Science and meets its 95% domestic needs and also exports as well its products to more than 80 countries. However, till date India is facing many health related problems, newer epidemics are creating the alert situations. I hope that the deliberation in the conference will find the solutions and suggest policy maker to develop mechanism to develop healthy state and country.

On behalf of the Bharati Vidyapeeth Deemed University, Pune, I welcome all delegates, teachers, scientists, industry professionals and students of polymer science and nanotechnology.

I convey my best wishes to the principal, secretary, convener and faculty members for success of this Conference.

**Dr. Patangrao Kadam**



## **Message from Vice Chancellor**

**Prof. Dr. Shivajirao Kadam**  
**Vice Chancellor, Bharati Vidyapeeth Deemed University, Pune**

I am happy to know that Bharati Vidyapeeth Deemed University, Poona college of Pharmacy, and Advanced Research Centre in Pharmaceutical Sciences & Applied Chemistry, Pune is organizing PolyTech - 2012: International Conference on Advanced Polymeric Materials and Nanotechnology, during December 15-17, 2012.

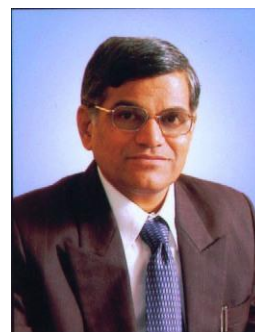
The 21<sup>st</sup> century is known as era of Techno-education. India is marching with global developments in almost all the professional and business developments like growth in Advance Polymeric Materials and Nanotechnology business.

In noble task of providing quality education, Bharati Vidyapeeth University has been taking proactive and determined role to provide best knowledge at par with national standards. I thank 'The Society for Polymer Science, India; National Chemical laboratory, Pune and C-MET, Pune for selecting this university for organizing PolyTech - 2012: International Conference on Advanced Polymeric Materials and Nanotechnology.

On behalf of the Bharati Vidyapeeth Deemed University, Pune, I welcome all delegates, teachers, scientists, industry professionals and students of polymer science and nanotechnology. I am sure that this conference would deliberate upon various issues related to innovative research and developments in Advanced Polymeric Materials and Nanotechnology.

I congratulate the Principal, Secretary, Convener and Faculty members of the college and organizing team and wish them grand success.  
With best wishes

**Prof. Dr. Shivajirao Kadam**



## **Message from the Principal**

**Prof. K. R. Mahadik**  
**Principal**  
**Poona College of Pharmacy**  
**Bharati Vidyapeeth Deemed University**  
**Pune**

Poona College of Pharmacy, Pune of Bharati Vidyapeeth Deemed University is pioneer and premier institute in the field of Pharmaceutical Sciences providing high quality education since 1981. We firmly believe that an academic institution can not grow unless the faculty is committed to research along with the teaching. Excellent infrastructure, state of art laboratories, sophisticated instruments and equipments, impressive research output, experienced and committed faculty are the backbones of Poona College of Pharmacy. We have filed 44 patents and published over 600 papers in national and international peer-reviewed journals. In Scopus survey our college ranks 9<sup>th</sup> in India.

The college has been routinely organizing seminars, conferences and workshops and conducts faculty developments programs every year. However, organizing PolyTech – 2012: International Conference on Advanced Polymeric Materials and Nanotechnology, during 15<sup>th</sup> – 17<sup>th</sup> December, 2012 is a special event for us, as it is an area of immense interest to scientists from academic and industry. This platform will help us to anchor many fruitful collaborations and exchange of innovative ideas in the fields of polymer Sciences and Nanotechnology which are the current thrust areas of research.

I place on record, my sincere appreciation of the efforts put in by our faculty members and students for the successful organization of this important event. I wish every success for the conference and fruitful participation for all delegates.

**Prof. K. R. Mahadik**



THE SOCIETY FOR POLYMER SCIENCE (INDIA)



**President**

*Dr. S.Sivaram (Pune)*

**Immediate Past President**

*Professor Ashok Misra (Mumbai)*

**Vice-President**

*Dr. C.P.R.Nair (Thiruvananthapuram)  
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**Message**

*I am delighted to know that Bharati Vidyapeeth University, Pune in association with CSIR-National Chemical Laboratory, Pune is organizing an International Conference on Advances in Polymeric Materials and Nanotechnology in Pune from December 15-17, 2012. I am indeed pleased that the Society of Polymer Science (India), the largest professional society serving the polymer science community in India, is a cosponsor of this meeting.*

*The scientific programme covering diverse areas of polymer science appears very exciting. I also observe that there are many distinguished speakers from overseas, sharing their perspectives. Thus, the Conference provides an excellent platform for interaction between established practitioners of science and young students and faculties, at the beginning of their research career. I compliment the organizers of the Conference for putting together an excellent scientific programme.*

*Polymer Science was born as a discipline only about seventy five years ago; yet, in this short span of time the discipline has seen major transformation – from an ability to make macromolecules with diverse range of structural and mechanical properties to the design and synthesis of functional macromolecules with interesting applications at the interface of polymer science with other disciplines, such as, material science and biology. Just like chemistry, polymer science is also becoming increasingly invisible, as component of systems that find many applications in areas such as, sustainable energy, health care, water, environment and management of natural resources.*

*Progress of science requires meaningful interaction with society at large. Of late, polymers have acquired a negative perception in the minds of people. As professionals, it is our responsibility to dispel this perception and present the positive elements of polymer science that significantly contributes to a better quality of life for all of us.*

*I wish the Conference all success.*

*(S. Sivaram)  
President,  
Society of Polymer Science (India)*





THE SOCIETY FOR POLYMER SCIENCE (INDIA)



**President**

*Dr. S.Sivaram (Pune)*

**Immediate Past President**

*Professor Ashok Misra (Mumbai)*

**Vice-President**

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**Message**

*I am delighted to know that Bharati Vidyapeeth University, Pune in association with CSIR-National Chemical Laboratory, Pune is organizing an International Conference on Advances in Polymeric Materials and Nanotechnology in Pune from December 15-17, 2012. I am indeed pleased that the Society of Polymer Science (India), the largest professional society serving the polymer science community in India, is a cosponsor of this meeting.*

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*I wish the Conference all success.*

*(S. Sivaram)*

*President,*

*Society of Polymer Science (India)*

*Dr. Sourav Pal*

*Director*

*CSIR-National Chemical Laboratory, Pune*

**MESSAGE**

The Society for Polymer Science, India along with Bharati Vidyapeeth University Poona College of Pharmacy, Pune, CSIR-National Chemical Laboratory, Pune and Centre-Materials for Electronics Technology (C-MET), Pune are organizing this PolyTech – 2012: International Conference on Advances in Polymeric Materials and Nanotechnology. I am very happy that this conference is being organized at the time when this topic has gained immense interest. The polymer science/nanomaterials is a cutting edge science and technology having impact on several areas like pharmacy, water, agriculture, transportation, composite materials, electronics materials, sensing, fuel cells etc. This conference will deliberate not only on the novel polymerization techniques, but also on modelling and simulation structure property relationship, which will help understanding the role of these materials in the above areas of interest. I am sure the deliberations involving the academia and industry over the two days at Bharati Vidyapeeth University Poona College of Pharmacy, Pune and CSIR-National Chemical Laboratory, Pune will be very fruitful and will lead to more collaborations specially between the academia and industry. I wish the conference a great success.

Dr. Sourav Pal  
Director, CSIR-NCL



## From the Secretary's Desk

**The Society for Polymer Science, India** in joint collaboration with BharatiVidyapeeth University, Pune; National Chemical Laboratory, Pune and C-MET, Pune is organising 'PolyTech – 2012: International Conference on Advances in Polymeric Materials and Nanotechnology' during December 15-17, 2012. The **Society** (SPSI) had a checkered history of more than three decades and was established as Professional Society in March 1979 at Anna University, Madras. The Society for Polymer Science, India was duly registered under 'The Societies Registration Act, Govt. of Maharashtra' at Pune and its Registration **No is :MAH/929/2001/Pune** dated August 16, 2001.

The 'PolyTech – 2012 aims to address teachers, scientists, industry professionals and students in Polymer Science and Nanotechnology. The lectures were designed to address the important wide aspects of polymers, advanced materials and the emerging areas of nanotechnology thus, covering both science and technology. Polymeric materials became a part of everyday life in the early fifties when they replaced natural materials. Today, polymers are inescapable component of renewable energy systems, information and communication technologies, purification of water, pharmaceuticals, healthcare and environment. In these areas, polymer science will interface with physics, biology, material science, atmospheric science and nanotechnology

The conference has a number of distinguished researchers from all over the country and abroad. We thank University Grant Commission, Council of Scientific & Industrial Research, DRDO, Solvay Specialities, RIL, Tata Chemicals and other private parties for recognizing the importance and sponsoring the event. I thank all the delegates, distinguished guests and participants for their interest and cooperation.

I am sure that the deliberations and discussions in the conference will strengthen the research activities in our academic/ research institutions and universities and will create research culture in the participants.

I wish an enjoyable and productive stay at Pune.

R.P.Singh  
Secretary, PolyTech – 2012  
Hon. Secretary, The Society for  
Polymer Science, India

## PROGRAMME

**Day-1: Saturday, 15<sup>th</sup> December, 2012**

**Venue: Bharati Vidyapeeth University, Erandawane Campus, Pune**

### Session-1

Time	Programme
8.00-9.30 hr	Registration
9.30-11.30 hr	<b>Inauguration Function</b>
11.30-11.45 hr	Tea Break
11.45-13.00 hr	<b>Chairman: Prof. Ajit D. Kelkar, USA and Prof. J.Lacoste, France</b> <b>Keynote Lecture: Dr. Sourav Pal; Director, CSIR-NCL, Pune</b>
13.00-14.00 hr	<b>Lunch</b>
13.00-14.00 hr	<b>Poster Display</b>

### Session-2

<b>Time</b>	<b>Hall-A</b>	
	<b>Chairman: Dr. Sourav Pal; CSIR-NCL, Pune and Prof. Anthony Guiseppi-Elie; USA</b>	
14.00 - 14.45 hr	<b>Plenary Lecture: Supramolecular Polymerization of Fluorescent <math>\pi</math>-Systems to Fibrillar Network Assemblies and Their Applications; Ayyappanpillai Ajayaghosh; CSIR-NIIST, Thiruvananthapuram, India</b>	
	<b>Hall-A</b>	<b>Hall-B</b>
	<b>Chairman: Prof. S. Thayumanavan, USA and Dr. Y.S.Negi, IIT, Roorkee</b>	<b>Chairman: Dr. Rajiv Kumar, Tata Chemicals Ltd., Pune and Prof. Satyendra Mishra, NMU, Jalgaon</b>
14.45-15.15 hr	<b>IT-1 Thermal Degradation and Fire Retardance of Polymer Nanocomposites; Giovanni Camino; Politechnic of Torino, Italy</b>	<b>IT- 2 Fuel Cell membranes : Challenges and opportunities; Veena Choudhary; I.I.T., New Delhi</b>
15.15-15.45 hr	<b>IT-3 Role of Solvent in Physical Gelation: Polymers vs Organogelators; J.M. Guenet; Institut Charles Sadron,</b>	<b>IT- 4 Controlling Microdomain Orientation and Long-Range Order in Block Copolymer Based Supramolecular Thin Films;E. Bhoje</b>

	<i>France</i>	<i>Gowd; CSIR-NIIST, Thiruvananthapuram</i>
15.45-16.15 hr	<b>IT- 5</b> ROMP is a Versatile Synthetic Tool for Making Functional Biopolymers; <i>S. Raja; IISER-Kolkatta, Mohanpur</i>	<b>IT- 6</b> Functionalized Single Walled Carbon Nanotubes Role on the Properties of Polyamide 6/Poly(Methyl Methacrylate) Blends; <i>A. V. Sessa Sainath; Polymers and Functional Materials Division, CSIR-Indian Institute of Chemical Technology, Hyderabad</i>
16.15-16.30 hr	Tea Break	

**Session-3**

<b>Time</b>	<b>Hall-A</b> <b>Chairman: Prof. K. R. Mahadik; BVU, Pune and Prof.K.Tashiro; Japan</b>	
16.30-17.15 hr	<b>Plenary Lecture:</b> Responsive Polymer Assemblies; <i>S. Thayumanavan; University of Massachusetts, Amherst, MA, USA</i>	
	<b>Hall-A</b> <b>Chairman: Prof. Tushar Jana, Hyderabad and Dr. Nikhil Singha; IIT, Kharagpur</b>	<b>Hall-B</b> <b>Chairman: Prof. Veena Choudhary; IIT, New Delhi and Prof. Robert Lochhead, USA</b>
17.15-17.45 hr	<b>IT-7</b> Visualization of Nanoworld Through Microscopic Techniques; <i>K. N. Pandey; CIPET, Lucknow</i>	<b>IT-8</b> Controlled Self-Assembly of Amphiphilic Block Copolymers into Multiple Morphologies; <i>Dr. Ashootosh V. Ambade; CSIR-NCL, Pune</i>
17.45-18.05 hr	<b>OP-1</b> Graphene Based Bionanocomposites: Green Materials for Advanced Applications; <i>Sunil Lonkar; University of Mons, Place du Parc, Belgium</i>	<b>OP-2</b> Dimensional Control of Solvent Vapor Induced Lamellar PS-B-P4VP Nanopatterns; <i>Atul Chaudhari; University College Cork, Ireland</i>
18.05-18.25 hr	<b>OP-3</b> In Vitro Investigation on PS:PLA and PS:PLA:OMMT Nanocomposites using Fungal Strain; <i>Navinchandra Shimpi; NMU, Jalgaon</i>	<b>OP-4</b> Biodegradable Bioepoxy Resin from Mahua Oil; <i>Omprakash S. Yemul; Swami RamanandTeerth Marathwada University, Nanded</i>

18.25 – 19.30 hr	<b>Poster Session: PP- 1 to PP-76</b>	
19..30-21.30 hr	<b>Dinner: BVU, Erandawane, Pune</b>	

**Day-2: Sunday, 16<sup>th</sup> December, 2012**

**Venue: CSIR-National Chemical Laboratory, Pashan, Pune**

**Session-4**

<b>Time</b>	<b>Hall-A</b> <b>Chairman: Dr. G. Camino, Italy and Dr. K. Krishnamoorthy, NCL, Pune</b>		
9.00-9.15hr	<b>Welcome and Brief Introduction of CSIR-NCL, Pune; Director, NCL, Pune</b>		
9.15- 10.00 hr	<b>Plenary Lecture: Hyperbranched Polyacetals and Polydithioacetals;</b> <b>S. Ramakrishnan, IISc, Bangalore</b>		
	<b>Hall-A</b> <b>Chairman: Dr. G. Camino, Italy and Dr. K. Krishnamoorthy, NCL, Pune</b>	<b>Hall-B</b> <b>Chairman: Prof. J. Lacoste, France and Dr. A.V. Sessa Sainath, IICT, Hyderabad</b>	<b>Hall-C</b> <b>Chairman: Prof. K. P. Singh, Pantnagar and Prof. Tarun K. Mandal, IACS, Kolkatta</b>
10.00-10.30 hr	<b>IT-9</b> Electroconductive Hydrogels For Biosensors, Bionics And Electorelease Devices; <b>Anthony Guiseppi-Elie; South Carolina, USA</b>	<b>IT-10</b> Template Assisted Self Assembly of Microstructures in Polymer Films; <b>M. Shelke; CSIR-NCL, Pune</b>	<b>IT-11</b> Photonic Crystal Sensing Materials Designed From Polymeric Nanoparticles And Hydrogels; <b>Tushar Jana; University of Hyderabad, Hyderabad</b>
10.30-11.00 hr	<b>IT-12</b> Characterization and Application of Fluorescent Poly(amido amine) Dendrimers; <b>T. Imae; National Taiwan University of Science and Technology, Taiwan</b>	<b>IT-13</b> Graphene/ Polymer Hybrids as Chemical and Biochemical Sensors; <b>A. K. Nandi; IACS, Jadavpur, Kolkata</b>	<b>IT-14</b> Thermal, Mechanical and Morphology of Surface Montmorillonite Modified Reinforced Viton Rubber Nanocomposites; <b>Satyendra Mishra; NMU,</b>

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			<b>Jalgaon</b>
11.00-11.30 hr	<b>IT-15</b> Discovery of New Melt Condensation Chemistry for Polymers Based on Amino Acids; <i>M. Jayakannan; IISER, Pune</i>	<b>IT-16</b> Polymerization of Plant Oils in Carbon Dioxide Media; <i>Zengshe Liu; Bio-Oils Research, Peoria, IL, USA</i>	<b>IT-17</b> Crossing Borders Between Natural and Synthetic Peptides; Shielding and Mediating of Hydrogen Bonding In Amide-Based (Macro) Molecules; <i>Sanjay Rastogi; Loughborough, U.K.</i>
11.30-11.45 hr	<b>Tea Break</b>		

**Session – 5**

<b>Time</b>	<b>Hall-A</b> <b>Chairman: Prof. Ayyappanpillai Ajayaghosh, CSIR-NIIST, Thiruvananthapuram and Dr. Sanjay Rastogi, UK</b>		
11.45-12.30 hr	<b>Plenary Lecture:</b> Biomaterial and Nano-Material Technology Indispensable for Regeneration Therapy and Stem Cell Research; <i>Yasuhiko Tabata; Kyoto University, Japan</i>		
	<b>Hall-A</b> <b>Chairman: Dr. Sanjay Rastogi, UK and Dr. K. Subrahmanya Bhat, Manipal</b>	<b>Hall-B</b> <b>Chairman: Dr. K. N. Pandey, CIPET, Lucknow and Dr. C. Gouri, VSSC, Thiruvananthapuram</b>	<b>Hall-C</b> <b>Chairman: Prof. P. K. Khanna, DIAT, Pune Dr. J. D. Sudha, CSIR-NIIST, Thiruvananthapuram</b>
12.30-13.00 hr	<b>IT-18</b> Comparative Studies on The Performance of Nanocomposites Based on PEEK/PEI Polymer Matrix Filled with MWCNT's Modified by Polycarbosilane and	<b>IT-19</b> Self-assembled Monolayer Based QCM Biosensor For the Detection of <i>E. Coli</i> ; <i>K. P. Singh; G. B. Pant University of Agriculture &amp; Technology, Pantnagar</i>	<b>IT-20</b> Clay Nanoparticles as <i>Pseudo-Pro-Oxidant</i> for Polyolefins Degradation; <i>Pratheep Kumar Annamalli; TenasiTech Pty Ltd, Australia</i>

	Polyphosphazene; <i>Vishal Verma; CIPET, Lucknow</i>		
13.00-13.15 hr	<b>OP-5</b> Synthesis and Characterization of Water Soluble CdSe/ZnS Q-Dots For Biomedical Applications; <i>Diksha Painuly; SCTIMST, Thiruvananthapuram</i>	<b>OP-6</b> Synthesis and Thermal Studies of Fumed Silica / Polybenzoxazole Nanocomposites; <i>Sarfaraz Alam; DMSRDE, Kanpur</i>	<b>OP-7</b> Porous and Crosslinked Cellulose Beads for Toxic Metal Removal-Hg(II) Ions; <i>Jyothi D. Mumbrekar; DIAT, Pune</i>
13.15-14.00 hr	<b>Lunch</b>		

**Session-6**

<b>Time</b>	<b>Hall-A</b> <b>Chairman: Prof. S. Ramakrishnan, IISc, Bangalore and Dr.B.B.Idage, CSIR-NCL, Pune</b>		
14.00-14.45hr	<b>Plenary Lecture:</b> Multifunctional Inorganic Polymers as Precursor Materials for Ultrahigh Temperature Applications; <i>Arvind Kumar Saxena; DMSRDE, Kanpur</i>		
	<b>Hall-A</b> <b>Chairman: Prof. S. Ramakrishnan, IISc, Bangalore and Dr.B.B.Idage, CSIR-NCL, Pune</b>	<b>Hall-B</b> <b>Chairman: Dr. B.Garnaik, CSIR-NCL, Pune and G.V.N. Rathna, CSIR-NCL, Pune</b>	<b>Hall-C</b> <b>Chairman: Dr. Arvind Kumar Saxena, DMSRDE, Kanpur and Dr. S.Raja, Kolkata</b>
14.45-15.15hr	<b>IT-21</b> Advances in Chitin and Chitosan Based Nanomedicine; <i>R. Jayakumar; Amrita Institute of Medical Sciences and Research Centre, Kochi</i>	<b>IT-22</b> Development of Phosphonated PEEK Membrane for Fuel Cell Applications; <i>Yuvraj Singh Negi; I.I.T., Roorkee</i>	<b>IT-23</b> Polymer nanocomposites for defence applications; <i>P. K. Khanna; DIAT, Pune</i>
15.15-15.30 hr	<b>OP-8</b> Nano-Calcium Carbonate (CaCO <sub>3</sub> )/Polystyrene (PS)	<b>OP-9</b> Detection Lung Cancer Biomarkers with Quantum Resistive	<b>OP-10</b> Recent Trends In Functionalised Polymer Systems For Industrial



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	Core-shell Nanoparticle: It's Effect on Properties of High Impact Polystyrene (HIPS); <b>Aniruddha Chatterjee; NMU Jalgaon, Maharashtra</b>	Vapour Sensors of Functionalized $\beta$ Cyclodextrin - Reduced Graphene Oxide; <b>Sananda Nag; European University of Brittany, Lorient, France</b>	Applications; <b>K. Balasubramanian; DIAT, Pune, India</b>
15.30-15.45 hr	<b>OP-11</b> Polymeric Coatings from Vegetable Oils as Renewable Sources; <b>V. V. Gite; NMU, Jalgaon, Maharashtra</b>	<b>OP-12</b> Preparation and the study of Zinc Polyacrylate Cement: Dental Cement Behavior and properties; <b>A.P. Gupta; Delhi College of Engineering, New Delhi</b>	<b>OP-13</b> Synthesis of Novel Quaternary Ammonium Polymerizable Surfactants from Tertiary Amines, Long Chain Alkyl Maleic Hemiesters, and Epoxy Resins; <b>G. John Dominic; Manipal University, Manipal</b>
15.45-16.15 hr	<b>IT-24</b> Functional Polymers by Controlled Radical Polymerization and "Thiol-ene" Reaction; <b>Nikhil K Singha; I.I.T., Kharagpur</b>	<b>IT-25</b> Polymer Silica Nanomaterial for Coating Industries; <b>Dr. Soumen Sensarma; TATA Chemicals Innovation Center, Pune</b>	<b>IT-26</b> Functional Polymers in Lithium-ion Batteries; <b>C. Gouri; VSSC, Thiruvananthapuram</b>
16.15-16.30 hr	Tea Break		

**Session -7**

Time	Hall-A	Hall-B	Hall-C
	<b>Chairman: Prof. A. K. Nandi, IACS, Kolkata and Dr. M.V.Shelke, CSIR-NCL, Pune</b>	<b>Chairman: Dr. Sunil Lonkar, Belgium and Dr. Vishal Verma, CIPET, Lucknow</b>	<b>Chairman: Prof. T. Imae, Taiwan and Prof. Varsha B. Pokharkar, BVU, Pune</b>

16.30-17.00 hr	<b>IT-27</b> Prediction of Glass Transition Temperature of EPON 862 (DGEGBF) cross-linked with Curing Agent W (DETDA) using MD Simulations; <i>Ajit D. Kelkar; School of Nanosci. &amp; NanoEngg., USA</i>	<b>IT-28</b> Electronic Devices from Conducting Polymers and TM-Phthalocyanines; <i>J.V. Yakhmi; HBNI, Mumbai</i>	<b>IT-29</b> Micelle –Assisted Synthesis of Electromagnetic Nanotapes by In Situ Self-Assembly Process; <i>J.D.Sudha; CSIR-NIIST, Thiruvananthapuram</i>
17.00-17.30 hr	<b>IT-30</b> Surface-Confined ATRP to Synthesize Functional Mesoporous Polymer / Carbon Nanospheres; <i>Tarun K. Mandal; IACS, Jadavpur, Kolkata</i>	<b>IT-31</b> Synthesis of some tri- and penta-block copolymers of styrene and methyl methacrylate via solution ATRP; <i>C. N. Murthy; Vadodara</i>	<b>IT- 32</b> Synthesis of Ibuprofen esters and nanoparticles preparation using Poly (L-lactide) s for controlled drug release; <i>Baijayantimala Garnaik; CSIR-NCL, Pune</i>
17.30-18.00 hr	<b>IT-33</b> Physical-Chemical approach of The Ageing, The Stabilization and The Long-Term Prediction Durability of Polymer; <i>J. Lacoste; ENSCCF France</i>	<b>IT-34</b> Synthesis of Polymers and Nanomaterials by Supercritical Carbon Dioxide; <i>Hullathy Subban Ganapathy; Kumamoto University, Japan</i>	<b>IT-35</b> Developments and Characterization of MoS <sub>2</sub> Filled Epoxy Nanocomposites; <i>S. K. Srivastava; I.I.T., Kharagpur</i>
18.00-18.15 hr	<b>OP-14</b> Studies on Design and Development of Gastrosparring Chimeric Derivative of Biphenylacetic Acid; <i>Manisha Kusurkar, BVU, Pune</i>	<b>OP-15</b> Studies on P- Aminosalicylic Acid-B- Cyclodextrin Conjugate for Colon Specific Delivery; <i>Samuel Soares, BVU, Pune</i>	<b>OP-16</b> A facile One-pot Reactive Solution Blending Approach for Main Chain Donor-Acceptor Polymeric Materials; <i>S. Kumari Nisha, CSIR-NCL, Pune</i>
18.15-18.30 hr	<b>OP-17</b> A New Approach for Degradation and Stabilization study of Proton Exchange Membranes Applicable in Fuel Cells; <i>Omkar Singh</i>	<b>OP-18</b> PVA Porous Membrane for Antibacterial Application; <i>Ramdayal; DIAT (DU), Pune</i>	<b>OP-19</b> Biodegradation of Medical Plastics Using Sewage, Muncible, and Radioactive Wastes: The Future Dream Challenge; <i>Sameh. A. S. Alariqi;</i>

	<i>Kushwaha; CSIR-NCL, Pune</i>		<i>University of Taiz, Taiz, Yemen</i>
19.30-21.30 hr	<b>Dinner: NCL Guest House</b>		

**Day-3: Monday, 17<sup>th</sup> December, 2012**

**Venue: Bharati Vidyapeeth University, Erandawane, Pune**

**Session-8**

<b>Time</b>	<b>Hall-A</b>	
	<b>Chairman: Prof. J. M. Guenet, France and Prof. Ram Mohan, USA</b>	
09.00- 09.45 hr	<b>Plenary Lecture:</b> Structural Evolution Processes in Phase Transitions of Crystalline Polymers as Investigated by Using a Newly-Developed Time-resolved Simultaneous Measurement System of WAXD, SAXS and FTIR Spectra; <i>Kohji Tashiro; Nagoya, Japan</i>	
	<b>Hall-A</b>	<b>Hall-B</b>
	<b>Chairman: Prof. J. M. Guenet, France Dr. Suneela Dhaneshwar, BVU, Pune</b>	<b>Chairman: Prof. Y.Tabata, Japan and Prof. M. Jayakannan, IISER, Pune</b>
09.45-10.15 hr	<b>IT-36</b> Nanomaterials for energy and environmental applications; <i>Satishchandra B. Ogale; CSIR-NCL, Pune</i>	<b>IT-37</b> Thin Film Devices Based on Polymes and Oligomers; <i>K. Krishnamoorthy, CSIR-NCL, Pune</i>
10.15-10.40 hr	<b>IT-38</b> Electrospun nanofibers: design, fabrication and applications; <i>G.V.N. Rathna, CSIR-NCL, Pune</i>	<b>IT-39</b> Conducting polymer nanomaterials: Current development and Opportunities ; <i>Vasant Chabukswar; Nowrosjee Wadia College, Pune</i>
10.40-11.05 hr	<b>IT-40</b> Role of Hydrogen-Bonding and Supramolecular Assembly of Small Molecules and Macromolecules; <i>Suhrit Ghosh; IACS, Jadavpur, Kolkata</i>	<b>IT-41</b> Thermal Characterization of Nanocomposites; <i>Vijai Kumar; CIPET, Lucknow</i>
11.05-11.15 hr	<b>Tea Break</b>	

**Session-9**

<b>Time</b>	<b>Hall-A</b>	<b>Hall-B</b>
	<b>Chairman: Dr.S.L.Bodhankar, BVU, Pune and Vasant Chabukswar; Nowrosjee Wadia College, Pune</b>	<b>Chairman: Prof.H.S.Ganapathy, Japan and Prof.A.P.Pawar, BVU, Pune</b>
11.15-11.45 hr	<b>IT-42</b> Polymer based nanocomposites for humidity sensing applications; <b>Parag V. Adhyapak; C-MET, Pune</b>	<b>IT-43</b> Biodegradable Polyurethane Nanocomposites as contact and non-contact Shape Memory advanced materials; <b>Niranjan Karak; Tezpur University</b>
11.45-12.15 hr	<b>IT-44</b> Polyamide 6-Inorganic/organo fillers: Effect of process conditions on mechanical and thermal properties; <b>S.S. Sonwanae; Visvesvaraya National Institute of Technology, Nagpur</b>	<b>IT-45</b> Self-Assembly and Cargo Release in Comb Polymers Probed By Fluorescence; <b>S. K. Asha; CSIR-NCL, Pune, India</b>
12.15-12.30 hr	<b>OP-20</b> Processing and Characterization of Epoxy- Graphite nanocomposites; <b>Subita Bhagat; Sant Longowal Institute of Engineering &amp; Technology, India</b>	<b>OP-21</b> Health monitoring in core of poly(epoxy)/glass fibre composites with Conductive Polymer Nano Composite Piezo-Resistive Sensors; <b>S. N. Chowdhury; Smart Plastics Group, European University of Brittany, Lorient, France</b>
12.30-12.45 hr	<b>OP-22</b> Highly Crystalline Nanostructured Comb Polymer of Perylenebisimide by Directed Self-Assembly; <b>N. Rekha; CSIR-NCL, Pune</b>	<b>OP-23</b> AB-Diblock Polymeric Vesicles and their Encapsulation Capabilities; <b>Smita Kashyap, IISER-Pune</b>
12.45-13.00 hr	<b>OP-24</b> Conjugated Polymer-Lanthanide Hybrid Temperature Sensors; <b>A. Balamurugan; IISER, Pune</b>	<b>OP-25</b> Synthesis and characterization of resole type polymer derived from 4-hydroxychalcone; <b>Carl Zschille; Manipal</b>

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# Keynote Lecture

## **Key Note Lecture**

**Dr. Sourav Pal**

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**Abstract Awaited**

# Plenary Lectures

# Supramolecular Polymerization of Fluorescent $\pi$ -Systems to Fibrillar Network Assemblies and Their Applications

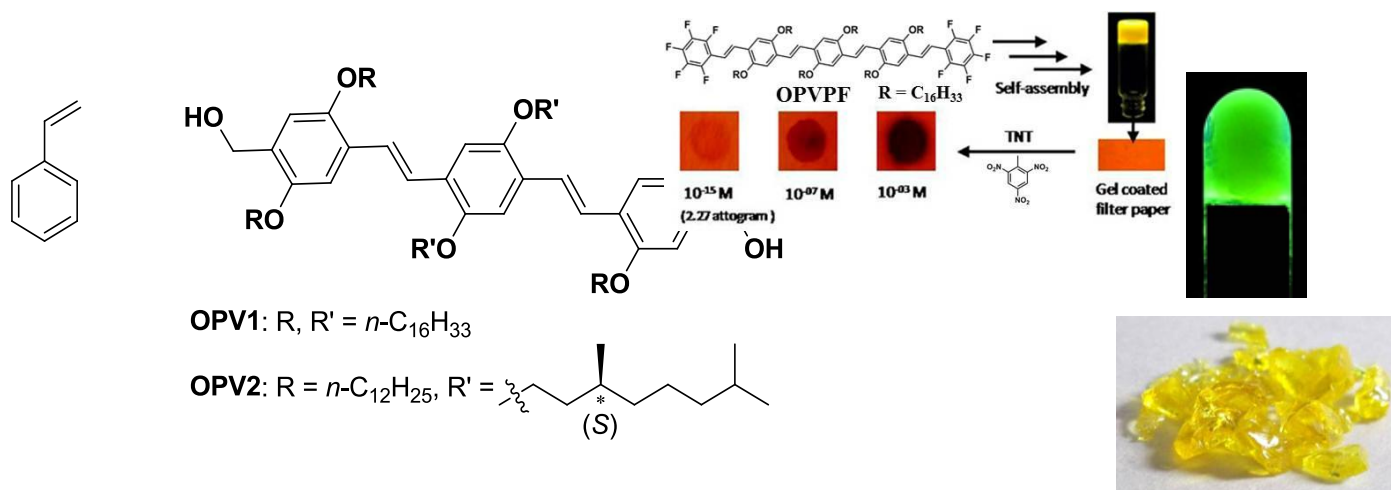
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## Abstract

Noncovalent interaction of  $\pi$ -conjugated molecules in general leads to elongated fibrillar structures which forms entangled networks. These are a kind of reversible macromolecular structures called supramolecular polymers. In most of the cases, these structures form soft materials in appropriate solvents leading to organogels. Even though supramolecular polymers are inferior to the conventional covalent polymers in mechanical properties, they show intriguing reversible properties such as self-healing, mechanochromism, fluorescence modulation etc. For example, in the case of fluorescent molecular gelators, self assembly leads to significant modulation of the emission properties which is reversible with solvents, analytes and temperature. In a recent report we have demonstrated the gelation of styrene using oligo (*p*-phenylene vinylenes) (OPVs) to prepare a composite polymer that is useful for reversible thermal imaging (Figure left). In another report a fluorescent OPV gelator has been used for the detection of TNT with attogram sensitivity (Figure right). Details of these studies will be discussed.



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## Responsive Polymer Assemblies

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### Abstract

Non-covalent encapsulation of guest molecules and their triggered release is of paramount importance in the field of drug delivery. Achieving such release characteristics using proteins as trigger would have significant implications in both drug delivery and bio-sensing, since protein imbalances are primary bases for the most of human diseases. Custom-designed facially amphiphilic dendrimers have been utilized for this purpose due to their unique ability of sequestering guest molecules through aggregation of several dendritic molecules.

Micellar assemblies, such as the ones above, are promising scaffolds to overcome many of the problems faced with traditional chemotherapies, because of their capacity for non-covalent, hydrophobic guest molecule binding. However, the stability of encapsulation with such self-assembled systems is limited during blood circulation because of a requisite concentration for assembly formation. Thus, deliberate molecular design for stable encapsulation, targeting and triggered release is required. For this purpose, we have developed a facile synthetic method for highly stable, polymeric nanogels using a simple intra/inter-chain crosslinking reaction. We show a simple, emulsion free method for the preparation of biocompatible nanogels that provides the ability to encapsulate hydrophobic guest molecules. The resulting nanogels show sizes of several hundred nanometers with well-defined shapes. The nanogel surfaces can be functionalized with specific groups, allowing for potential functionalization for targeted delivery. We show that the non-covalently encapsulated guest molecules can be released in response to a biologically relevant stimulus. The release of the guest molecules can be tuned by crosslinking density and in situ release was observed through in vitro fluorescence resonance energy transfer (FRET) experiments. Hence, the reversible nanogel formation using self crosslinking polymers and the corresponding method of surface modification are a promising platform for creating polymer nanogels for a range of biomedical applications, from drug delivery to biosensing.

## Hyperbranched Polyacetals and Polydithioacetals

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### Abstract

Hyperbranched polymers could be considered as the structurally imperfect analogues of the more symmetric Dendrimers; however, several of the interesting and useful properties of Dendrimers are also exhibited by analogous HBPs, but at a fraction of the effort to prepare them. One of the common methods for the preparation of HBPs is by the self-condensation of AB<sub>2</sub> type monomers; this approach has been used to prepare a wide variety of polymers, ranging from polyesters, polyethers, polyamides, polyurethanes, etc. We have recently developed a melt trans-acetalization method to prepare hyperbranched polyacetals from 4-hydroxymethyl benzaldehyde, dimethylacetal; by changing the structure of the monomer we successfully varied the terminal units from a simple dimethylacetal to dihexylacetal. These HB polyacetals were shown to be acid-labile and completely degraded to the corresponding hydroxyl-aldehyde; the rate of degradation was shown to depend on the hydrophobicity of the terminal groups, which suggested that the penetration of water could be the controlling factor in degradation rates. More recently, by adding a nitro-group on the aromatic ring, the HB polyacetal was made photo-degradable; this enabled us to develop the first HB photoresist material. Replacing the hydroxymethyl group with a mercaptomethyl unit enabled to generate HB polydithioacetal; the unique feature of this polymerization is that the polymers formed were seen to have no linear defects, suggesting the formation of HBP with a degree of branching (DB) of 100 %. A detailed study of the mechanism of polymerization demonstrated that the intermediate monothioacetal is relatively labile and is rapidly transformed to the dithioacetal; this appears to occur faster than the reaction of the starting dimethylacetal monomer. An additional virtue of this approach is that the numerous terminal dimethylacetal groups are very labile and can be quantitatively transformed by treatment with a variety of functional thiols; the terminal dimethylacetals were, thus, reacted with various thiols, such as dodecanethiol, benzyl mercaptan, ethylmercaptopropionate etc., to demonstrate the versatility of these systems as sulphur-rich hyperscaffolds to anchor different kinds of functionality on their periphery. The talk will focus on the design and development of these two novel classes of HBPs and their potential applications.

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## **Biomaterial and Nano-Material Technology Indispensable for Regeneration Therapy and Stem Cell Research**

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### **Abstract**

As the third choice of advanced medical therapy following reconstruction surgery and organ transplantation, a new therapeutic trial based on the natural potential of body to induce tissues regeneration and repairing, has been recently expected. To realize this regeneration therapy, there are two practical approaches; cell therapy and tissue engineering. The idea of tissue engineering is to artificially create a local environment which enables cells to enhance their proliferation and differentiation, resulting in cell-induced tissue regeneration. For this purpose, biomaterials are being used as the cell scaffold and delivery carrier of biosignaling molecules (growth factor and gene). If a key growth factor is supplied to the right place at the right time period and concentration, it is no doubt that the body system will initiate to physiologically function, resulting in the cell-based natural induction of tissue regeneration. One practically possible way to enhance the in vivo therapeutic efficacy of un-stable growth factor with in vivo short half-life period is to make use of drug delivery system (DDS) technology.

We have designed biodegradable hydrogels for the controlled release of growth factors and succeeded in the growth factor-induced regeneration and repairing of various tissues. Some tissue regeneration therapies with the release technology of biomaterials have been clinically started to demonstrate the good therapeutic efficacy. The release system can be combined with cells or/and the cell scaffold to promote the therapeutic efficacy of tissue regeneration. The combination with the growth factor release augmented the survival rate of cells transplanted and the consequent biological functions, resulting in enhanced therapeutic efficacy of cell transplantation. On the other hand, the controlled release of plasmid DNA and small interference RNA (siRNA) was effective in enhancing the in vivo activity and prolonging the duration time period. The cationized polysaccharide of nano-sized non-viral carrier enabled plasmid DNA to genetically engineer cells and enhance the efficacy of cell therapy in tissue regeneration (cell-gene hybrid therapy). If a fibrotic tissue can be digested by any DDS method to loosen or disappear,

it is highly expected that the tissue is regenerated and repaired based on the natural healing potential of the surrounding healthy tissue. This is a new approach of regeneration therapy to treat chronic fibrotic diseases.

The biomaterial and nano-material technology of cell scaffold and DDS can be also applied to the basic researches of biology and medicine for stem cells which scientifically support future regeneration therapy. The cell scaffold technology can provide cells with a local environment similar to that present in the body. The gene transfection with plasmid DNA and siRNAs is one of the important technologies to manipulate cells and make clear the mechanism of cell proliferation and differentiation. It is undoubted that these biomaterials and nano-materials certainly contribute to the further development of stem cell researches.

In this paper, several concrete experimental data on promoted regeneration of various tissues and stem cell biology with the cell scaffold and DDS technologies are presented to emphasize scientific and clinical significance of biomaterial-induced tissue engineering to realize tissue regeneration therapy as well as the stem cell research for future therapy..

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## Multifunctional Inorganic Polymers as Precursor Materials for Ultrahigh Temperature Applications

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### Abstract

With the growing interest in aerospace technology both from civil and defence point of view, the demand of such materials, which can withstand above 1000 °C upto 2500 °C, is greatly increasing. Though the ceramics and ceramic matrix composites are capable to withstand such temperature but the intractable nature of these materials restricts their application for making complicated engineering structures. Hence, such type of materials are required which are melt able and soluble so these can be fabricated easily in desired shape and size structures and which on further processing yields the desired material (Specially ceramic) engineering structures with the retention of shape and size.

Polysilane and polycarbosilanes are very interesting class of such Multifunctional Inorganic Polymers which yield a variety of SiC poly types on pyrolysis and found several applications in the form of monoliths, high tech continuous fibre ceramic composites, ceramic matrix composites, ceramic fibers, high temperature semiconductors, coating materials for oxidation prone substances, high temperature thermal barrier coatings, high temperature magnetic ceramics, refractory materials in the form of foams and SiC nano materials etc.

We have successfully developed pilot scale synthesis of polysilanes and polycarbosilanes and exploited their applications as mentioned above.

# Structural Evolution Processes in Phase Transitions of Crystalline Polymers as Investigated by Using a Newly-Developed Time-resolved Simultaneous Measurement System of WAXD, SAXS and FTIR Spectra

Kohji Tashiro

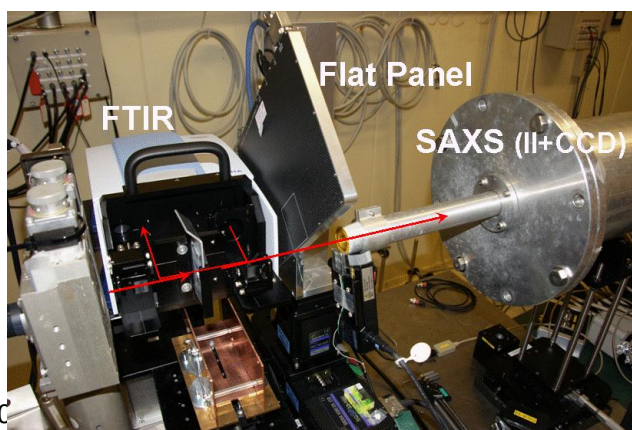
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## Abstract

A simultaneous measurement system of wide-angle X-ray diffraction (WAXD), small-angle X-ray scattering (SAXS) and transmission-type Fourier-transform infrared spectra has been developed in order to clarify the static and dynamic hierarchical structural changes of polymer materials subjected to the various external conditional changes. (Case Study 1) Figure 1 shows a schematic illustration of the hierarchical structural changes which was successfully derived from the quantitative analysis of all the data collected in the stress-induced phase transition of the oriented PTMT sample. Under the tension free state, the  $\alpha$ crystalline lamellae were stacked together with the lamellar normal tilted from the draw axis. The  $\alpha$ crystal lattice transformed to the  $\beta$  crystal lattice when the tensile stress was beyond a critical value. The content of the  $\beta$ form increased almost linearly in proportion to the sample strain. Important notice is that the  $\alpha$ -to-  $\beta$  transition of PTMT occurred with the lamellar tilting angle kept almost constant. Once the transition was mostly completed, then the tilting angle became zero and the lamellae stood with the normal vector parallel along the draw axis. This phenomenon occurred reversibly. PTMT is known to be mechanically quite tough in a reversible mechanical deformation. The reason may come from such a characteristic structural transition feature that the higher-order structure is kept unchanged during the phase transition in the crystal lattice. The externally-applied



mechanical energy is consumed by this phase transition and the direct breakage of the higher-order structure is avoided.

(Case Study 2) The structural evolution processes in isothermal crystallization of PE and Gutta Percha (green polymer) and in the phase transition of aliphatic nylons have been also investigated by using this simultaneous measurement system. The concrete lamellar formation processes have been derived by quantitative analysis of SAXS data.

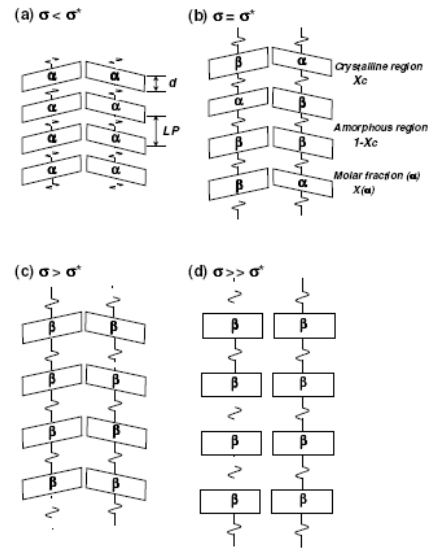


Figure 1. SAXS/WAXD/FTIR simultaneous measurement system

# Invited Lectures

## Thermal Degradation and Fire Retardance of Polymer Nanocomposites

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### Abstract

In the last half century, the development of advanced and mature technologies as well as the massive production of consumers goods have been based on the extensive use of polymer materials which has expanded at a rate never experienced before for traditional materials

However, flammability of polymers still represents a major limitation to their use and to the ensuing beneficial effect on industrial development. Indeed, flammability is related to fire risk (probability of fire occurrence) and hazard (consequences of a fire) in a number of applications of polymer materials such as in the electrical-electronic (E&E), transportation, building and furniture sectors.

The concern about negative impact on environment and on health by well established, versatile and effective halogenated Fire Retardants (FRs) has driven the enforcement of new European regulations progressively restricting their use since the years 2000. Some halogenated compounds (e.g. penta- and octa-bromodiphenyl ether) are already banned, whereas some other FRs are currently undergoing a risk assessment procedure. Moreover, the use of brominated fire retardants is discouraged by the Directive 2002/96/EC of the European Parliament on waste electrical and electronic equipment (WEEE) requiring separation of brominated fire retarded plastics from E&E equipment prior to recovery and recycling which has become mandatory for end of life electrical and electronic equipments.

Although a number of halogenated fire retardants have been recognised to be safe for health and environment on the basis of an extensive risk assessment, the general feeling of materials producers and of end users is that halogen-free fire retardants should be developed, that however show at least the same effectiveness of halogenated systems. The scientific rationale behind this request is related to the mechanism of fire retardance of halogen-based fire retardants. Indeed they slow down thermal radical chain oxidation reactions in the gas phase by trapping radical chain carriers which reduces the rate of heat released during combustion. Heat feedback to the condensed phase may thus be reduced below self-sustaining limit. However, the resulting incomplete oxidation of products of degradation of the polymer material, inevitably leads to increase of CO and of obscuring smokes production during combustion and flame extinction. This increases the fire hazard in scenarios involving the presence of people and makes

fire extinguishment by human intervention more dangerous and difficult. Corrosive gaseous products simultaneously evolved, jeopardise structures and devices which may be of strategic relevant importance.

To comply with these requests, new fire retardant strategies are being developed aiming at materials characterised by both low fire risk and hazard which simultaneously comply also with the modern environmental requirements globally defined as “sustainable development”. As a result, the fire retardant approach is shifting from flame extinguishment typical of early developed fire retardants, to flame prevention by creation of flame starvation conditions during polymer combustion. Most promising approaches involve polymer surface protection promoted by heat of the flame, thus reducing the rate of thermal degradation of the polymer, which supplies the fuel to the gas phase. In particular, a breakthrough could come from surface ceramisation and charring taking place in the combustion of polymer nanocomposites.

Indeed, during combustion of nanocomposites, polymer ablation rapidly leads to the accumulation of a network of floccules on the surface, mainly made of nanoparticles, whatever their chemical composition and aspect ratio, combined with a relatively small fraction of carbonaceous char. Partial charring of burning polymer induced by the presence of nanofillers is a typical result of nanocomposites combustion, particularly evident in the case of polymer matrices which do not produce charred residue when burned by themselves.

This thermally stable ceramic-char surface layer is able to act as a thermal shield by surface re-irradiation and as a barrier to heat and oxygen transfer from flame to the material and of degradation products from the material to the flame. Thus, the overall rate of flame feeding by combustible products from polymer pyrolysis and thermo-oxidation is decreased. Hence rate of combustion and of heat release are decreased accordingly.

Thus, nanocomposites make a step forward towards reduction of fire hazard for polymers because they avoid flame spreading by flaming dripping and reduce the rate of combustion. For the first time in polymer fire retardant history, we have polymer materials available in which fire hazard is reduced by a small amount of filler (ca. 2-3 %) with simultaneous improvement of other polymer material properties and using an environmentally friendly technology. Whereas, most of the fire retardants used now have to be loaded to polymers in relatively large amount (10-70% by wt.) with negative effects on polymer physical and mechanical properties and on environmental issues.



## Fuel Cell membranes: Challenges and opportunities

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### Abstract

Energy is one of the most important and fundamental requirements for the development of any country. Fossil fuels which are being abundantly used for the production of energy have potential adverse effects on our environment, namely global warming, ozone layer depletion etc. In this 21<sup>st</sup> century, we have reached to a point where we need effective and efficient substitution for fossil fuels which would also have additional advantages of being benign to environment. Development of fuel cell technologies is a significant breakthrough on alternative energy generation devices. Fuel cells are poised to make a vast revolutionary change in the field of energy because it renders certain advantages like very low emissions, higher efficiency, low noise etc. compared to other energy conversion devices.

Proton exchange membrane fuel cells (PEMFCs) in particular are experiencing an upsurge. They have high power density and can vary their output quickly to meet shifts in power demand. The main obstacles to greater commercialization of polymer electrolyte fuel cells are mostly related to the low-proton conductivity at relatively low humidity levels, high methanol permeability and poor mechanical properties at higher temperatures. A fuel cell membrane must exhibit relatively high proton conductivity, must present an adequate barrier to mixing of fuel and reactant gases and must be chemically and mechanically stable in the fuel cell environment. Typically, the membranes for PEM fuel cells are made of perfluorocarbon- sulfonic acid (PSA) ionomer. Despite the good characteristics and performance of fluorinated ionomer membranes, these materials have high production costs and the fluorine-chemistry involved in the polymerization. The improvement of the existent polymer electrolyte membranes for fuel cells and the development of new ones is key issue for commercialization of PEMFC processes

Widespread effort is underway to develop alternative, more economical, non fluorinated PEMs for fuel cells. The combination of the thermo-oxidation, chemical and hydrolytic stability of PEEK backbone with the presence of a protogenic source (the sulfonic acid groups) makes SPEEK a suitable candidate for the fuel cell application. The preparation and characterization of SPEEK has been carried out by incorporation of diols and inorganic filler such as polyhedral oligosilsesquioxane (POSS). In this lecture I

will discuss the various approaches which has been used to improve the performance of membranes based on sulfonated poly(ether ether ketone) [PEEK] for applications in fuel cells.

## Role of Solvent in Physical Gelation: Polymers Vs Organogelators

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### Abstract

In the past decade, the library of soft materials has been enriched by a wide variety of molecules which can spontaneously self assemble or crystallize from their solution while producing fibrillar organogels, of which some form functional superstructures<sup>1</sup>. In this category, the  $\pi$ -oligomers stand most probably as the most remarkable as they may find potential applications in organic electronics, light harvesters, bio-imaging, non-linear optics<sup>2-7</sup> and the like.

Organogelation of  $\pi$ -oligomers causes a quenching or enhancement of fluorescence<sup>1</sup> as reported by Ajayaghosh and co-worker with oligo-(p-phenylene vinylene) (OPV). These molecules typically consist of a paraffinic moiety (6 aliphatic wings) linked through oxygen atoms to a central core of alternating phenyl rings and double bonds. The solutions of these molecules exhibit a large red-shift of emitted light when undergoing SOL-GEL gel transition along with a concurrent fluorescence quenching.

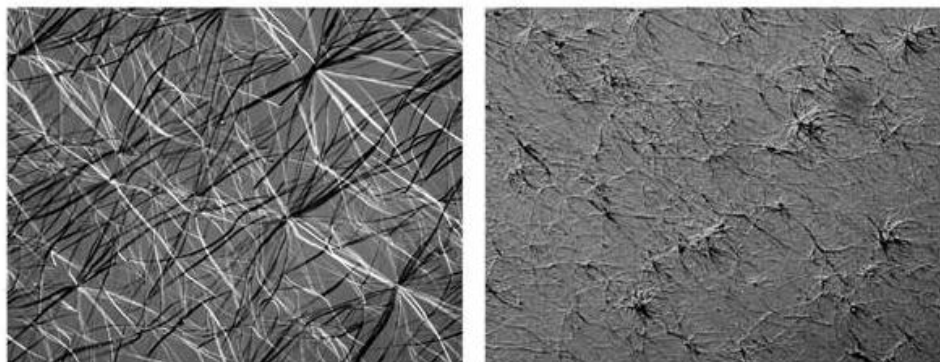


Figure 2. Stress-induced crystalline phase transition and higher-order structure change of PTMT

Our group has recently reported the large interplay between molecular design, solvent type and the resulting network architectures<sup>2,3</sup> in the case of OPVs displaying different terminal groups located at each end of the central core. In particular, the possible formation of an OPV/benzyl alcohol molecular compound was contemplated in the case of OPVs with OH terminal groups in order to explain the thermodynamic behavior of these systems as well as their unique morphological features. The formation

of a molecular compound is supposed to arise from the close relation between the molecular structure of benzyl alcohol and the tips of the central core due to the presence of the OH groups<sup>2</sup>. The role of solvent is occasionally raised as a very important issue both in polymer<sup>4</sup> or small molecules assembly. Investigations have been performed with various techniques (DSC, transmission electron microscopy, scanning electron microscopy AFM, X-ray diffraction, UV-Vis and fluorescence spectroscopy). We will again emphasize the important role of the solvent on the organogel morphology, the molecular structure, the thermodynamic properties and the optical properties by studying a structurally different OPV gelator molecule. These outcomes will be discussed by examining the interactions of the solvent with the different moieties of the organogelator.

# Controlling Microdomain Orientation and Long-Range Order in Block Copolymer Based Supramolecular Thin Films

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## INTRODUCTION

Fabrication of laterally ordered ultradense arrays of nanoscopic elements using self-organizing systems is a highly relevant and interesting topic of research today, owing to its potential contributions to device miniaturization with revolutionary applications ranging from electronics to biomedicine. Self-assembly of polymers is emerging as a promising route to generate templates and scaffolds for the fabrication of nanostructured materials, since self-assembly is highly parallel, versatile, and easy to implement. The self-assembly of block copolymers is potentially most interesting due to their ability to self-organize into well ordered periodic structures. In these nanostructures, the feature size and feature spacing can be controlled by the molecular weight of the block copolymer, which typically ranges from 10 to 100 nm. However, these nanostructures lack long-range order because the typical “grain size” over which the block copolymer features are ordered is in the submicron range. Many practical applications such as patterned magnetic recording media require nanostructures with long-range positional order. There is, therefore, an interest in developing fabrication methods for long-range ordered nanostructures from these self-assembled systems.

In the present work, we successfully identified new additives, which can form SMA with PS-*b*-P4VP block copolymer. For that purpose, we have chosen rigid additives and investigated the microphase separation in thin films of SMA. Our search of additives was based mainly on a qualitative analysis of hydrogen bonding with PS-*b*-P4VP, a capability to form mesophases, and a capability for the selective extraction from the block copolymer matrix. We successfully demonstrated that 4-hydroxybiphenyl is a suitable additive to form SMA with PS-*b*-P4VP and to obtain thin films with desired orientation and lateral ordering of the microdomain.

## EXPERIMENTAL

**Materials.** Two different PS-*b*-P4VP with number averaged molecular masses ( $M_n$ ): PS 35500 g/mol, P4VP 4400 g/mol,  $M_w/M_n = 1.06$  for both blocks, and ( $M_n$ ): PS 32900 g/mol, P4VP 8000 g/mol,  $M_w/M_n = 1.06$  for both blocks were purchased from Polymer Source, Inc. 4-hydroxybiphenyl, biphenyl-4-carboxylic acid and 4'-hydroxyl-4-biphenyl carboxylic acid were purchased from Sigma-Aldrich. All the solvents used were purchased from Acros Organics and were used without further purification.

**Sample Preparation.** The supramolecular assembly of PS-*b*-P4VP and the additive was prepared at a constant copolymer concentration of 1 wt% in a mixture of toluene/tetrahydrofuran (THF) (75/25 v/v) in various additives to copolymer ratios. Thin films were prepared by dip-coating from the solution filtered through 0.2  $\mu\text{m}$  teflon filters. Porous templates were fabricated by washing the thin films in methanol.

**Characterization.** Scanning force microscopy (SFM) imaging was performed using a Dimension 3100 scanning force microscope (Digital Instruments, Inc., Santa Barbara) in the tapping mode. FTIR spectra were taken with Bruker IFS 66v/s FTIR spectrometer in transmission mode. GISAXS measurements were carried out at the beamline BW4 of the DORIS III storage ring at HASYLAB (DESY, Hamburg, Germany).

## RESULTS AND DISCUSSION

The block copolymer (BC) with number averaged molecular masses ( $M_n$ ): PS 32900 g/mol, P4VP 8000 g/mol,  $M_w/M_n = 1.06$  for both blocks used in this study has a P4VP volume fraction of 0.2, which gives cylindrical morphology in bulk. Thin films of this BC were deposited on silicon wafer from toluene/THF (75/25 v/v) solution and films were further annealed in 1,4-dioxane vapors. Since, the film morphology is hidden under the thin layer of PS, the lateral structure of these films was revealed by surface reconstruction process. SEM image suggests that the cylindrical domains of the P4VP are oriented normal to the film surface in a hexagonal lattice with a periodicity of  $\sim 25$  nm. The Fourier transform of the SEM image shows more than six-point patterns due to lack of long-range order and presence of poly grains. It is worth mentioning here that the orientation of the P4VP cylindrical domains can be easily switched upon annealing in vapors of an appropriate solvent. Sidorenko et al. demonstrated such switching phenomena in SMA based on PS-*b*-P4VP diblock copolymer with 2-(4'-hydroxybenzeneazo) benzoic acid.

## ROMP is a Versatile Synthetic Tool for Making Functional Biopolymers

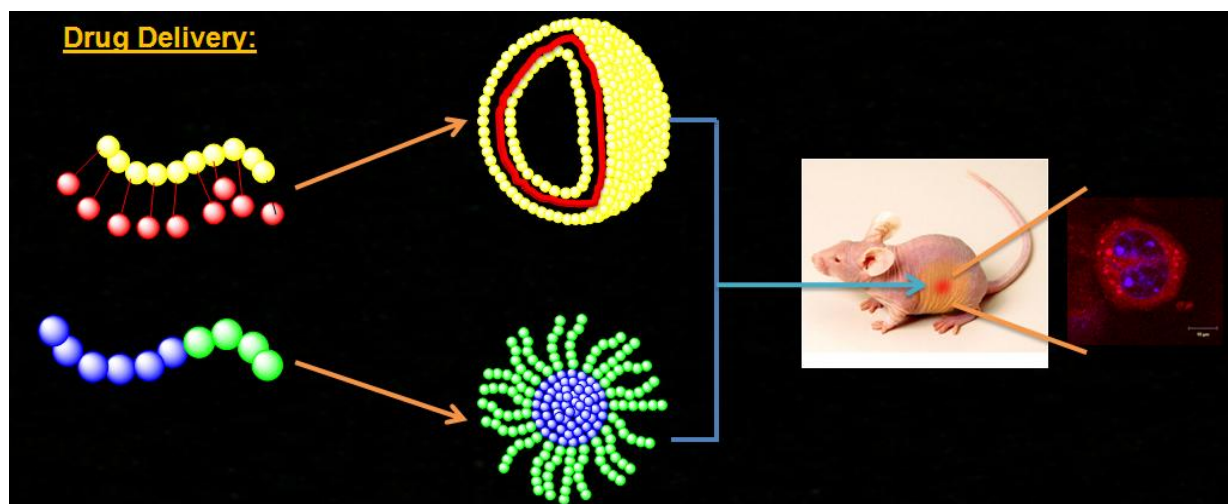
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### Abstract

Polymers that have potential application in the field of drug delivery with anti tumor prodrugs are being developed. Controlled/living polymerization techniques such as ROMP will be used to synthesize random and block copolymers where the composition of the copolymer length that contain drugs can be controlled. The advantage of ongoing work in designing prodrugs is that one block is linked to the nanoparticle so the drug-carrier's path can be influenced by external stimuli like magnetic force, thus drug delivery can be targeted. Preliminary enzymatic cleavage of drug from the polymer is studied using spectroscopic and chromatographic techniques. The preliminary results on monomer synthesis are shown here. We also develop CdSe nanoparticles and carbon nano tube (CNT) containing polymers that are used to sense heavy metals such as arsenic and mercury.



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## Functionalized Single Walled Carbon Nanotubes Role On The Properties Of Polyamide 6/Poly(Methyl Methacrylate) Blends

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### Abstract

In recent years, there are potential opportunities in the development of nanocomposites based on carbon nanotubes (CNTs) or nanoplatelets due to their wide range of engineering applications. The CNTs play a role of reinforcing fillers which significantly improve mechanical properties of the polymers due to high young's modulus and tensile strength of nanotubes. Such exceptional features of CNTs are intriguing to study CNTs based polymer composites and to develop high performance materials with enhanced properties. Even though potential benefits associated with CNTs have been confirmed, the interfacial interactions still remain critical in obtaining uniformly dispersed CNTs in the polymer matrices in exploiting the superior properties of CNTs. This is due to large surface area and strong van der Waal's forces of the CNTs tending to form aggregation in the polymer matrix. These aggregations may act as the stress concentration points that affect the mechanical properties of the nanocomposites.

The stress transfer from the matrix to the reinforcement components depends on interfacial strength and dispersion of CNTs in the blend matrix. Processing conditions also influence on the sate of dispersion of CNTs in polymer blend. However, the dispersion of CNTs and the interfacial adhesion between CNTs and polymer matrix is usually poor. Therefore, several routes were reported to minimize the interfacial tension between the blend components and to enhance uniform dispersion and interfacial adhesion of CNTs, such as use of surfactants, compatibilizers and functionalized and encapsulated CNTs in polymer/CNTs composites. It has been reported that poly(*n*-butyl acrylate) (PBA) encapsulated multi-walled CNTs (MWCNTs) melt-mixed with polyamide 6 (PA6) enhanced the interfacial adhesion between

PA6 and PBA encapsulated MWCNTs. The concept of reactive compatibilization was demonstrated in melt-processed PA6 and polyamide 12 with SMA encapsulated SWCNTs. The enhanced interfacial adhesion between polyamide and SWCNTs was explained by enhanced mechanical properties.

Covalent functionalization of CNTs is considered as one of the most effective means for homogeneous dispersion of CNTs in solution as well as melt-mixing method, to produce nanocomposite. Polystyrene with functionalized SWCNTs (SWCNTs-*f*), and the MWCNTs with multifunctional amines with epoxy resin led to a reduced agglomeration and improved interaction between CNTs and polymer. Addition of a compatibilizer is also reported in order to improve the dispersion of CNTs in polymer matrix. For instance, maleic anhydride-grafted-polypropylene (PP-*g*-MA) used as a compatibilizer to fabricate PP/CNTs composites in order to promote dispersion and interaction of CNTs and to improve the compatibility between PP and CNTs. The amphiphilic MWCNTs play dual role as reinforcing agent and compatibilizer in the immiscible poly( $\epsilon$ -caprolactone)/polylactide blends. The compatibilizer resides at the interface and reduces the interfacial tension between the blend components and prevents coalescence.

The compatibilization occurs through the formation of covalent bonds and the secondary interactions such as hydrogen bonds between blend components. Secondary interactions may arise by the complimentary structures having appropriate interactive functional groups (e. g., COOH and OH) of the blend components and improves miscibility or compatibility among the blend components. Poly(ethylene oxide) (PEO)-*b*-polyamide, the random and alternative copolymers of styrene and maleic anhydride and organomodifiednanoclay were used as compatibilizers in PA6/PMMA blend to achieve better dispersion of PMMA in PA6. Recently, the authors reported that the SWCNTs-COOH acted as compatibilizer in PA6/PMMA blend, for the first time. In this presentation, we present the influence of COOH- and OH-functionalized SWCNTs and non-functionalized SWCNTs incorporation into a PA6/PMMA blend, on the compatibility between PA6 and PMMA, morphology, thermal, mechanical and dynamic properties.

A series of PA6/PMMA nanocomposites with different compositions were prepared by melt-mixing method by the incorporation of non-functionalized SWCNTs and SWCNTs-*f* (*f*: COOH and OH). The FT-IR analysis of nanocomposites shows the formation of hydrogen-bond interactions among PA6, PMMA and SWCNTs-*f*. Thermal studies of nanocomposites exhibited higher thermal stability and increased crystallinity of PA6 with respect to the blends. The X-ray diffraction analyses of nanocomposites indicate that the  $\alpha_{II}$  phase of PA6 was shifted towards  $\beta$  phase. Melt flow index (MFI) values decreased with increasing the PMMA content in blends and nanocomposites compare to the PA6 and these MFI values are shown in Table 1. All nanocomposites exhibit lower MFI values with respect to their corresponding blends. It indicates that the viscosity of the nanocomposites was increased by the addition of 1 wt% of functionalized and non-functionalized SWCNTs in PA6/PMMA blends.

Table 1. Melt flow index and mechanical properties of PA6, PMMA, blends and nanocomposites.

Sample	MFI g/10 min	Storage		tan $\delta_{\text{peak}}$ <sup>a)</sup>	Tensile modulus /MPa	Yield stress /MPa	Elongation at break /%
		modulus <sup>a)</sup> /GPa					
		-30°C	+30°C				
PA6	20.56	2.68	1.98	0.1	814.1	72.77	562.22
80/20							
PA6/PMMA	15.43	2.41	2.34	0.128, 0.186	841.7	29.22	42.41
79.5/19.5/1							
PA6/PMMA/SWCNTs-OH	12.47	2.75	2.18	0.109, 0.194	840.4	33.54	63.92
PA6/PMMA/SWCNTs-	11.1	2.67	2.11	0.109, 0.235	871.4	31.34	31.65
COOH							
50/50							
PA6/PMMA	3.56	2.72	2.44	0.113, 0.381	939.3	21.16	6.46
49.5/49.5/1							
PA6/PMMA/SWCNTs	2.67	2.96	2.63	0.107, 0.334	918.5	22.79	5.88
PA6/PMMA/SWCNTs-OH	1.85	2.85	2.55	0.102, 0.376	1011.9	19.27	4.34
PA6/PMMA/SWCNTs-	2.13	2.72	2.56	0.105, 0.333	964.0	24.28	6.05
COOH							
20/80							
PA6/PMMA	0.62	3.62	2.96	0.093, 0.669	1093.3	28.51	5.18
19.5/79.5/1							
PA6/PMMA/SWCNTs	0.27	3.36	2.9	0.09, 0.646	1155.7	35.71	5.89
PA6/PMMA/SWCNTs-OH	0.36	3.58	2.92	0.083, 0.666	1198.7	30.41	4.83
PA6/PMMA/SWCNTs-	0.27	3.11	2.78	0.088, 0.604	1219.0	38.03	6.10
COOH							
PMMA	0.32	-	-	-	-	-	-

<sup>a)</sup> Calculated from DMA curves

The tensile characteristics of the blends and nanocomposites in terms of tensile modulus, yield stress and elongation at break are given in Table 1. The tensile modulus of the blends and nanocomposites were

increased with increasing the content of PMMA as shown in Figure 1. The yield stress and elongation at break reduced with increasing PMMA content in the blends and nanocomposites compare to the pure PA6. However, the yield stress of all the nanocomposites was higher compare to the respective PA6/PMMA blends. On the other hand, among all specimens, nanocomposite of PA6/PMMA/SWCNTs-COOH 19.5/79.5/1 was exhibited higher yield stress, 38 MPa and tensile modulus, 1219 MPa compare to the all blends and nanocomposites. The PA6/PMMA having SWCNTs-*f* specimens show higher tensile modulus compare to the non-functionalized SWCNTs in the weight ratio of 49.5/49.5/1 and 79.5/19.5/1 as shown in Table 2. These increments could be attributed due to the hydrogen bonding interactions among PA6 interactive groups of NH and C=O, PMMA of C=O and O and SWCNTs functional groups of OH and COOH. The scanning electron microscope (SEM) images of nanocomposites showed improved compatibility of nanocomposites than the blends. The SWCNTs-*f* are considered as compatibilizers in PA6/PMMA blends.

Key words: functionalized single walled carbon nanotubes, PA6 blends, nanocomposites, mechanical properties, and compatibilizer.

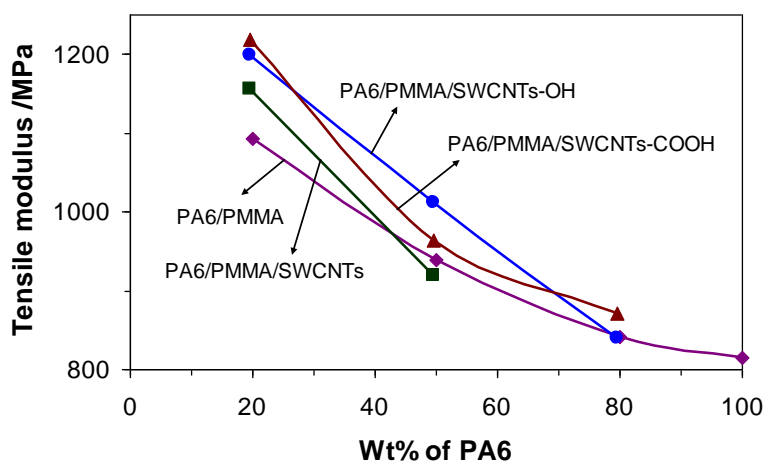


Figure 1. The variation of tensile modulus as a fraction of wt% of PA6 in blends and nanocomposites.

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## Visualization of Nanoworld through Microscopic Techniques

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### Abstract

Research related to nanotechnology is one of the most exciting and popular activities in almost all the disciplines. In this field the investigations cover a wide range of materials for diversified applications. This would include nanoelectronics as the threshold dimension scale for modern devices is now below under 100nm. Other areas include polymer blends, nanocomposites, electrospun nanofibres, layer-by-layer self assembled polymer films, polymer based biomaterials, imprint lithography, fuel cell electrode, polymer bound catalysts and nanoparticles in drug delivery. Truly speaking in the field of nanocomposites, a wide domain of research & development activities prevail including composites reinforcement, barrier properties, flame resistance, electro-optical properties etc. Phase separated polymer blends often achieve nanoscale phase dimensions, block co-polymer domain morphology in nanoscale level and interfacial phenomena in blends and composites involve nanoscale dimension. In the present scenario, MWCNT's and various nanoclays reinforcement of elastomers and other polymer matrix such as PEEK, PEI, PES etc. and other blends are attracting greater attention of the investigators.

Microstructural characterization on nanoscale has become very important for all types of materials in recent times. Microstructural characterization in large domain includes ascertaining the morphology of phases, number of phases, structure of phases, composition of phase dispersion of nanofillers and detection of crystallographic defects. Several microscopic techniques are available such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM), scanning tunneling microscopy (STM) etc, which can render information from the region at nanometer level. The fact is that TEM has emerged as the exclusive technique, which can be used for complete characterization of nanostructured materials. Morphological properties evaluation through above techniques will be discussed.

**Key words:** Microscopic techniques, Microstructures, SEM, TEM, AFM

## Controlled Self-Assembly of Amphiphilic Block Copolymers into Multiple Morphologies

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### Abstract

Amphiphilic block copolymers that comprise a hydrophilic segment attached to a hydrophobic chain are an important class of polymeric materials known for their interesting phase separation behaviour. This property leads to self-assembly of block copolymers into a variety of morphologies. Tuning the morphology is important for a variety of applications such as drug delivery and templates for nanomaterials. In this direction, the primary strategy has been to explore variety of molecular architectures for the amphiphilic copolymer building block. An alternative strategy that circumvents tedious synthesis is to use binary mixtures of block copolymers. I will present our work that uses both these approaches. We have synthesized novel dendron-coil-rod amphiphilic glycopolymers viz. glycopolyptide-dendron conjugates that self-assemble into nanorods and micelles and also yield organogels depending on the block lengths. These assemblies displaying carbohydrates on the surfaces are bioactive and can encapsulate guest molecules. As an example of the binary mixture approach, we have blended two linear block copolymers of asymmetric compositions and shown control of morphology using molar ratio of the two components. A complete change in morphology from vesicles to micelles is observed.

# Electroconductive Hydrogels for Biosensors, Bionics and Electrorelease Devices

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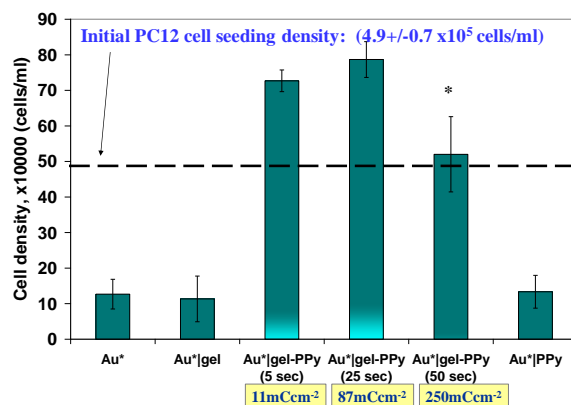
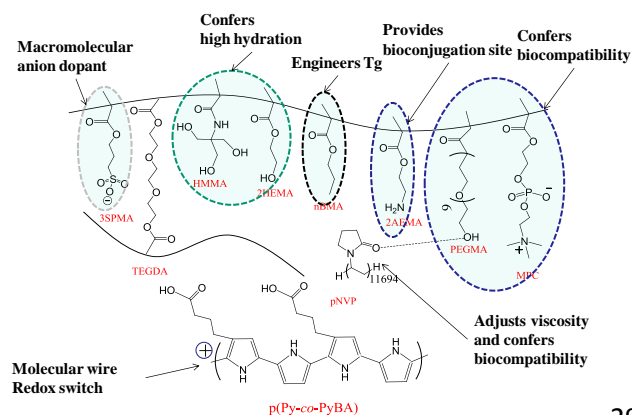
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## Abstract

Conductive electroactive polymers (CEPs) such as polypyrrole (PPy) and polyaniline (PAn) have been successfully combined with biomimetic and bioactive hydrogels to yield *plural functional polymers* with diverse biotechnology roles; i) as bioreceptor hosting membranes of enzyme-based implantable biosensors [i], ii) as biomimetically inspired biocompatible coatings on intraocular bionic implants, and iii) as voltage stimulated devices for the electro-stimulated release of biologically important factors and drugs. These electroconductive hydrogels (ECH) are interpenetrating networks or co-networks of the CEP synthesized within the hydrogel using oxidative chemical or electrochemical means [ii]. Electrical, voltametric, impedimetric and optical characterization confirm synthesis of the CEPs within the hydrogel **Figure 1L**. Electropolymerization has been shown to be a convenient and effective method to direct the immobilization of multiple biomolecules (enzymes) within hydrogel-coated microlithographically fabricated devices that may be multi-analyte biotransducers or intraocular implants. PPy-poly(HEMA)





ECHs have been used as the enzyme hosting membrane in implantable enzyme-amperometric biotransducers [iii]. The PPy-hydrogels have demonstrated effective screening of endogenous interferents [iv] and have shown *in vitro* biocompatibility through growth and proliferation of PC12 neuronal cells and RMS 13 muscle fibroblasts [v] **Figure 1R**.

**Figure 1.** *Left:* Schematic illustration of an interpenetrating network of poly(pyrrole-co-4-3 pyrrolyl butyric acid) and a poly(HEMA)-based hydrogel. *Right:* Growth and proliferation of PC12 cells on the ECH composite.

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## Template assisted self assembly of microstructures in polymer films

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### Abstract

Micro-patterned polymers are being increasingly used in micro-nanodevices, bio-mimetics, tissue engineering scaffolds, and biosensors. Features such as squares, rectangles, and cylinders can be readily fabricated with conventional fabrication techniques. More complex topologies such as spheres or ellipsoids are difficult to fabricate and creative modifications of existing techniques as well as innovative approaches are needed to develop cost competitive solutions which can be practiced on large scales. Such complex patterns are often desired for the fabrication of tissue engineering scaffolds for directed growth, microdevices for drug delivery, microbioreactors and many other applications. We developed a simple new approach for the creation of unique highly ordered mixed micro-cavity pattern comprising of the replica of the parent mold and an additional correlated self-generated one (not present in the parent mold) through template modulated solvent vapor back-pressure.

## Photonic Crystal Sensing Materials Designed From Polymeric Nanoparticles and Hydrogels

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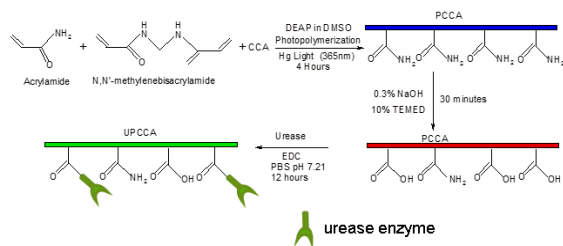
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### Abstract

Concerns over the toxicity of mercury have motivated the search of rapid, precise and reliable methods for monitoring, sensing and quantification of traces amount of mercury ion ( $\text{Hg}^{+2}$ ) in water.<sup>1,2</sup> The current techniques involve expensive equipment, complicated time consuming experiments, poor selectivity, irreversibility, slow response, incompatibility with aqueous solution, high levels of operator's skill and in addition they are user unfriendly and not cost effective.<sup>3</sup> Most often, the detection limit of the  $\text{Hg}^{2+}$  ion sensors reported in the literature are higher than the maximum contamination limit (MCL) as suggested by EPA, USA. Therefore, a sensor which rectifies all the above issues is of great demand and development of this still remains a great challenge for the chemists. Very recently, we have developed and reported a novel reusable sensor which addresses all the problems discussed above, for the determination of  $\text{Hg}^{2+}$  ion in aqueous medium.<sup>4</sup> The visible light diffracting self-assembled polymeric nanoparticles, often called as crystalline colloidal array (CCA), are embedded inside stimuli responsive polymer hydrogel matrix to fabricate this novel photonic crystal material. This presentation will highlight the design, development and the sensing behaviour of this novel sensor.

This new sensing material optically reports the  $\text{Hg}^{2+}$  concentration in water via diffraction of visible light from polymerized crystalline colloidal array (PCCA). The PCCA consists of light diffracting CCA of monodisperse, highly charged polystyrene nanoparticles, which are polymerized within the polyacrylamide hydrogel. The preparation of PCCA based light diffracting sensor material for the sensing of mercury involves three major steps as follows and presented in Scheme 1. The steps involved are: (1) preparation of PCCA, (2) preparation of ions responsive PCCA (carboxylated PCCA), and (3) preparation of urease coupled (UPCCA) sensor for mercury.



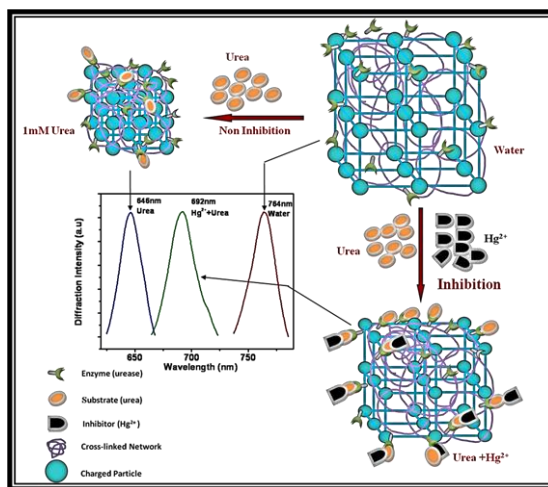
**Scheme 1.** Preparation of urease coupled polymerized crystalline colloidal array (UPCCA) for the sensing of  $\text{Hg}^{2+}$

It has been demonstrated that the net change in the total free energy of the hydrogel in response to the various environmental stimuli such as change in pH and ionic strength is the driving force for the volume change of the hydrogel which alters the lattice spacing of self-assembled polymeric nanoparticles (CCA) and hence shifts the diffraction wavelength of light.

We have developed a PCCA based sensor which detects  $\text{Hg}^{2+}$  in water very selectively using enzymatic hydrolysis of the substrate and its inhibition by the  $\text{Hg}^{2+}$  ion.<sup>4</sup> Our sensor mechanism is the combination of enzyme-substrate reaction and its inhibition by the inhibitor. We have made a sensor which respond to the substrate concentration and this response can be interfered quantitatively by the suitable inhibitor of the enzyme. Hence the interference of the sensor response by the inhibitor to the fixed substrate concentration can be quantified as an inhibitor concentration.

We have utilized urease (enzyme)-urea (substrate) reaction and followed by the inhibition by the mercury ion  $\text{Hg}^{2+}$  to achieve the PCCA based sensing motif. Urea specific enzyme urease is coupled to the ions responsive PCCA (carboxyaled) and this UPCCA hydrolyzes the urea and produces  $\text{NH}_4^+$  and  $\text{HCO}_3^-$  ions within the UPCCA hydrogel over that outside.<sup>4</sup> The production of ions within hydrogel induces the charge-screening between the carboxylate groups of the polyacrylamide backbone. As this occurs, the carboxylates experience less electrostatic repulsion between themselves and the ionic polyacrylamide backbone relaxes, causing the hydrogel to shrink. As a result the UPCCA shows diffraction blue shifting. Hence the diffraction blue shift can be monitored as a function of urea concentration. When an inhibitor (such as  $\text{Hg}^{2+}$ ) is introduced into the solution, it binds to the urease and deactivates the enzyme functionality by inhibiting the enzyme-substrate reaction. This inhibition process intervene the production of ions and hence the hydrogel shrinking suppresses. This suppression results the further diffraction red shifting of UPCCA from the blue shifted UPCCA when it was exposed to the urea only. Therefore the suppression of hydrogel shrinking can be controlled as a function of inhibitor concentration ( $\text{Hg}^{2+}$  here) for a fixed concentration of substrate (urea here). Hence the net change in the diffraction wavelength shift (red shift) from the initial blue shift with the fixed urea concentration can be

quantitatively monitored as a function of inhibitor concentration.<sup>4</sup> Figure 1 represents the sensing motif of our sensor.



**Figure 1.** UPCCA sensor concept in which sensing motif is relied on two steps coupled spontaneous processes.

This UPCCA photonic crystal sensor detects ultra-low (1 ppb) concentration of  $\text{Hg}^{2+}$  in water, exhibits reversibility and displays very high selectivity towards  $\text{Hg}^{2+}$ . The uncompetitive inhibition nature of the urease enzyme, when it is covalently attached in the polymer hydrogel backbone, is the driving force for the very high selectivity and reversibility of the UPCCA sensor<sup>4</sup>

A novel photonic crystal sensor material, made of self-assembled polymeric nanoparticles and hydrogel, has been developed for the determination of toxic  $\text{Hg}^{+2}$  concentrations in water. The sensor detection limit is 1 ppb ( $1\mu\text{g}/\text{liter}$ ), which is well below the MCL (2 ppb) recommended by the EPA, USA for the safe drinking of water.

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## Characterization and Application of Fluorescent Poly(amido amine) Dendrimers

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### Abstract

Fluorescent probes are extensively used as convenient and excellent markers in biological and medical sciences because of the easy detection and the highly-sensitive power. A green fluorescent protein (GFP) is now popular as a biocompatible fluorescent dye, and fluorescent nanoparticles are also the targeted drugs on the diagnostic imaging. These fluorescent markers always fall on issues of the influence to biological organisms. Therefore, scientists are still demanded the development of adequate markers. Then amine-branched dendrimers are one of expected biocompatible phosphors.

The strong blue luminescence from poly(amido amine) (PAMAM) dendrimers has been confirmed in 2004 and later [1-3]. Similar strong fluorescence is discovered even for other amine-branched dendrimers [3,4]. The investigation is carried out at different conditions, and the origin of the luminescence has been discussed on the basis of the experimental evidences. In association with the origin of fluorescence of amine-branched dendrimers, the formation of an “exciplex” between two species, namely, a tertiary amine and an oxygen atom is first presumed as a driving force for the intrinsic fluorescence emission of the dendrimers [5]. Another possibility is the formation of a peroxy radical, which should be originated from tertiary amine and oxygen [6].

It should be noted that the visualization of fluorescent dendrimers is possible and indispensable for the utilization as an imaging agent. Dendritic nanohydrogels fabricated by the polymerization of PAMAM dendrons [7], cotton fibers dyed by PAMAM dendrimers [3] and porous silica particles (beads) surface-modified by PAMAM dendrons [5] are visualized by a fluorescence microscope. The selective electrostatic adsorption of fluorescent dendrimers is visually observed on the substrates with counter ionic patterns and hydrophobic patterns [8]. An avidin molecule is labeled with G4.5 PAMAM dendrimers through the amide chemical bond, and the visual observation of fluorescent dendrimers confirms avidins bound fluorescent dendrimers interact selectively with biotin immobilized on the patterned substrates [9]. Gene delivery and transfection toward rat C6 glioma cell lines are successfully evaluated by

mediation of blue fluorescent PAMAM dendrimer [10]. These results suggest that the photoluminescent dendritic polymers are valuable as biocompatible and chemically-stable fluorescent markers without quenching by oxygen.

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## Graphene/ Polymer hybrids as Chemical and biochemical Sensors

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### Abstract

Graphene oxide (GO) in acidic medium (pH = 4) emits blue light but in neutral and alkaline medium (pH=7 and 9.2) the emission is negligible. On addition of methyl cellulose (MC) by 0.85, 1.7 and 3.4 % (w/v) to GO solution (0.005 % w/v) the emission intensity increases dramatically in every pH but with increase in pH the PL (photoluminescence) intensity decreases for every composition of the hybrid solution. The average lifetime of GO at pH = 4 increases on addition of MC. Fluorescent microscopic images of GO-MC hybrids for different MC content indicate that the morphology of the hybrids at pH 4 is ribbon type but at pH 7 and 9.2 no characteristic morphology is produced. The decrease of glass transition temperature by 9<sup>0</sup> C of the GMC0.85 system (produced from drying GO-MC hybrid solution containing 0.85% MC solution) from that of pure MC suggests the presence of supramolecular interaction in the system. There is a drastic decrease in PL intensity on addition of nitroaromatics to the GMC0.85 system and it is very large (91%) for the addition of picric acid. Thus the hybrid system acts as a good sensor for the detection of nitro aromatics by instantaneous photoluminescence quenching with a detectable limit of 2 ppm. Graphene oxide / poly(vinyl alcohol) hybrid in acidic medium (pH=4) is highly fluorescent due to passivation by H-bonding as evident from FTIR & Raman spectra, and the fluorescence property can be used as a tool for selective sensing of Au (III) ions with a detectable limit of ~ 275 ppb.

Sulfonated graphene (SG) and graphene oxide (GO) are used as binding platform of ethidium bromide (EtBr, E), to preferentially sense DNA (D) amongst the other biomolecules like RNA (R), bovine serum albumin (BSA, P) and glucose (G) using spectroscopic techniques. EtBr has lost its intrinsic fluorescence property after binding with SG. DNA can “turn on” the quenched fluorescence of SG-EtBr hybrid to a greater extent compared to the RNA, BSA and glucose. Compare to GO-EtBr, SG-EtBr hybrid is superior



to preferentially sense DNA An analysis of Raman spectral data indicates that the interaction of EtBr in its adsorbed state on SG template is greater with DNA than that with RNA

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## **Thermal, mechanical and morphological properties of surface modified montmorillonite (MMT) reinforced viton rubber nanocomposites**

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### **Abstract**

Thermal, mechanical and morphological properties of surface modified montmorillonite (OMMT) reinforced viton rubber nanocomposites were studied. Surface of montmorillonite was modified by column chromatography technique using quaternary long chain ammonium salt as an intercalent, which resulted uniform exchange of ions between MMT and ion exchange resin, and increased d- spacing to 22 Å. This improved d-spacing was due to ion exchange column of sufficient length (35 cm) and diameter (5 cm) with maximum retention time for exchange of ions. The viton nanocomposites reinforced with OMMT (3-12 wt %) were prepared on two roll mill and molded on compression molding machine. The mechanical properties like tensile strength increased 317 % and elongation at break from 500 to 600 % respectively for 9 wt % loading of OMMT in comparison to pristine viton rubber. The results of DSC and TGA revealed that loading of OMMT greatly improved the thermal stability. The increase in properties with increase in amount of OMMT loading was due to incertion of rubber chains between the OMMT plates with good wet ability. Overall, at optimum amount of 9 wt % OMMT loading the properties of viton rubber nanocomposites improved and subsequently decreased at 12 wt % due to agglomeration of OMMT as resulted by SEM and AFM images.

**Keywords:** Viton rubber, organically modified MMT (OMMT), Thermo-mechanical properties, Morphological structure.

## Discovery of New Melt Condensation Chemistry for Polymers Based on Amino acids

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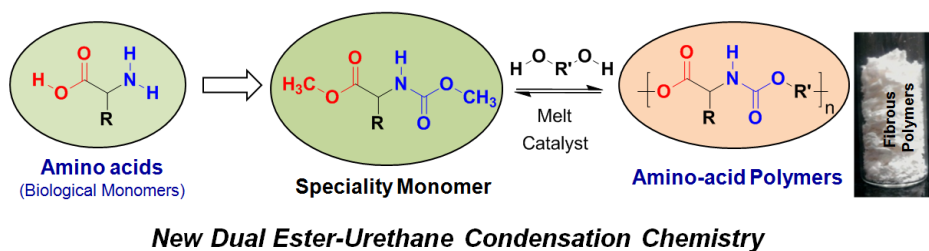
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### Abstract

Synthetic polymers based on amino acids have been great interest in chemistry-biology interface due to their potential application in therapeutics, cosmetics, biodegradable and biocompatible engineering thermoplastics. Ring opening polymerization of amino acids via N-carboxyanhydride (NCA) intermediate was another important approach to make linear, block and star-shaped polypeptides. However, the interference of functional groups in multi-functional amino acids (like serine) with the catalyst restricted this approach to a limited range of amino acids. As a consequence, amino acid based polymers as thermoplastics or application in biomedical industry is very far from reality. Recently, we have developed, for the first, time, a dual ester-urethane process for amino acid polymers under solvent free melt condensation. In this new process, amino acids were readily converted into dual ester-urethane monomers and polycondensed with diols under melt conditions to produce high molecular weight polymers. The new synthetic process was tested for more than half-dozen of amino acids and diols. L-amino acids were converted into their corresponding ester-urethane monomers by simple tailor made approach.



The new dual ester-urethane condensation approach was demonstrated for variety of amino acids: glycine,  $\beta$ -alanine, L-alanine, L-leucine, L-phenylalanine and L-valine along with commercial diols: di-, tri- and tetraethylene glycols, 1,12-dodecanol (linear aliphatic diols) and 1,4-cyclohexanedimethanol (cycloaliphatic diols). The end group analysis by MALDI-TOF confirmed that the amino acid functional

groups were very much thermally stable in the dual ester-urethane melt polymerization process and produced high molecular weight polymers. The thermal properties of the new polymers such as glass transition temperature and crystallinity could be easily fine-tuned by choosing appropriate L-amino acid monomers or diol in the feed. Thus, the new melt condensation approach will open up new platform of research activates based on amino acids in polymer synthetic literature.

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## Polymerization of plant oils in carbon dioxide media

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### Abstract

The conversion of plant oils to polymers has attracted renewed attention in recent years to replace or augment the traditional petro-chemical based polymers and resins. This is because of concerning the environment, waste disposal, and depletion of fossil and non renewable feedstocks. Usually polymers obtained from agricultural raw materials are biodegradable and inexpensive. Here we report polymerization of plant oils, such soybean oil, euphorbia oil, jojoba oil and epoxidized soybean oil in carbon dioxide media (liquid and supercritical condition) catalyzed by Lewis acid. The resulted polymers were characterized by FTIR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, solid state <sup>13</sup>C-NMR spectroscopies, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and gel permeation chromatography (GPC). The application of these functionalized polymers will be explored.

## Crossing Borders between Natural and Synthetic Peptides; Shielding and Mediating Of Hydrogen Bonding In Amide-Based (Macro) Molecules

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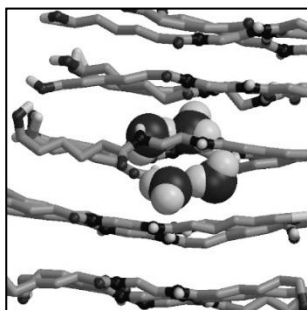
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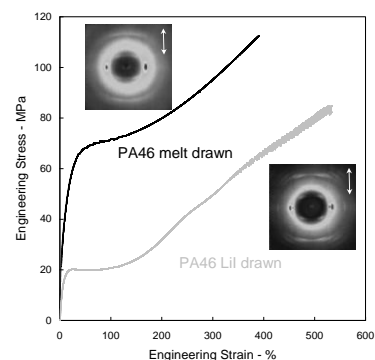
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### Abstract

High performance fibers of polymeric origin benefit from the high energy required to distort covalent bonds along the molecular axis. The polymer molecules exist in extended conformation perfectly aligned in the fiber direction. In case of polyethylene (PE) only weak van der Waals forces reside between the molecules in the extended crystals, but with sufficient length of the molecules the sum of these weak secondary interactions between the molecules entails sufficient frictional forces between the chains that the stress is transferred to the covalent bonds in the main chain upon deformation, resulting in high strength and stiffness. In processing polyamides (PA) cooling induces crystallization into chain folded crystals that are comparable with stacks of  $\beta$ -sheets in proteins, for example silk. Because of strong interchain hydrogen bonding the chain folded crystals cannot be unfolded like in the case of PE. Temporarily shielding of hydrogen bonding during spinning and drawing may lead to ideally aligned and extended chain crystals upon restoration of hydrogen bonding. Based on water, which in the superheated state acts as a good solvent [1], and inspired by natural silk spinning, where in the glands of spiders and silk worms hydrogen bonded moieties of the proteins are shielded and mediated by water molecules, ions and pH [2], a new reversible shielding route in polyamide processing is explored.



**Figure 1: Shielding of amide moieties in EDHA (stick model) by four water molecules (ball model) [5]**



**Figure 2: Strain induced crystallization and structure development (WAXD) in melt (black) and LiI drawn PA46 (gray).**

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**Comparative studies on the performance of nanocomposites based on PEEK/PEI polymer matrix filled with MWCNT's modified by Polycarbosilane and Polyphosphazene**

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**Abstract**

The field of nanotechnology is one of the most demanded areas for current research and development in almost all technical disciplines. Nanotechnology is not new to polymer science as prior studies before the age of nanotechnology involved nanoscale dimensions but were not specifically referred to as nanotechnology until recently. Phase separated polymer blends often achieve nanoscale phase dimensions, block copolymer domain morphology is usually at the nanoscale level, asymmetric membranes often have nanoscale void structure, miniemulsion particles are below 100nm, and interfacial phenomena in blends and composites involve nano scale dimensions. The nanoscale of dimensions is the transition zone between the macro level and molecular level. Recently polymer matrix based nano composites have become a prominent area of current research activity with interesting observation. More recent studies involve carbon nanotubes, carbon nanofibres, graphene, nanocrystalline metals and various nanoscale inorganic filler or fibre modifications.

Poly (ether-ether) ketone (PEEK) is a semicrystalline thermoplastic polymer with excellent thermal and chemical stability, specially used in a wide range of applications in automobile and aerospace industries. It is suitable for use as a matrix material in the preparation of thermoplastic composites owing to its good adhesion to glass and carbon fibres. Blending of PEEK/Polyetherimide (PEI) combines the synergistic properties of both of them. It has been established that PEEK/PEI are molecularly miscible in the amorphous state.

The present study is aimed to modify multiwall carbon nanotube (MWCNT's) with polycarbosilane (PCS) and poly phosphazene (PPh) separately and to compare the performance of developed nanocomposites based on PEEK/PEI polymer matrix filled with varied loading of coated MWCNT's.

PEEK/PEI (50:50) blend has been prepared by the melt blending. The thermal stability of the composites has been studied by thermogravimetric analysis (TGA) which demonstrates an increase in the decomposition temperature of PEEK/PEI blends at higher loading of PCS and PPh coated MWCNT's. Differential scanning calorimetry (DSC) studies reveal that the melting temperature ( $T_m$ ) has increased with higher loading of PCS and PPh coated MWCNT's in PEEK/PEI blends. From SEM studies, it has been demonstrated that strong interfacial adhesion between matrix and disperse phase of PEEK/PEI blends has been observed at higher loading of coated MWCNT's. XRD results indicate a compact crystalline structure of the composites. Comparatively nanocomposite filled with PCS coated MWCNT's give better performance as compared to PPh coated MWCNT's.

Key words: PEEK/PEI, MWCNT's, Polycarbosilane, Polyphosphazene



## Self-assembled monolayer based QCM biosensor for the detection of *E. Coli*

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### Abstract

The self-assembled monolayer based Quartz Crystal Microbalance (QCM) biosensor was developed for the rapid detection of some water-borne pathogens. The developed biosensor is also called a piezoelectric immunosensor. This study includes the fabrication of a QCM based biosensor for the detection of *E. Coli* using self assembled monolayer (SAM) of antigen and antibodies attached on thiolated gold surface of a quartz crystal. The biosensor setup measures the change in frequency corresponding and non corresponding using RQCM (Maxtek, Inc. USA). The whole detection procedure is comprised of cleaning, thiolation, activation, and immobilization steps.

In this biosensor system the affinity purified antibody i.e.  $\beta$ -gal was immobilized onto the monolayer of 16-Mercaptohexadecanoic acid (MHDA), a long chain carboxylic acid terminating alkanethiol self-assembled on a gold electrode surface of 5 MHz AT-cut quartz crystal and then the thiolated crystal was activated by the treatment of 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) and N-Hydroxysuccinimide (NHS). This EDC-NHS treatment improves the stability of the linker compounds and has been commonly used in antibody immobilization as reactive intermediate.

The immersion-dry-immersion method was applied on the course of entire experiment. The binding events were determined by decreasing resonant frequency of the quartz crystal mounted onto the quartz crystal microbalance (QCM). The decrement in the frequency was directly proportional to the concentration of mass added onto the crystal's gold electrode surface. The surface coverage obtained with QCM was 0.234, 0.073, and 0.386  $\mu\text{g}/\text{cm}^2$ ; for the layers of MHDA, EDC-NHS, and antibodies, respectively. The developed biosensor setup is a label free, cost effective, reusable and quick method of detection of *E. coli* and can be employed to other pathogens also.

## Clay nanoparticles as *pseudo*-pro-oxidant for polyolefins degradation

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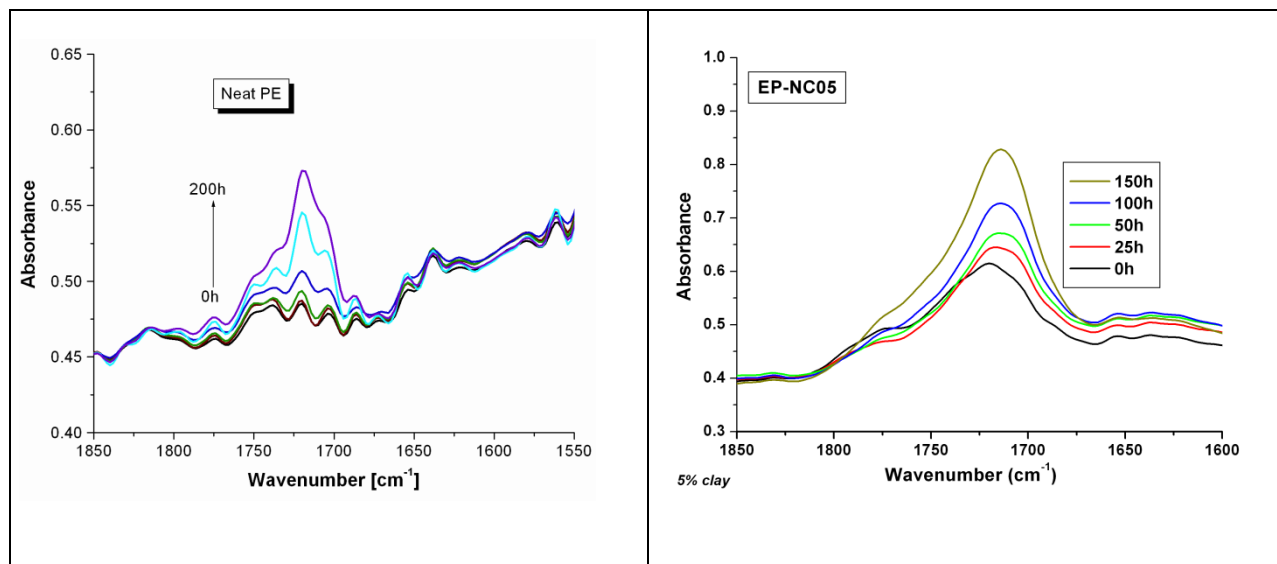
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### Abstract

Over the past 50 years in plastic industry, the success of thermoplastics of polyolefins based on petroleum resources can be attributed not only to the reliable raw materials basis, but also to their versatile applications (packaging and biomedical devices) and to their melt-processability. The inertness and durability of polyolefins which have made them a material of choice for many applications are seemingly a disadvantage when it comes to their disposal. This present investigation aimed at using clay (layered silicates) nanoparticles as pseudo-pro-oxidant for enhancing the photo-oxidative degradation of polyolefins (PE, PP and their copolymers). The strategy involved here is preparing nanocomposites of polyolefins with clay as reinforcing nanoscale filler and pseudo-pro-oxidant and microcrystalline cellulose as biodegradable additive for enhancing the biodegradation. Investigation on mechanical properties and FTIR spectroscopy (Figure) upon photo-irradiation suggested that the clay-incorporated samples are more susceptible towards photo-oxidation than the neat polymer and polymer-cellulose composites. Biodegradation studies by composting method indicated that the though incorporation of clay has no direct and significant effect on earlier stage of weight loss, show higher level of biodisintegration when they are already photo-oxidated. Since the clay incorporated samples showed their vulnerability to photo-oxidation which is pre-requirement for biodegradation of polyolefins, we suggest that the acceptable level of biodegradation can be achieved by incorporation clay followed by photo-oxidation.



## Advances in Chitin and Chitosan Based Nanomedicine

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### Abstract

Chitin and chitosan are biodegradable and biocompatible biopolymers. They are being used for several biomedical applications such as drug delivery, tissue engineering and wound healing [1, 2]. These biopolymers can be easily processed into different forms such as beads, nanofibers, nanogels, nanoparticles, microgel, microparticles, sponges and scaffolds. Research on the chitin and chitosan based nanomedicine has grown significantly worldwide. In our laboratory, we have developed chitin and chitosan based nanofibers, nanogels, nanoparticles, microgels and nanocomposite scaffolds for drug delivery, tissue engineering and wound healing applications. This presentation will discuss about the various synthesis routes and applications of selected chitin and chitosan based nanomaterials.

Biocompatible chitin nanogel was developed by regeneration chemistry without the use of any surfactant or cross-linker. The prepared chitin nanogel was very suitable for encapsulating quantum dots [3], anticancer [4] and antifungal [5] drugs. The details about the drug delivery, imaging, sensing and cancer therapy applications of quantum dots, anticancer and antifungal drugs encapsulated chitin nanogels will be discussed in detail.

We also developed a novel drug delivery system comprising of *O*-carboxymethyl chitosan (*O*-CMC) nanoparticles and surface-conjugated with Cetuximab (Cet) for targeted delivery of paclitaxel (PTXL) to cancer cells [6]. The selective cytotoxicity and uptake of Cet-PTXL-*O*-CMC nanoparticles by EGFR over-expressing cancer cells compared to EGFR negative cells will also be discussed.

In continuation we also prepared tetracycline encapsulated *O*-carboxymethyl chitosan nanoparticles (Tet-*O*-CMC Nps) [7] for intracellular bacterial infections. These infections are recurrent, persistent and difficult to treat because of poor penetration and limited availability of antibiotics within macrophages and epithelial cells. The efficacy of the Tet-*O*-CMC Nps in killing intracellular *S. aureus* compared to Tet alone will be discussed.

In addition, we have also developed chitosan hydrogel/nano fibrin [8], chitosan hydrogel/nanoZnO [9] and chitin hydrogel/nanoZnO [10] composite bandages for wound healing

applications. The *in vitro* and *in vivo* animal studies of the prepared chitosan hydrogel/nano fibrin, chitosan hydrogel/nanoZnO and chitin hydrogel/nanoZnO composite bandages will also be discussed.

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## Development of Phosphonated PEEK Membrane for Fuel Cell Applications

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### Abstract

Polyelectrolyte membrane (PEM) for fuel cell application has been the interesting and progressive field of research. Various types of perfluorinated and sulphonated polymers have been used in the past decade however Nafionis the only membrane commercially available which gives the satisfactory result for low temperature application in polyelectrolyte membrane fuel cell (PEMFC). PEMFC of relatively high working temperature, durability, power output, high efficiency, and long self life under relatively constant operating conditions for fuel cell is the prime requirement in futuristic applications. Owing to these requirements the thermally stable engineering polymer materials are the centre of attention in fuel cell research area. Poly (ether ether ketone) (PEEK) is one of the high performance engineering polymers which caters the requirement of excellent thermal stability and mechanical properties at high temperatures. Many of such efforts have been exercised to use Sulphonated PEEK and its composites in the past. In this research we have prepared phosphoric acid functionalized PEEK polymer which was further characterized by various technique. The proton conductivity was measured using impedance spectra. Satisfactory results will be reported for new PEM fuel cell.

## Polymer Nanocomposites for Defence Applications

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### Abstract

Nanometer-size particles have attracted a lot of research interest, mainly due to the size-quantization effect by which the material properties are tunable by the particle size. For application in electronics and photonic devices as well as industrial applications such as various additives, surface coatings and environmentally stable flexible boards for advertisement as well as in rubber technology. The net result of such development is the immense scope of these materials in defence sector. Nano-technologists' desire to be able to cast the nano-particles into films by easy process is a common but important requirement. To handle associated challenges, polymers are best choice for encapsulation of nano-particles due to two factors i) ready processability of polymer films and ii) homogeneous/uniform distribution of the particles. In defence sector there are number of nano-materials used for a range of application including the nano-particles–polymer composites. Modern military operations and tactics necessitate the development of advanced ballistic protection body armor systems. High performance polyethylene (HPPE), Epoxy resins, Poly(methyl methacrylate) (PMMA) are useful polymers for ballistic applications. Normally, Silver, Titanium dioxide, Zinc oxide and Zirconia nano-particles are used as ballistic fillers. Similarly, war tanks, electronic circuits etc need to be protected from corrosion for increasing their life and to reduce life-cycle cost. Polymer nano-composites are used for coating metal and alloy parts to increase their working life by reducing corrosion. Nano-crystalline particles are also useful for killing the fire, polymer nano-composite shows excellent gas barrier properties hence block access for gas molecules generated from combustion and heat during fire thus preventing materials from burning. There are several electronic devices for defence application which arise out of use of nano-particles e.g. chemical sensors based on metal-oxide nano-particles play great role in identifying various war gases that generally contain NO<sub>2</sub>, NH<sub>3</sub>, etc. Additionally, fluorescent tags for identifying defence personnel in distant location can be developed by use of semiconductor quantum dots e.g. shape and size dependence CdSe and ZnSe quantum dots can be applied for identification of personnel by way of different colour light emission. Synthesis and characterization of a few of these useful nano-particles will be discussed in this lecture.

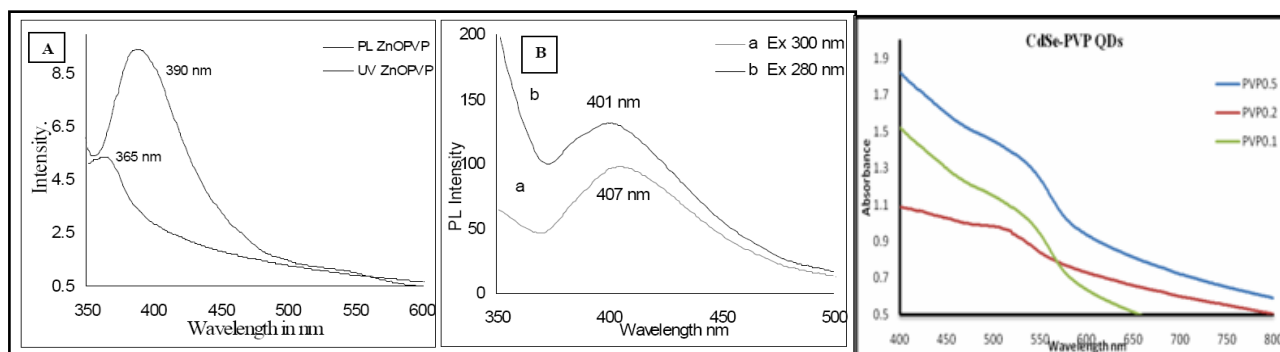


Figure showing UV (A) and PL(B) of ZnOnano-particles and UV of CdSe QDs coated with a polymer



## **Functional Polymers by Controlled Radical Polymerization and “Thiol-ene” Reaction**

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### **Abstract**

Polymers bearing specialty functional groups are being used in smart materials, self-healing, strategic materials and in different biomedical applications. Conventional free radical polymerization of the functional monomers lead in polymers with uncontrolled molecular weights and broad polydispersity index and thus it results in poor processing and inferior mechanical properties. This investigation reports the preparation of tailor-made functional polyacrylates via atom transfer radical polymerization and thiol-ene reaction.

## **Polymer Silica Nanomaterial for Coating Industries**

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### **Abstract**

Products that contain nanoparticle dispersions are finding increasing applications in coatings, personal and health care, paints and inks, plastics and several other industries. A good and uniform dispersion of nanoparticle is a very parameter for all the above applications, in particular when used in coatings. Resin based coating systems used in automotive, floor, tiles are one of the most important industrial products in use today. However, there is one significant limitation with most industrial resin systems: the difficulty of coating polymers to provide additional capabilities such as improved scratch resistance. Particle agglomeration hinders each individual nanoparticle to interact with the surrounding media. Use of nanoparticle in clear coating formulation and retaining optical clarity is one of the greatest challenge industry is facing today. The present talk will highlight mainly the nanotechnology opportunity, market potential and its use in clear coat industry to obtain antiscratch property.

## Functional Polymers in Lithium-ion Batteries

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### Abstract

Lithium-ion batteries (LIBs) have taken the lead position among the various energy storage devices being used in consumer electronics including portable gadgets. The high capacity variants of LIBs are the preferred secondary power source for satellites. They are also emerging fast as the power sources for electric and hybrid-electric vehicles. LIBs gained wide spread acceptance for such varied applications because of their unique properties including high specific energy (both in terms of mass and volume), low self-discharge, high calendar life, high cycle life and high-power capability. The LIB technology is based on the shuttling of  $\text{Li}^+$  ions between the electrodes during charge-discharge reactions through the ion-conducting separator. The performance of LIB is decided mainly by the properties of cathode, anode, electrolyte and separator. The LIB technology offers immense scope for developing new electrode materials, separators as well as evolving new cell design concepts.

Polymers play a crucial role in LIBs. Different polymers are used as cell components such as separator, binder, electrolyte, electrode-active material, insulating material and pouch packing material. Thus, several new developments in LIB originate from the advancements achieved in polymer science and technology. A separator is an important component of LIB which separates direct contact between the anode and cathode, thus preventing short circuits, and provides internal passage for  $\text{Li}^+$  ions. The promising separators are those with high electrolyte permeability and mechanical strength, as well as good thermal, chemical, and electrochemical stability. Polypropylene and polyethylene as ultra thin membranes (of about 25  $\mu$  thickness) are the most commonly used separators. In the case of a polymer LIB, polymer plays the dual role of separator and electrolyte. Here, the porous structure of the polymer is swollen with a  $\text{Li}^+$  ion conducting liquid electrolyte to form a gel polymer electrolyte (GPE). Solid polymer electrolytes (SPEs) have also been widely investigated in LIB for their non-leaking and non-flammable nature. Polyethyleneoxide (PEO), poly(methylmethacrylate) (PMMA), poly(acrylonitrile)

(PAN) and poly(vinylidene fluoride) (PVdF) have been of interest in developing GPEs and SPEs. The nature and properties of these polymer membranes vary with their formation techniques. Composite polymer membranes with inorganic fillers, functionalized derivatives of PEO, etc. are also studied as PEs. Latest technologies like electro-spinning are also being investigated to realize host membrane for PEs with desired properties. Another key component used in LIB electrode processing is the polymeric binder. The binder is added to the electrode-active materials which are in the form of fine powders, to form slurry and help its deposition on the metal current collector by improving adhesion. Various polymers like PVdF and PTFE are widely employed as binders.

Functionalized polymers have been developed and found promising as electrode-active materials for LIBs in place of the conventional inorganic materials. Polymers as active materials impart light weight, flexibility and processability to the electrodes and help to realize ultrathin batteries. Electrically conducting polymers with  $\pi$ -conjugated skeleton structures, such as polyaniline, polypyrrole, polythiophene, and their related derivatives, have been explored as electrode-active materials. However, the success of these  $\pi$ -conjugated polymers is limited by their insufficient doping levels, resulting in low redox capacities and fluctuation of the cell voltage through the doping/de-doping process. Redox-active radical polymers are emerging electrode-active materials. Polymers with pendent nitroxide radicals such as tetramethylpiperidineoxyl (TEMPO) derivatives and the oxygen radicals such as phenoxy and galvinoxyls are typically examined as electrode-active materials. The radical polymers allow fabrication of flexible thin-film batteries with excellent rate performance which allows instant full charging. Polymer-Carbon nano tube composite electrodes are also emerging candidates as electrodes.

## Prediction of Glass Transition Temperature of EPON 862 (DGEBF) cross-linked with Curing Agent W (DETDA) using MD Simulations

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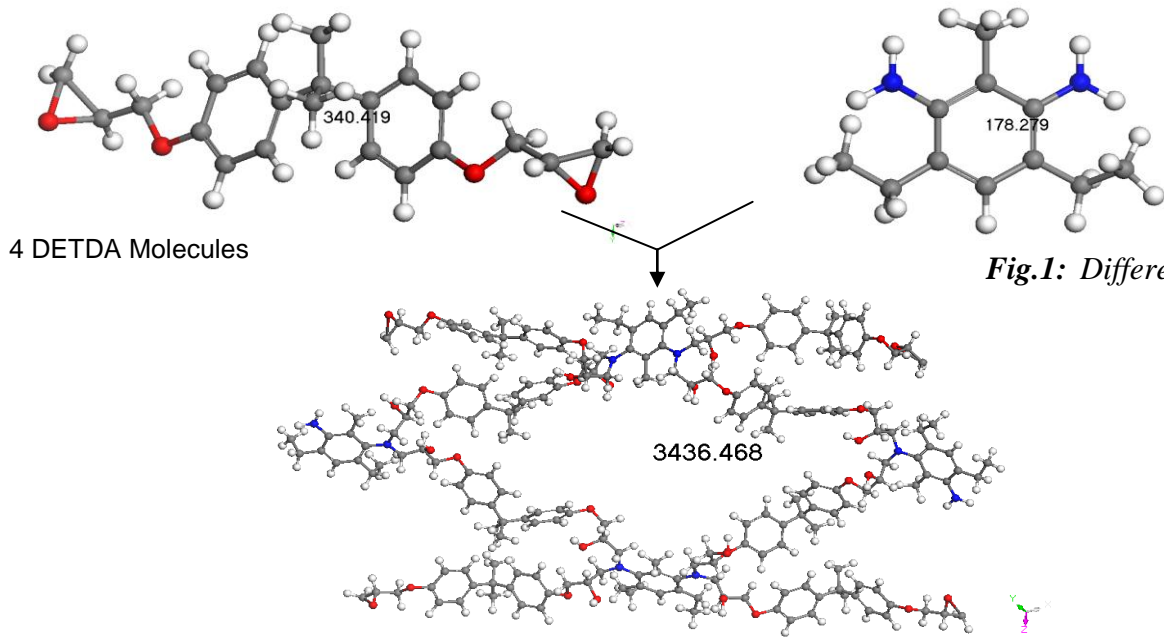
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### Abstract

The present study focuses on the prediction of glass transition temperature ( $T_g$ ) of the cured epoxy resin (DGEBF) cross-linked with curing agent W (DETDA). A quad oligomer of DEGBF cross-linked with DETDA was used for the calculations (see Figure 1). MD model of the epoxy was built using the amorphous module of Material Studio (Accelrys Inc.). The Polymer Consistent Force Field (PCFF) was used in the simulation. The amorphous structure was achieved by giving periodic boundary conditions and then subjected to an energy minimization using the ensemble of the constant-volume and temperature (NVT). The structure was equilibrated for 100 picoseconds (ps) and then followed by a MD equilibration at room temperature for another 200 ps. Since at room temperature most of the atoms are in static mode, the atoms were excited using simulation temperatures above the glass transition temperatures. In an attempt of finding global energy minimum, simulated annealing runs were then carried out starting at elevated temperatures at atmospheric pressure using the ensembles of the constant number of particles, constant-pressure and constant temperature (NPT). Temperature was then gradually lowered to a room temperature. Each subsequent simulation was started from the final configuration obtained at the preceding temperature. Density of the epoxy at each temperature was calculated from the average specific volume and glass transition temperature ( $T_g$ ) was estimated based on the discontinuity in the slope of the density-temperature plot. Amorphous structure obtained at room temperature was analyzed to determine the fundamental mechanical

properties of EPON 862-W.



Keywords: atomistic modeling, molecular dynamics, glass transition temperature, EPON 862-w, Accelrys, annealing

## "Electronic Devices from Conducting Polymers and TM-Phthalocyanines"

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### **Abstract**

In this talk, we describe efforts made by our group at Bhabha Atomic Research Centre (BARC) to prepare molecular electronic devices from thin films of conducting polymers or transition-metal phthalocyanines. These devices include actuators, sensors, or electronic devices such as diodes, FETs, etc. The main focus of this talk will be the growth strategies adopted by us to deposit high-quality mono- or multi-layers, in order to obtain desirable physical characteristics, including high mobility of charge carriers in them as well as good bonding of these films to the substrates.

## Micelle –Assisted Synthesis of Electromagnetic Nanotapes by In Situ Self-Assembly Process

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### Abstract

Electromagnetic nanocomposite materials have attracted increasing attention because they offer the possibility of a new generation of nanostructure materials with diverse applications. Polyaniline is one of the most technologically important materials because of its environmental stability in the conductive form, unique redox properties and high conductivity. There has been increasing interest in the preparation of conductive inorganic hybrid composites. Conducting polymers incorporating magnetic materials will possess the potential of multifunctional applications such as sensors and electromagnetic interference shielding materials. Despite a few of papers concerning the preparation of magnetic nanocomposite and their application, their practical application is limited due to the agglomeration of magnetic particles originating from the strong interaction between these particles which will diminish its magnetic properties. Therefore, it is fundamental importance to develop a method to synthesise novel electro-magnetite composites for high technological applications. In the present work, we report a facile one-pot synthesis of electro-magnetic polyaniline composite through 3- pentadecyl phenol micelle assisted synthesis by in situ self-assembly method. The presence of PDPSA can effectively prevent the formation of larger particles, thereby producing nanometre sized particles. During polymerisation, in presence of aniline, they will form nanotapes by self-assembly process. During the formation of PPICS, 3-PDPSA serves multifunctional role of micelle template, capping agent, structure directing agent, dopant etc which was manifested from various studies like particle size, morphology, electrical conductivity etc. Studies revealed the formation of nanotapes having electrical conductivity  $\sim 100 \text{ S m}^{-1}$  and saturation magnetization of  $1 \text{ emu g}^{-1}$  with coercivity of  $\sim 50 \text{ Oe}$  which makes them promising multifunctional candidate for high technological applications.



## Surface-Confined ATRP to Synthesize Functional Mesoporous Polymer/Carbon Nanospheres

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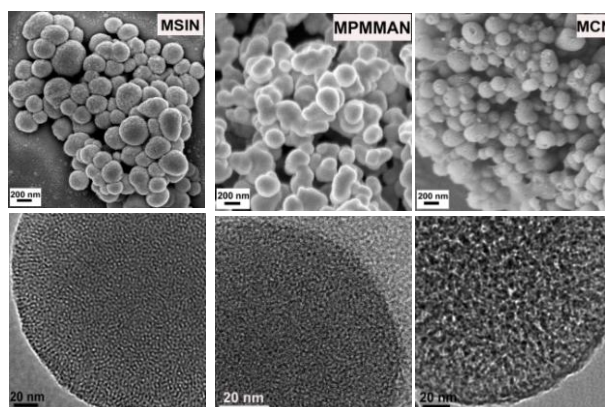
### Abstract

Over the last few years, the interest in ordered mesoporous materials (pore size: 2-50 nm) with high surface area and large pore volume has grown exponentially due to their diverse applications in separation, adsorption, sensors, catalysis, and energy storage. Among them, mesoporous polymer (MP) materials are used in electronics, controlled release and heterogeneous catalysis. Mesoporous carbon (MC) materials have applications as an adsorbent of bio and organic molecules, component of fuel cells and component of Li ion batteries. Due to these diverse applications of these materials, researchers have developed several synthetic strategies to produce MP/MC materials. For example, a template-free approach has been used for the synthesis of MP materials by self-assembly of diblock copolymers. These MP materials were converted into MC materials by carbonization. Recently, mesoporous silica materials are used as a hard template to prepare MP/MC materials. But, poor grafting of organic moiety was observed into the pores of silica because the initiation sites on silica template were created by post functionalization technique. Again, all the existing reports mostly deal with the production of MP or MC powdery materials, that is, powders with no definite shape. On the other hand, the synthesis of materials with controlled and tunable morphologies, especially via shape replication is one of the biggest challenges of the present time. Furthermore, from the application point of view, the fabrication of functional MP materials is very important and highly relevant.

This talk will highlight some of our very recent research on a facile approach for the production of mesoporous polymer nanospheres (MPN) and mesoporous carbon nanospheres (MCN) with complete shape retention of the original template via surface-confined atom transfer radical polymerization (SC-ATRP) of various methacrylate monomers from initiator-modified hard mesoporous silica nanospheres (MSIN) template. MSIN are synthesized by hydrolysis/co-condensation reaction of tetraethyl orthosilicate (TEOS) and ((chloromethyl)phenylethyl)trimethoxysilane (CMPE-TMS) at a basic pH (~12) in presence of cetyltrimethylammonium bromide (CTAB) as the template and subsequently removing the template by an acid extraction. Mesoporous silica-polymer hybrid nanospheres (MSPN) are then prepared via SC-

ATRP of methacrylate monomers from the MSIN material using CuCl/CuCl<sub>2</sub>/PMDETA as the catalyst in xylene at 105 °C. Subsequent removal of the hard silica template results in the formation of MPN. Furthermore, carbonization of the MSPN hybrid, followed by removal of the silica template by HF results in the production of MCN. These mesoporous materials are characterized by FTIR, nitrogen adsorption, powder X-ray diffraction and thermogravimetry techniques. FESEM and TEM analyses of the obtained MPN/MCN materials show that they completely retain the size, shape and mesoporous network of the original template MSIN nanospheres. The synthesized mesoporous poly(methyl methacrylate) nanospheres (MPMMA) and MCN materials have high surface area of 520 and 658 m<sup>2</sup> g<sup>-1</sup> respectively. The silica free polymers (MPN) have controlled molecular weights and low polydispersities (PDI = M<sub>w</sub>/M<sub>n</sub> ≤ 1.3), as determined by gel permeation chromatography (GPC). Kinetics study of the polymerization reveals that the number average molecular weight (M<sub>n</sub>) of the grafted polymer increases linearly with time maintaining low PDIs, indicating the living nature of the polymerization. The as-synthesized MPN material have low dielectric constants and hence have potential use as a promising material in microelectronics. This technique further allows fabrication of functional MPN material. These functional MPN materials are successfully used as “clickable” mesoporous materials for the synthesis of triazole functionality with potential antimicrobial activity, in efficient removal of ionic contaminants with binding capacity of 0.345 mmol g<sup>-1</sup> and in glucose-sensing with a high binding capacity of 29.6 mmol g<sup>-1</sup>.

We further extend this work to generate heterogeneous supported catalyst by immobilizing palladium<sup>II</sup> 2-aminopyridine complex onto the surface of MSIN through the it's chlorine functional group. This catalytic system exhibits excellent activity in Suzuki-Miyauracross-coupling reactions of aryl iodides, aryl bromides and also aryl chlorides with phenylboronic acids in water medium with high yields. The supported catalyst could be quantitatively recovered by simple filtration and is found to be highly active without the any significant loss of its catalytic activity in eight consecutive runs.



FESEM images of different mesoporous nanospheres (upper panel). The high magnification TEM images of the corresponding nanospheres (lower panel).

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## Synthesis of some tri- and penta-block copolymers of styrene and methyl methacrylate via solution ATRP

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### Abstract

Block copolymers of methyl methacrylate and styrene are challenging synthetically because of their interesting properties like morphology & mechanical properties. The versatility of ATRP to synthesize such blocks has been attempted in this work by the way of synthesis of different tri- and pentablock copolymers of styrene, n-butyl methacrylate and methyl methacrylate. Thus, poly (n-butyl methacrylate-b-styrene-b-n-butyl methacrylate) and poly(methyl methacrylate-b-n-butyl methacrylate-b-styrene-b-n-butyl methacrylate-b-methyl methacrylate) linear tri- and pentablock copolymers were synthesized with control on the molecular weights. The synthesis of poly (n-BMA-*b*-styrene-*b*-n-BMA) and poly(MMA-*b*-n-BMA-*b*-Styrene-*b*-n-BMA-*b*-MMA) linear tri- and pentablock copolymers were carried out by using copper halide as the transition-metal catalyst and PMDETA as the complexing ligand and were synthesized in three steps. The thermal analysis of these blocks copolymers showed distinct glass transition temperatures ( $T_g$ 's) of PnBMA at 35 °C and 96 °C for PS in case of triblock copolymer. Different polymerization conditions such as different reaction mediums and halogen exchange were utilized to achieve the desired well-defined homo and block copolymers. Both the block copolymers showed core-shell type flower-like micellar structures when toluene was used as a selective solvent for one of the blocks.

## Synthesis of Ibuprofen Esters and Nanoparticles Preparation Using Poly (L-lactide) s for Controlled Drug Release

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### Abstract

Ibuprofen esters were synthesized and the nanoparticles were prepared using Poly (L-lactide) s. Poly (L-lactide) s were synthesized by ring opening polymerization using biocompatible zinc proline catalyst. The nanoparticles were prepared by the modified emulsion solvent evaporation method. The physicochemical analysis of nanoparticles were studied by determining the % poly (vinyl alcohol) (PVA) adsorbed at the surface of nanoparticles, encapsulation efficiency and drug release pattern. Residual PVA percentage and encapsulation efficiency of ibuprofen were found to be similar. The effect of basic process parameters like the concentration of polyvinyl alcohol (PVA) in the nonsolvent, the concentration of ibuprofen or esters of ibuprofen in the organic phase, the emulsion temperature, the time period and power input of ultrasonication on the particle size of the nanoparticles were investigated systematically and the optimal values were 0.2%, 50 mg/ml, below 4°C, 10 min and 400W respectively. The morphology of nanoparticles was found to be spherical in shape with the size ranging from 200 to 700 nm by scanning electron microscopy (SEM). The X-ray diffraction (XRD) patterns demonstrated the absence of self crystallization of ibuprofen even in every different proportion of PLA-drug or PLA-ester ratios (2:1; 3:1 and 4:1). The differential scanning calorimetry (DSC) analysis showed the reduced values of  $T_g$  and  $T_m$  attributing to plasticization effect and formation of newly ordered structure of drug-polymer molecules in the nanoform. The *in vitro* release of ibuprofen esters from nanoparticles was investigated.

## Physical-Chemical Approach of the Ageing, the Stabilization and the Long-Term Prediction Durability of Polymer Materials

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### Abstract

The polymer materials, by the diversity of their properties and by the ease of their implementation, continue to be inescapable sources of innovation in all the sectors of our industry. However two properties: fire resistance and abiotic ageing resistance, limit their applications and must be mostly improved during the key stage of their formulation. This presentation will be focused on the ageing resistance.

The most common polymer ageing is of chemical origin. The external constraints (light, heat, oxygen) generate free radicals which are going to react with the polymer to modify its chemical structure: organic oxidized functional groups (ketones, alcohols, acids, esters), chain scissions, crosslinkings, can then appear. Generally, some pourcents of progress of these reactions is enough to affect the nominal properties of materials (mechanical properties, aspect).

Contrary to the empirical methods which were able to be imagined to estimate an ageing, a physical-chemical approach of the thermal and (or) photochemical ageing, which is developed by our research center (CNEP) for 25 years, allows at the same time a cognitive approach and a predictive approach of ageing. It has recently just been comforted by a ISO standard (10-640 of August, 2011).

The presentation will review the contribution of the physico-chemical methods on several aspects of the ageing: the knowledge of the mechanisms of degradation, the laboratory analysis of both ageing itself or stabilisers lost, and finally the prediction of the long-term behavior of the polymer materials based on accelerated and ultra-accelerated methods representative of environmental ageing.

## Synthesis of Polymers and Nanomaterials by Supercritical Carbon Dioxide

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### Abstract

Over the past ten years, environmental concern has prompted the scientific community to consider strategies for decreasing the burden caused by volatile organic compounds (VOCs). Accordingly, an intense research activity concentrated in the last decade has demonstrated that supercritical carbon dioxide (scCO<sub>2</sub>) can be used as an attractive alternative replacement for the aqueous and organic solvents. Apart from the key advantages such as the lack of toxic solvent residues and the ease of product recovery, CO<sub>2</sub> is inexpensive, inert, nontoxic, and non flammable, which makes it as a unique medium with tunable solvent properties. Additionally, CO<sub>2</sub> separates the products from polymerization by simply depressurizing it, leading to a clean and dry product and thus could reduce a large amount of cost for the product recovery at industrial scale. While scCO<sub>2</sub> has been proved to be a commercially viable solvent for the synthesis of industrially important organics and isolation of natural products, it has also been explored as a promising medium for protein extraction, bioconversion, polymer synthesis, material processing, and particle engineering in pharmaceuticals.

In this study, we have used scCO<sub>2</sub> as a solvent for different type of polymerizations, such as oxidative polymerization of thiophenes to prepare functionalized conducting polymers, ring-opening polymerization of L-lactide to prepare biodegradable polymers, and also the free-radical dispersion polymerizations of various methacrylates. The polymerization results were compared with those obtained from conventional organic solvents. In addition, we have investigated the synthesis of polymeric nanoparticles and carbon nanofibers by supercritical fluid technology. The rapid expansion of supercritical carbon dioxide solutions into liquid solvent (RESS or RESOLV) method was used to produce conducting polymeric nanoparticles of substituted

polythiophenes. In general, rapid expansion of supercritical solutions containing solutes into ambient air (RESS) or liquid (RESOLV), through a small heated micro-orifice, produces an abrupt decrease in dissolving capacity of the  $scCO_2$ , and thus results in the nucleation and growth of particles in the nozzle prior to reaching the free jet expansion. The high degree of supersaturation accompanying the rapid pressure reduction in the expansion results in homogenous nucleation and thereby the formation of well-dispersed nanoparticles. We have demonstrated the use of supercritical fluid process to produce the aqueous suspension of functionalized conducting polymers such as fluorinated polythiophene nanoparticles. These materials were shown to have promising applications in molecular electronics and nanofabrications. Using this simple method, we have also obtained polyacrylonitrile (PAN) nanofibers, which were subsequently converted into carbon nanofibers.

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## Developments and Characterization of MoS<sub>2</sub> Filled Epoxy Nanocomposites

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### Abstract

Epoxy resins constitutes one of the important types of high-performance thermosetting polymer matrix commonly used as coatings, adhesives and matrices in fiber composites for a wide range of advanced applications such as in the field of automotive, aerospace, marine and electronics, ballistic protection, wear resistant slide joints, nuclear power plants, defense, tribological field, i.e. bearings, coatings, dental restoratives, etc. However, epoxy resin is brittle in comparison to the metals and hence it is important to improve its fracture as well as other mechanical properties by incorporating different fillers. The other aspects which determine the applications of epoxy are related to the improvements in the tribological properties and thermal stability. Therefore, it would be interesting to develop filler(s) with a unique combination of these properties and balance without compromising much in terms of its processability and dimensional stability to ensure better safety and economic growth. In the present work, the molybdenum disulfide (MoS<sub>2</sub>) nanoparticles are reinforced in the epoxy resin and characterized. It is observed that with varying amounts (<0.2 wt%) provides unique combination results in the simultaneous improvements in and mechanical properties, thermal stability, friction and wear resistance of the epoxy/MoS<sub>2</sub> nanocomposites.

## Nanomaterials for Energy and Environmental Applications

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### **Abstract**

The fields of energy and environment are intertwined in many complex ways through our excessive dependence on polluting fuels. In the face of the unavoidable increasing demand for energy we must necessarily seek clean forms of energy. Solar energy is the most abundant and clean energy source which can be harnessed in various interesting and effective ways. It was considered uneconomic for a long time, but with new inventions emanating largely from nanoscience and nanotechnology, the solar economics are gyrating towards favourable domains. In this talk I will discuss this scenario taking some examples from our own research on Dye and Quantum Dot Sensitized Solar Cells, photo-electrochemical (PEC) water splitting and visible light photocatalysis. I will also discuss research in allied fields such as energy storage batteries and supercapacitors, with innovative inclusion of functional carbon. Further, I will discuss some examples of the use of suitably engineered high surface area carbon for water purification.

Work supported by CSIR, DIT, DST, Govt. of India.

## Thin Film Devices Based on Polymes and Oligomers

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### Abstract

Conjugated polymers (CPs) have been widely explored for myriad of applications. CPs have been active materials in electronic devices and host for guest molecules. In this talk, I will discuss reversible disassembly and assembly of micelles using rigid, charge bearing and insoluble polymer films. Supramolecular complexes involving nanoscopic amphiphilic assemblies (AAs) and polyelectrolytes (flexible and semi rigid) have been used to prepare a variety of materials, wherein the dynamic AAs retain the structural features, but the polyelectrolytes undergo conformational changes. Here, we show that a charge bearing rigid conjugated polymer can alter the structural features and disassemble AAs. We also demonstrate reversible assembly and disassembly of AAs by controlling the number of charges on the rigid polymer. Furthermore, during the disassembly the polymer surface becomes hydrophobic. The surface hydrophobicity can be controlled by controlling the oxidation potential of the polymer.

In the second part of my talk, I will discuss about the Field Effect Transistors fabricated using thin films of small molecules. These small molecules are based on triphenylamine donors and i-indigo acceptors. The impact of the nature of transistor gate oxide on the charge carrier mobility will be discussed. I will discuss as how binding of metals with charge transport ligands lead to the formation of ordered lamellae structures. These nanostructures are stable even after charges are created by chemical doping. On the contrary, nanostructures of the ligands alone are not stable. These materials formed by metal assisted assembly showed high charge carrier mobility under atmospheric conditions. The device also works at a very low operating voltage.

## Electrospun Nanofibers: Design, Fabrication and Applications

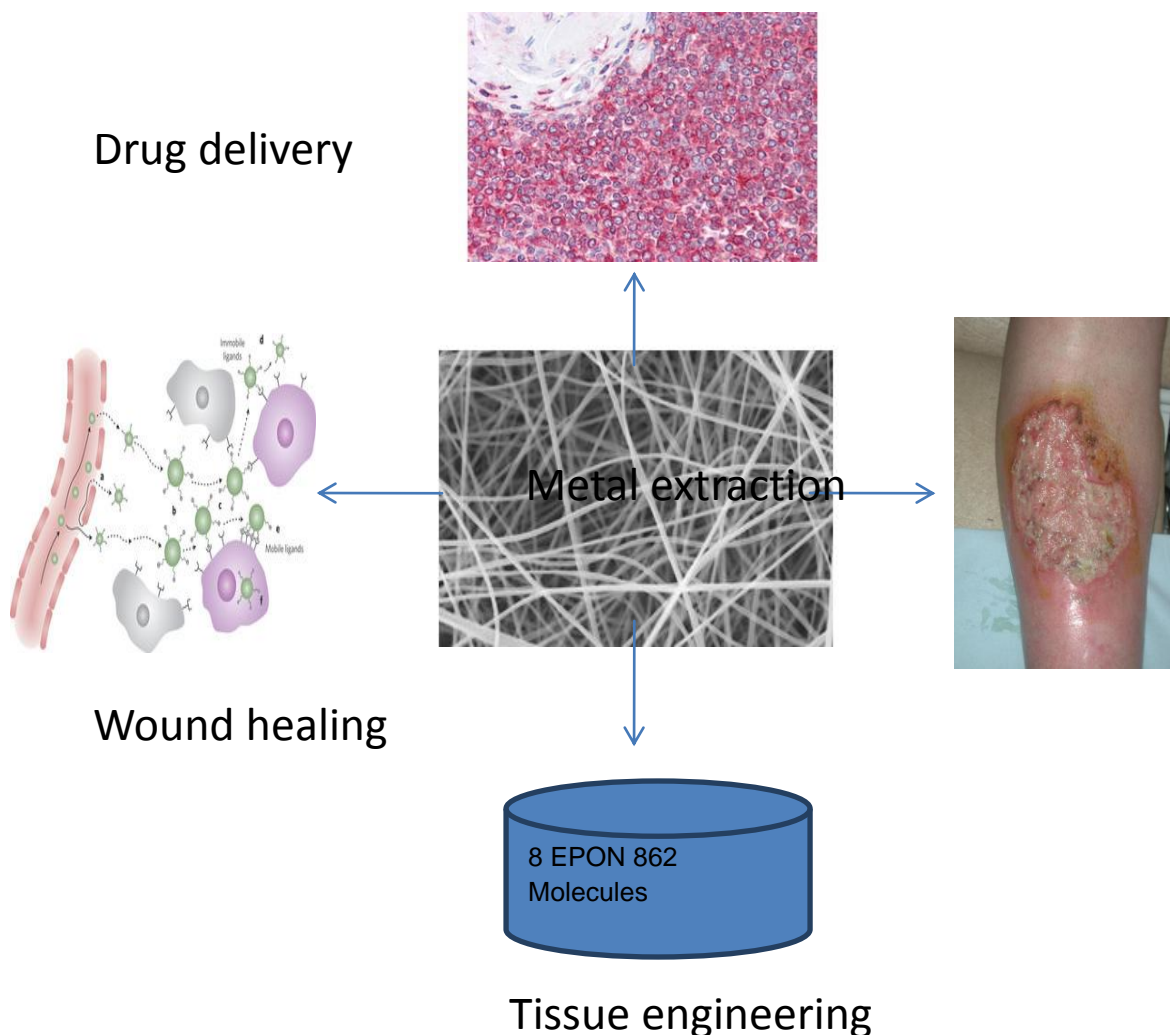
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### **Abstract**

Several methods such as, template-directed, solution-phase growth, melt blown non-woven, nanolithography, self-assembly and electrospinning are used for development of non-woven nanofibers. Among those, the electrospinning is considered to be one of the good methods because it is simple, easy, versatile, controllable, economical and scalable technique to fabricate nanofibers. Currently, electrospun nanofibers are being developed for several applications. The electrospinning method is exploited more for biomedical applications such as, tissue engineering, drug delivery and for wound healing applications because, obtained nanofibers are close resemblance to extracellular matrix (ECM) and hence more compatible. Several biocompatible polymers are being used for fabrication of these materials however, there is always need for new and improved materials for these applications. Hence, in our lab we designed new nanomaterials for their utility in tissue engineering, wound healing and drug delivery applications. In addition, we explored the utility of the developed electrospun nanofibers for industrial applications such as metal extraction. The findings related to these studies will be presented in this talk.



## Conducting Polymer Nanomaterials: Current Development and Opportunities

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### Abstract

Conducting polymers, an attractive subject of research was initiated because of the interesting properties and numerous application possibilities. Conducting polymers nanostructures combine the advantages of synthetic conductors and metallic properties and therefore should yield many interesting physicochemical properties. Nanoparticles can therefore be much more reactive than larger volumes of the same substance. They are relatively cheap and can be manufactured in large quantities. The unique chemical and physical properties of nanoparticles make them extremely suitable for designing new potent applications in number of growing technologies in opto-electronic, telecommunication, sensor, biosensors, biological activity, and catalysis of organic reactions. Present paper review on various aspects of conducting polymers, viz, synthesis, and processing and proposed utility for future scientific and technological applications. Details are provided for the different synthesis methodology used to obtain a high quality, small diameter nano structured materials in large quantities. The effect of various process parameter such as dopant, nature of oxidizing agents, temperatures etc have been studied. A detailed discussion on the mechanism of conductivity of polymer and the factor those influence the structural properties, morphology, conductivity and solubility in common organic a solvent is also included. The important functions provided by polymer nano structured materials included the biological activity, the catalysis of organic synthetic reactions, electrochemical sensor and biosensors. Additionally, this paper addresses recent advances in nanoparticles based chemical sensor, biosensor and summarizes the main functions of polymer nanostructure materials in the biological activity studies.

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**Role of Hydrogen-Bonding and Supramolecular Assembly of Small Molecules  
and Macromolecules**

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**Abstract**

Abstract: Assembly of amphiphilic molecules and macromolecules has been an intense area of research in interdisciplinary domain ranging from biology to materials science. A natural step towards enriching their structural diversity would be to make multiple directional non-covalent forces (H-bonding,  $\pi$ -stacking, CT-interaction) work in tandem. However examples of H-bonding-directed self-assembly of abiotic building blocks in aqueous medium are still rare presumably because of the inherent difficulty associated with competitive H-bonding interaction with the water molecules.

We have recently reported spontaneous vesicular assembly of a naphthalene-diimide (NDI)-based non-ionic bolaamphiphile in water by  $\pi$ -stacking and H-bonding. Site isolation of the hydrogen bonding functionality (hydrazide), a strategy that has been adopted so elegantly in nature, has been demonstrated with perfection to protect them from bulk water so that distinct role of hydrogen-bonding in self-assembly could be realized even in aqueous solution. Further, we showed electron-deficient NDI-bolaamphiphile could be engaged in donor-acceptor (D-A) charge-transfer (CT) interaction with water-insoluble electron rich pyrene donor by perfect intercalation which eventually resulted in rupturing of the membrane to form 1D fiber leading to gelation. Effective pyrene intercalation was also exploited for spontaneous *insitu* multi-functionalization of the vesicular membrane. More recently we have moved to amphiphilic polymeric conjugates of functionalized NDI-chromophores and demonstrated precise role of H-bonding interaction even for dictating self-assembly of large-macromolecules. Our recent results in this area with specific emphasis on optimization of structural parameters of the building block for realizing H-bonding in aqueous medium will be included in this presentation.

**Keywords:** Self-assembly, H-Bonding in Aqueous Medium,  $\pi$ -Conjugated and Polymeric Amphiphiles, Hydrogel.

## **Thermal Characterization of Nanocomposites**

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**Abstract**



The incorporation of fillers and reinforcements has played key role in the polymer industries. Various types of fillers have been added in polymers to provide superlative degree of enhancement to processability and end use properties such as tensile, heat distortion temperature, coefficient of thermal expansion, thermal stability, thermal and electrical conductivities and gas barrier properties. Over the last few decades, the addition of nano-sized particulate and layered fillers in polymers have been found to offer improvements to the above mentioned property with just a minute quantity, typically in the range of 2-5 wt%. Layered silicate layers have been found to be essential in the design and development of nanocomposites to their lamellar elements that have inplane strength and stiffness and high aspect ratio. The clay material has a very high surface area of about 750 m<sup>2</sup>/g (montmorillonite). In the past decade, there has been tremendous interest in carbon nanotubes filled nanocomposites because of unique combination of promising properties. These nanocomposites exhibit the superior mechanical, thermal and electrical properties.

It is a well established fact that due to incorporation of nano-sized particulate/layered/carbon nanotubes in polymer matrix give rise to the decrease in damping (tan $\delta$ ), increase in storage modulus, enhanced glass-transition temperature (T<sub>g</sub>), excellent improvement in thermal stability and variation in many other thermal properties. In the light of the above mentioned thermal properties of nanocomposites, the present talk is devoted to demonstrate the usefulness of various thermal techniques (TGA, DSC, DMA& TMA) for their characterization.

**Key words: Nanocomposites, Layered fillers, CNT's, DMA, TGA.**

## **Polymer Based Nanocomposites for Humidity Sensing Applications**

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**Abstract**

The advancement in science and technology led greater emphasis on the measurement and control of humidity in many areas such as weather prediction, agriculture, industrial, process control, household electric appliances, medical field and research. Depending on the need, humidity sensing is carried out by different methods such as resistive, capacitive or optical. Among these, the sensor devices based on electrical properties such as impedance, resistance or capacitance are best suited to modern automatic control systems. Therefore, electrical detection is the most commonly used method which is based on the change in resistance or capacitance of the sensor on exposure to water vapors. Recently variety of materials such as ceramics, carbon nanotubes, organic/conducting polymers and hybrid polymer/inorganic systems have been extensively investigated and used as humidity sensors based on their capacitive or resistive response. The advantages of polymer based sensors are that they can be used at room temperature in comparison with inorganic sensors which normally operate at high temperatures. Moreover, with amalgamation of nanostructures with suitable polymer, it is possible to control the chemical nature of the composite material, and thereby the selectivity of sensor device, while the physical properties of the nanostructures can be utilized for signal transduction. Secondly, due to the high surface-to-volume ratio of nanostructured materials, a significant number of atoms are located at interface. Therefore, the overall material properties are dominated by surface properties, which can be strongly affected by the interaction with analyte molecule. Polymer based sensors also provides good mechanical properties, ease of processing and high sensitivity but suffers from slow response, low accuracy at high humidity and limited long term stability. These limitations can possibly overcome by incorporating nanostructure inside polymeric system. The present talk covers the synthesis and characterization of metal/polymer nanocomposites based on individual and core-shell Ag and Au nanostructures and their application in humidity sensing.

## **Biodegradable Polyurethane Nanocomposites as Contact and Non-Contact Shape Memory Advanced Materials**

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**Abstract**

Shape memory biodegradable polyurethanes and their nanocomposites are emerging as smart stimuli responsive intelligent materials, which can fix the desired deformed shape and remember their original shape. Shape memory polymers are used in various sectors from artificial muscles to self-disassembling mobile phones including robotic, actuators, self healing, biomedical device, auto-repairing, heat-shrinkable tubes for electronics or films for packaging, etc. In this international conference various aspects of shape memory polyurethane nanocomposites including concept, mechanism, factors, design protocol, processing, characterization, properties, testing and applications will be highlighted. The results of various researchers including the present author's group show that the biodegradable shape memory polyurethane nanocomposites are the most desired materials in this field, especially for biomedical applications. The emphasis will be given on the results obtained from Advanced Polymer and Nanomaterial laboratory of Tezpur University, India, where vegetable oil based biodegradable hyperbranched polyurethanes and their nanocomposites with different types of nanomaterials such as OMMT, functionalized MWCNT, GO, RGO, MNP, etc. have been studied for the said purpose in both contact and non-contact modes. Minimal energy consumption, considerably minimal environmental pollution during production and service and ease of processability, and most importantly the 'nano-effect' are the key guidelines of this work.

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**Polyamide 6-Inorganic/Organo Fillers: Effect of Process Conditions on  
Mechanical and Thermal Properties**

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**Abstract**

Polymers with unique properties can be prepared with addition of nanoparticles usually less than 10% in amount. Nanofibres are the polyfibres which have diameter 500 nm or less, due to this characteristic it possesses specific and unique characteristics such as high specific surface, small pore sizes, and high porosity. Electrospinning has been recognised as an efficient technique for the fabrication of polymer nanofibers. Polyamide-6 is a classic example of it, due to fibrous structures it has low surface roughness, a superior mechanical performance a high liquid absorption capacity and higher wicking rates. It has applications in many field nanofibrous mats for biomedical applications, good filtration due to fibre fineness, protective clothing from eletrospun fibres, good thermal, electrical and optical properties. The polyamide-6 has lead in usability over commonly used polymers due to its unique properties. Optimisation was done in processing regarding technology limitations to prepare PA-6 with better structure for unique property properties to study the limitations of parameters in uniform and steady technique in electrospinning. The ratio of polyamide in a solution is very dominant factor in determining the properties such as fibre diameter and other thermal, mechanical and optical properties. The characterisation of the surface structure and morphology is done by X-Ray Diffraction (XRD), Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Tensile Testing.

**Key words:** Polyamide6, nanofibre, electrospun

## **Self-Assembly and Cargo Release in Comb Polymers Probed By Fluorescence**

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### Abstract

Urethane methacrylate comb polymers having pendant bulky hydrophobic units like tricyclodecane, 3-pentadecyl phenol, pyrene etc, exhibited the ability to self-assemble into vesicles, spheres, rods etc upon drop casting from different solvents. The driving force for the self assembly in such fully hydrophobic polymers is an interplay of extensive hydrophobic interactions of the bulky pendant units with the hydrogen bonding interactions of the urethane groups. Using pyrene as a fluorescent handle the self-assembly in these systems were probed under very dilute conditions and it was established that intramolecular pyrene excimer emission occurred even at very dilute concentrations ( $10^{-6}$  M) as a consequence of the polymer design with pendant pyrene units on every side chain. Random copolymers incorporating pyrene (Py) and 3-pentadecyl phenol (PDP) units as pendants were developed by direct one-pot free radical random copolymerization. These copolymers and corresponding homopolymers spontaneously self-organized into microspheres upon drop casting from solvents like DMF and tetrahydrofuran (THF). Stable microspheres were obtained in water by dialyzing THF solution of the polymers against water in dialysis bags with molecular weight cutoff of  $\sim 2000$ . The hollow nature of the spheres was confirmed by rhodamine B (RhB) encapsulation followed by Förster resonance energy transfer (FRET) based fluorescence emission from RhB upon exciting pyrene. The microenvironment inside the capsule was probed by following the I1/I3 ratio of pyrene emission as well as RhB release as a function of temperature. These results demonstrate a simple approach to produce polymer hollow capsules, and using varying pyrene incorporation the microenvironment inside the capsules could be traced using fluorescence spectroscopy.

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# Oral Presentations

## **Graphene Based Bionanocomposites: Green Materials for Advanced Applications**

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### **Abstract**

There are compelling environmental and economic reasons for using renewable materials like bioplastics in numerous applications and considerable research is now devoted to devising advanced yet green materials with improved performance. Therefore, to improve properties and ability of bioplastics suitable for advanced applications is a vital task. Biobased materials in conjunction with nanotechnology can warrant reliable solution which are set to create new materials of commercial value and will thus be an integral part of the next industrial revolution. In advent of developing new multifunctional bionanocomposites for advanced applications, we have used Graphene as potential nano-reinforcement to the bio-resourced polymers like polylactic acid (PLA). High level of graphene dispersion was achieved by using supramolecular approach. We anticipate that with this new concept it will be possible to provide environmentally benign green material with tunable properties like thermo-electric conductivity, thermo-mechanical stability, gas barrier and biodegradability under specific conditions. Such materials offer an enormous potential for advanced applications in e.g. electronics, automotive, construction, packaging etc. and also expected to offer green and sustainable alternative to the conductive composites based on plastics from petroleum resources.



## Dimensional Control of Solvent Vapor Induced Lamellar PS-B-P4VP Nanopatterns

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### Abstract

Diblock copolymer (BCP) self-assembly at interfaces enables the generation of nanoscale structures in a parallel, scalable, bottom-up fashion with vast applicability in the nanofabrication industry[1]. The high Flory-Huggins parameter ( $\chi \sim 0.18$ ) of PS-b-P4VP at room temperature makes it an ideal BCP system for self-assembly and template fabrication in comparison to other BCPs. Such high  $\chi$  BCP system requires precise fine-tuning of interfacial energies achieved by surface treatment and that improves the wetting property, ordering, and minimizes defect densities. Herein, we describe the microdomain orientation of different PS-P4VP BCP (20k-17k, 9.8k-10k, 7.4k-7.7k and 5k-5k) thin films on silicon substrate induced by solvent vapor annealing. The effects of the casting and annealing solvents, annealing temperature and time etc. have been demonstrated in terms of ordering, pitch size and coverage of the film on substrate. The substrate is covered with sub-20 nm features with perpendicular lamellae of thickness around 30 nm. No surface treatment is required to microphase separate the blocks. While the substrate surface were also modified with polystyrene and ethylene glycol brushes which form self-assembled monolayer on substrate in a simple way to study the consequences on the wetting property of the BCP, ordering and coverage of the thin films.

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## In vitro investigation on PS: PLA and PS: PLA: OMMTNanocomposites Using Fungal Strain

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### Abstract

The environmental issues related to the synthetic polymers have been resolved using biodegradation under controlled conditions. The polymeric composites of a) polystyrene (PS) and poly (lactic acid) (PLA) (PS:PLA), and b) PS: PLA filled with organically modified montmorillonite (OMMT) (PS:PLA:OMMT) were prepared. Initially, PS was dissolved in benzene (10:90) and allowed for overnight digestion. PLA was synthesized using L-lactic acid under controlled ultrasonic cavitation technique and dried at 100 °C for 15 minutes to make it moisture free and then mixed with the PS solution. Meanwhile, the surface of montmorillonite (MMT) was modified using column chromatographic technique, due to this d-spacing was improved (22 Å). A variable amount of PLA (10, 15, 20, 25, & 30 %) and OMMT (0.5 to 5 mass %) was used for the preparation of PS:PLA composites and PS:PLA:OMMT nanocomposites, respectively under controlled sonication. The sheets (5 X 5 cm) of PS:PLA and PS:PLA:OMMT were subjected to degradation in minimal medium using *Phanerochaete chrysosporium* microorganism under controlled conditions for 28 days. The growth of microorganism and fractures inside the polymer matrix before and after degradation was observed using scanning electron microscopy (SEM). Moreover, change in extra cellular protein content, biomass production and % degradation with respective time (up to 28 days) of incubated samples were also studied.

**Keywords:** Biodegradation, Poly (lactic acid) (PLA), and *Phanerochaete chrysosporium*.

## Biodegradable Bioepoxy Resin from Mahua oil

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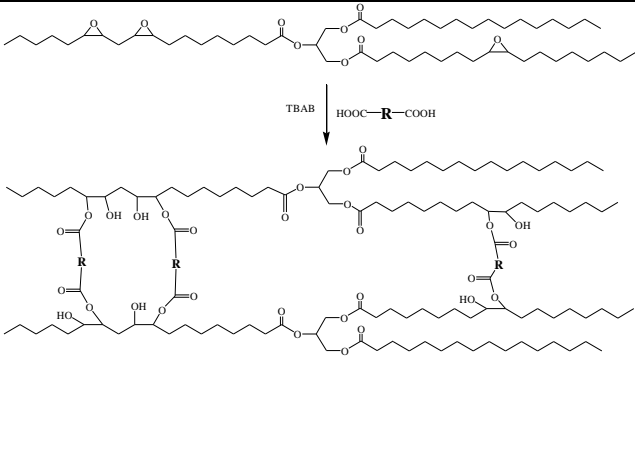

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### Abstract

Polymers derived from renewable resources are gaining a great interest due to rarefaction of fossil raw material and environmental issues related to fossil based products. Among the renewable resources available in the world plant product rank very high. Vegetable oil attracted attention toward the material science due to great versatility due to functional group like ester, hydroxyl and unsaturation i.e. presence of double bond. In the recent years development of bio based material from vegetable oil is the very important because vegetable oil are good raw material for development of new polymer, chemicals and biodiesel.

Mahua tree is locally grown in marathwada region of Maharashtra. Mahua oil contains the suitable lipid profile for further functionalization to get different polymers. Epoxidation of Mahua oil is a industrial process can be carried using peracetic acid. Triglycerides (fatty acids) are aliphatic in nature. The advantage of aliphatic epoxy resins is their high reactivity, flexibility, and resistance to UV light. In the present study we have attempted to obtain epoxy mahua oil which was further reacted with diacids like citric acid forming epoxy resin. The fully biobased epoxy was able to get good transparent thin films from solution casting and is completely biodegradable within 15days using soil bacteria in bacterial consortium broth culture. The various properties of biobased epoxy resin have been compared with petroleum analogues. Mahua oil is valuable source of making biodegradable polymers for various applications which will find value added products and can generate the local industry based on agriculture.

	
<p>Reaction between epoxy mahua oil and diacid forming bioepoxy resin</p>	<p>Photo showing progressive stages of biodegradation of epoxy resin film from mahua oil</p>

**Key words:** Mahua oil, bio-epoxy resin, citric acid, tartaric acid, biodegradation

## Synthesis and Characterization of Water Soluble CdSe/ZnS Q-Dots for Biomedical Applications

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### Abstract

Fluorescent quantum dots (Q-dots) are promising candidates for imaging, diagnostic and therapeutic applications. In the recent years, numerous attempts have been made out to synthesize these Q-dots in aqueous medium. CdSe Q-dots are one of the important II-VI semiconductors used for life science applications. However, the bare nanocrystalline semiconductors have surface defects, which need to be passivated using an outer coating, which can be organic or inorganic. The organically capped nanocrystals may still have a large number of surface sites, which quench luminescence to some extent. Inorganically capped core-shell quantum dots have been proposed as an alternative to the organically capped quantum dots for enhanced luminescence efficiency. Core-Shell (CS) nanocrystals have been prepared by passivating the surface of a narrow gap semiconductor core with a shell of wider band gap material. The overall benefit visualized enhanced luminescence efficiency and stability.

Present study aims to modify the thioacid capped CdSe Q-dots surface by ZnS coating by direct synthesis in aqueous medium. Characterization of wet chemically synthesized CS was carried out using photoluminescence (PL) spectroscopy, X-ray diffraction (XRD), Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS). CS formation was confirmed by red shift as well as enhancement in the luminescence peak compared to bare Q-dots. Effects of processing parameters during the shell preparation such as core concentration and sulphur concentration on the PL properties of CS have been studied. Processing parameters have been optimized at maximum luminescence efficiency. DLS studies showed the Q-dots and CS to be stable even after aging for 8 days. Cytocompatibility and hemocompatibility behavior was found to be better for CS compared to their bare Q-dots counterpart after evaluation. Cytotoxicity of CS has been further evaluated by changing the sulphur concentration and after aging for 8 days.

## Synthesis and Thermal Studies of Fumed Silica / Polybenzoxazole Nanocomposites

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### Abstract

Novel nanocomposites of fumed silica and polybenzoxazole (PBO) have been prepared by two step thermal conversion of hydroxyl containing polyimides to PBO. This two step PBO synthesis has been successfully used to fabricate PBO films and their nanocomposites over the past decade. These find use in microelectronic industry, buffer coatings in IC chips, substrates for flexible printed circuit boards and high end electronic packaging material. Different proportions of silica have been mixed with polyhydroxyamide (PHA) precursor and subsequently subjected to ring closure to form PBO nanocomposites. These PBO films and their nanocomposites have been characterized by Infra-red Spectroscopy and Nuclear Magnetic Resonance and their thermal properties are studied by DSC, TGA and TMA.

**Keywords:** polybenzoxazole, nanocomposite, thermal analysis.

## Porous And Crosslinked Cellulose Beads for Toxic Metal Removal-Hg(II) Ions

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### Abstract

Heavy metal poisoning is one of the major threats to the ecosystem. Mercury which is a heavy metal poses threat to the ecosystem when it gets deposited in the environment. Mercury is one of the highly toxic and hazardous pollutants even in trace amounts and compared to other heavy metals, mercury even at low concentrations is highly neurotoxic. According to USEPA standards, mercury content in drinking water should not exceed 2.0ug/L and the permitted discharge level of mercury in waste water is 10.0ug/L. So it becomes necessary to remove it from the aqueous systems which has been a subject of interest for researchers for a long time now. In this study, we have synthesised highly porous and cross-linked cellulose beads magnetised with ferric oxide to remove Hg(II) ions from aqueous systems by the process of adsorption. These beads are prepared by solution polymerization using different solvents viz DMSO and N,N-Dimethyl Acetamide:Acetone. The beads were characterised using FTIR and SEM for functional group determination and surface morphology respectively.

Various parameters affecting adsorption such as pH of the solution, percentage of ferric oxide, dose, time and concentration of the Hg(II) ions were all investigated. Optimum pH for the maximum amount of uptake of Hg(II) ions is found to be pH 6.0. Among various w/w % of Fe<sub>2</sub>O<sub>3</sub> (1w/w% - 20w/w%), the beads with 5w/w% of Fe<sub>2</sub>O<sub>3</sub> were found to adsorb maximum amount of Hg(II) ions from aqueous solutions which can be correlated to the degree of dispersion of Fe<sub>2</sub>O<sub>3</sub> particles in the polymeric matrix. As the percentage of Fe<sub>2</sub>O<sub>3</sub> in the beads increased, adsorption also increased till 5w/w% and further increase in the percentage of Fe<sub>2</sub>O<sub>3</sub> had no effect on the adsorption since the degree of dispersion of Fe<sub>2</sub>O<sub>3</sub> in the polymeric solution was good upto 5 w/w% of Fe<sub>2</sub>O<sub>3</sub>. But beyond 5w/w% of Fe<sub>2</sub>O<sub>3</sub> it was observed that Fe<sub>2</sub>O<sub>3</sub> particles agglomerated. Also it was noticed that beyond 5w/w% of Fe<sub>2</sub>O<sub>3</sub> in the solution, the viscosity of the solution increased drastically. Time dependant study of intake of Hg(II) ions by polymeric beads from aqueous solutions of Hg(II) ions with different initial concentrations was

carried out and the concentration of Hg(II) ions was monitored spectrophotometrically using UV-Visible Spectrophotometer. Various isotherm models were tested among which Freundlich adsorption isotherm was found to be suitable. The process of adsorption followed pseudo second order kinetics.

Eventhough there is no much difference in the results using beads prepared with DMSO and N,N-Dimethyl Acetamide:Acetone as solvents, the ecofriendliness of the N,N-Dimethyl Acetamide:Acetone system makes it a better solvent to be used commercially. These beads which are formed from a natural material, Cellulose, can find good applications in removing Hg(II) ions from aqueous systems.

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## Nano-Calcium Carbonate (CaCO<sub>3</sub>)/Polystyrene (PS) Core-shell Nanoparticle: It's Effect on Properties of High Impact Polystyrene (HIPS)

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### Abstract

Rheological, thermal, mechanical and morphological properties of core-shell [Calcium carbonate (CaCO<sub>3</sub>)/Polystyrene (PS)]/High impact polystyrene (HIPS) as well as bare nano-CaCO<sub>3</sub>/HIPS nanocomposites with different wt% loading were investigated in this paper. All composites were prepared individually by incorporating nano-CaCO<sub>3</sub>/PS hybrid nanoparticles and bare nano-CaCO<sub>3</sub> with 0.10-5.0 wt% loading on Brabender Plastograph. It was shown from the experimental results that rheological, thermal, mechanical and morphological properties were improved as hybrid nano-CaCO<sub>3</sub>/PS particles reinforced in HIPS matrix. The interaction between nano-CaCO<sub>3</sub> particles and HIPS matrix was significantly improved when the nano-CaCO<sub>3</sub> nanoparticles were grafted with PS. SEM (scanning electron microscope) and AFM (atomic force microscope) images showed a perfect dispersion of the nano-CaCO<sub>3</sub> particles in PP matrix.

*Keywords:* Core-shell nanoparticles; High impact polystyrene (HIPS); Thermal properties; Rheological properties; Mechanical properties

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## Detection of Some Lung Cancer Biomarkers with Quantum Resistive Vapour Sensors Made of Functionalized $\beta$ Cyclodextrin - Reduced Graphene Oxide

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### Abstract

Cancer kills more than seven million people every year. The current 5-year survival rate for lung cancer is 15 %, but this rate may rise to 49 % if the cancer could be diagnosed when it is still localized [1]. Since the survival of cancer patients depends on early detection of tumour cells, developing technologies applicable for rapid and effective differentiation between cancer and normal cells is an important challenge for the cancer researchers. The analysis of specific VOC in exhaled breath (defined as biomarkers of specific disease) can provide non-invasive and potentially inexpensive anticipated diagnosis of lung cancer, as the breath extract of lung cancer patients are found to display elevated levels of several volatile organic compounds (VOC), mostly C<sub>4</sub> to C<sub>20</sub> monomethylated alkanes, in addition to certain benzene derivatives [2, 3].

In the present study, a novel chemo-resistive vapour sensor, comprising of functionalized  $\beta$  cyclodextrin-reduced graphene oxide hybrid transducer has been developed.  $\beta$  Cyclodextrin modified graphene can be considered as a functional hybrid material which can take combined benefits of high specific surface and good electrical conductivity of graphene as well as host-guest inclusion complex formation ability and variable selective chemical modification possibility of  $\beta$  cyclodextrin. The key goal of this present work is, to be able to tune the molecular selectivity of  $\beta$  cyclodextrin modified graphene based sensors by utilizing the specific chemical functionality on  $\beta$  cyclodextrin and finally to construct a high performance chemical sensor with distinct selectivity for a targeted lung cancer biomarker VOC.

**Key Words:** Functionalized  $\beta$  cyclodextrin; Lung cancer biomarker; VOC Detection; Graphene; Quantum Resistive Sensor;

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## Recent Trends in Functionalised Polymer Systems for Industrial Applications

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### Abstract

The study of functionalised polymer system offers numerous opportunities in basic science and engineering applications. Polymer surfaces can be engineered to achieve specific goals on its properties like adhesion, wettability, friction, chemical resistance and absorption. Our research area specifically focuses on the properties of functionalised polymer systems for medical, waste water treatment, coating and defence applications. Functionalised polymer system with Poly vinyl alcohol and natural herbs like azadirachta indica, curcuma longa etc, is significantly effective against the *E.coli*, *P.monas* and *S.aureus* bacteria and found to be a promising candidate for the treatment of injuries, burns in medical field. Laboratory studies of surface modified cellulose with iron oxide proved to be cost effective and more capable of adsorbing metal ions from waste water and thereby reducing the hazardous impact of these metal ions on our environment. Our demonstration of hydrophobic coatings based on modified polystyrene system from waste polystyrene products, shows very impressive results in coating applications in marine field and is eco friendly. We are working on functionalised healing system containing nano reinforcing agents that can heal composites under room temperature, when subjected to cracks. We are also developing anti slash gels that respond to sudden impact by locking the functionalised polymeric system into solid form, which can be extended to ballistic fabrics. These developments in functionalised polymer systems open a new window to explore and utilise their capabilities to tailor for industrial applications.

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## Polymeric Coatings from Vegetable Oils as Renewable Sources

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### Abstract

Preparation of polymers from renewable resources has found great potential in a variety of industrial applications and can contribute to sustainable development in the future due to the environmental concerns, hike of prices and depleting of petroleum resources. Therefore exploration of renewable and non-conventional raw materials for preparation of polymers is one of the prime targets to researchers. Cellulose and vegetable oils are the most important and largely available raw materials to substitutes for petrochemicals in preparation of polymers. Vegetable oils are triglycerides of fatty acids and properties of oil are decided by the composition of fatty acids present. Normally linseed, cotton seed, rice bran, nahar seed, etc. were the oils of focus for preparation of coatings. Due to their varying properties and possibility of easy conversion into resins, they are used as polymeric resins suitable for paint and coatings applications. Basic forms of vegetable oils used as polymeric binders cover alkyd resins, epoxy resins, polyurethane resins, polyesters, polyesteramides, etc.

Vegetable oils are abundantly available as far as India is concerned. In the present study, cottonseed, linseed, coconut, rice bran, sunflower and castor oils based one and two pack coatings have been prepared and their performance tested in terms of coating properties, thermal stability and chemical resistance.

In the present study waste cooking oil from (university canteen) has been used to obtain epoxy vegetable oil which was further reacted with different diacids like citric acid, tartaric acid, succinic acid, sebacic acid and glycine forming epoxy resin. The fully biobased epoxy was able to get good transparent thin films from solution casting and is completely biodegradable within 2 - 5 weeks using soil bacteria in culture. The various properties of biobased epoxy resin have been compared with petroleum analogues. Waste cooking oil is valuable source of making biodegradable polymers for various applications.

## Preparation and the study of Zinc Polyacrylate Cement: Dental Cement Behavior and properties

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### Abstract

The solution polymerization method at 90<sup>0</sup>C was performed for the synthesis of Polyacrylic acid (PA) and the deactivated Zinc Oxide (ZnO) was obtained by heating at 1000<sup>0</sup>C and powdered. These powdered pre-materials were used for the development of the dental cement. The deactivated ZnO powder (approx. 75mm particle size) mixed with 40% aqueous polyacrylic acid with ratio of 1.5:1 (powder: liquid) to develop the polycarboxylate cement. The polyacrylic acid and polycarboxylate cement were characterized by TGA, DTA, FTIR, SEM and XRD studies. The viscosity average molecular mass of polyacrylic acid was determined for better result. The thermal stability of the polymer and the cement was evaluated by analyzing the TGA data. Which provides the various kinetic parameters like activation energy, Arrhenius (frequency) factor and entropy changes associated with the thermal decomposition of polyacrylic acid and polycarboxylate cement. It is inferred from the DTA and XRD data that incorporation of Zn<sup>2+</sup> ions (from ZnO) significantly enhanced the degree of crystallinity in the polycarboxylate cement. The setting time, compressive strength and diametral tensile strength of polycarboxylate cement was evaluated in this research article.

Keywords: Polyacrylic acid (PA), Zinc Oxide, Dental cement, TGA, DTA, FTIR, SEM and XRD

## Synthesis of Novel Quaternary Ammonium Polymerizable Surfactants from Tertiary Amines, Long Chain Alkyl Maleic Hemiesters, and Epoxy Resins

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### Abstract

The quaternary ammonium polymerizable surfactants (QAPS) are known for their wide industrial applications. The QAPS with long alkyl chains has got biocidal property. Mostly the long alkyl chain is attached to the amine group making the QAPS to have its own limitations in biocidal effect. But, a new synthetic route has been disclosed where the long alkyl chain is linked to other functional groups which are then linked to the tertiary amines hence forming QAPS. These surfactants have well exposed quaternary ammonium groups making them much more lethal towards the microbes.



## Studies on Design and Development of Gastro sparing Chimeric Derivative of Biphenylacetic Acid

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### Abstract

Rheumatoid Arthritis (RA) is an autoimmune disease characterized by chronic inflammation of multiple joints. In spite of severe GI side effects; NSAIDs are still used as the mainstay treatment for RA. Prostaglandin inhibition and local irritant effect due to free carboxylic group are the two major mechanisms of GI toxicity. Many prodrugs are reported in literature to overcome GI toxicity of NSAIDs.

The present work focuses on design and development of carrier-linked chimeric prodrug of biphenyl acetic acid and D-phenylalanine (BP-1) with the objectives of reducing its ulcerogenicity, enhancing its anti-inflammatory activity and bioavailability.

BP-1 was stable in HCl buffer & stomach homogenate. In phosphate buffer BP-1 furnished 33% BPA, in small intestinal homogenates 42% BPA and in 80% human plasma 56% BPA, over a period of 8 h. *In vivo* release studies of BP-1 in blood indicated 40 % release of BPA over 24h indicating delivery of intact prodrug to colon where it might have hydrolyzed by N- acyl amidases resulting in the release of BPA that might have entered into systemic circulation after absorption through colonic mucosa. 3.5% of BPA was observed in 24h urine and feces.

BP-1 exhibited better analgesic, anti-inflammatory and anti-arthritic activity than BPA and fenbufen, individual amino acids and physical mixture in various acute and chronic models of arthritis. BP-1 significantly decreased bone loss, showed organ protective effects and also restored the altered haematological profile. The prodrug had excellent gastro-sparing profiles than BPA, fenbufen and physical mixture.

## Studies on P-Aminosalicylic Acid-B-Cyclodextrin Conjugate for Colon Specific Delivery

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### Abstract

Cyclodextrins find extensive use in drug targeting to colon either in the form of solid inclusion complexes or sterically hindered prodrugs. We give here an account of the synthesis, *in vitro* release kinetics of the  $\beta$ -cyclodextrin prodrug of p-aminosalicylic acid and its pharmacological evaluation in 2, 4, 6-trinitrobenzenesulphonic acid- induced colitis in rats. Protection chemistry and CDI coupling were used for the synthesis of this prodrug after which it was subjected to characterization by IR, <sup>1</sup>H-NMR and LC-MS. *In vitro* stability and release characteristics were assessed in buffers (pH 1.2 and 7.4), stomach/small intestinal homogenates and rat cecal/fecal matters. The prodrug withstood pH-dependent hydrolysis. The extent of release in stomach and small intestinal homogenates was 20-23% while substantial release (68% and 92%) was observed in rat cecal and fecal matters. The alleviating effect of 4-A $\beta$ Cyd on colitis was moderate when judged against sulfasalazine or 4/5-ASA given rectally, but it was similar to that of aminosalicylates given orally, implying that the delivery of 4-ASA to the colon is incomplete due to partial hydrolysis of the prodrug in the upper GIT. The histological evaluation of the pancreas and the liver of the prodrug-treated animals demonstrated no pathological changes signifying its improved safety profile as compared to that of sulfasalazine or oral 5-ASA. The prodrug resulted in noteworthy reduction in ulcer index when compared to aminosalicylates insinuating significant enhancement in gastro-protective effect than oral aminosalicylates.

## A facile one-pot Reactive Solution Blending Approach for Main Chain Donor-Acceptor Polymeric Materials

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### Abstract

A high temperature solution blending process has been used to synthesize a series of copolymers incorporating varying mole ratios of Perylenebisimide (PBI) into the backbone of an engineering thermoplastic polyester [Poly(1,4-cyclohexylenedimethylene-1,4-cyclohexanedicarboxylate)] (PCCD). A random donor-acceptor copolymer incorporating oligo(p-phenylene vinylene) (OPV) and PBI was also synthesized. The chemical incorporation of these chromophores into PCCD was confirmed by carrying out the melt condensation using 1,4-cyclohexanedimethanol (CHDM) and 1,4-dimethylcyclohexane dicarboxylate (DMCD) with hydroxyl functionalized PBI and OPV derivatives. The PBI polymers produced using the two different approaches exhibited structural variations. Polymers synthesized using solution blending approach possesses the required thin film processability for organic solar cell where they can replace the poor film forming fullerene derivatives as the electron acceptor and transport material in plastic solar cells. The covalent incorporation of both donor and acceptor moieties are also expected to improve the morphology of the resultant polymer. Thus the reactive solution blending approach to covalently incorporate the desired chromophores into high molecular weight polymer backbones has the potential to develop polymers for applications like organic solar cells and luminescent solar collectors.

## A New Approach for Degradation and Stabilization Study of Proton Exchange Membranes Applicable in Fuel Cells

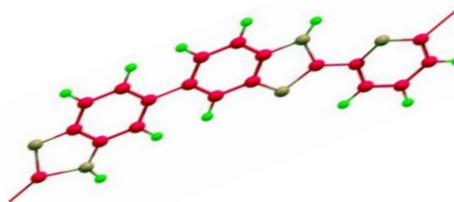
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### Abstract

Fuel Cells are high energy efficient devices without emission of green house gases. Polybenzimidazole membranes have emerged as the promising polymer material for high temperature fuel cells. There are various derivatives of PBI have been synthesized and reported in the literature. We report here a new approach to study degradation and stabilization of Proton Exchange Membranes (PEMs). Thermal and photo treatments were given to the aromatic derivatives of PBI membranes. The stability of these membranes was tested and the results were correlated to the fuel cell performance.



It has been observed that the conditions of fuel cells are very similar (oxidizing) to those generated by thermal treatment and SEPAP 12 Instrument. All the aromatic derivatives of PBI membrane were thermally treated and photo-irradiated and characterized by using FT-IR, NMR, XRD, SEM and Contact angle measurements to monitor the changes occurred by UV-irradiation. The correlation between thermal-photo and Fenton's results were also made and summarized. It has been found that thermal-photo degradation is a good technique to evaluate the performance of fuel cell membranes. The results show that all membranes suffer by thermal-photo-irradiation treatment and develop nano-dimensional structures may result in performance deterioration of fuel cells.

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## PVA Porous Membrane for Antibacterial Application

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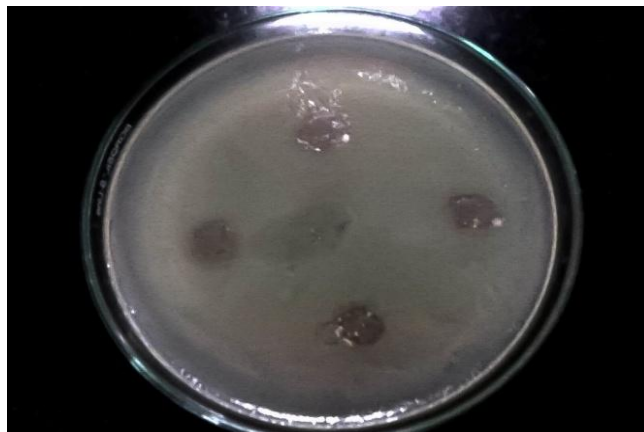
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### Abstract

Most textile materials currently used in military are conducive to cross-infections or the transmission of diseases caused by microorganisms. These infections are mainly caused by Gram positive *Staphylococcus aureus* (*S. aureus*), *Bacillus subtilis* (*B. subtilis*), and Gram negative *Pseudomonas aeruginosa* (*P. aeruginosa*) and *Escherichia coli* (*E. coli*). To avoid infections, antimicrobial properties can be imparted to textile material by incorporating functional agents in fibers and fabrics. Usually, antibacterial loading in micro/nanoparticle can be achieved by incorporating additives during the preparation of the particles or after the formation of the particles by incubating additives with fibers. The ability to fabricate a variety of antibacterial constructs with the different morphology such as films, gels, foams, patches and fibers contributes to a broad application spectrum of the biomaterials.

In this study, high molecular weight poly(vinyl alcohol) (PVA) fiber of the diameter 70-80  $\mu\text{m}$  were prepared by adding antibacterial additives like curcuma longa, mangiferaindica, azadirachta indica, Cu nano particles,  $\text{TiO}_2$  and  $\text{ZrO}_2$ . Known concentration of antibacterial additives was solution mixed and viscosity of the solution was tailored such that a fiber can be produced by nozzle. Simultaneously, inexpensive and biofriendly foaming agents like sodium chloride and sodium bi-carbonate etc were added to impart porosity on fiber for improving its efficacy of nano/micro additives for antibacterial properties. Beyond 2 Wt% loading of nano/micro additives like curcuma longa, mangiferaindica, azadirachta indica, Cu nano,  $\text{TiO}_2$  and  $\text{ZrO}_2$ , the melt strength of PVA was affected, which resulted in poor fibers. Agglomeration of the additives in the fiber was also noticed. Antibacterial assessments were carried out against *E. coli*, *S. aureus* and *P. aeruginosa*. Filter paper disk method was used to determine the area of zone of inhibition formed by fibers. The obtained result showed that azadirachta indica possessed larger zone of inhibition compared to other additives as shown in figure-1.



## Nanofibers

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## Biodegradation of Medical Plastics Using Sewage, Muncible, and Radioactive Wastes: The Future Dream Challenge

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### Abstract

Since the world is suffering from huge wastes amount such as medical plastic, radioactive, municipal wastes and spend a lot of money for treating them separately. It will be a wonderful aspect to use technology to separate radioactive wastes as a source of gamma radiation which is used for irradiating plastic waste and use the municipal waste to prepare compost by optimal growth of microorganisms to consume the medical plastics via biodegradation technique. It will be a brilliant method to get rid of the three hazardous wastes, which the world is suffering from, eradicate themselves miraculously. Our previous studies aimed to investigate the biodegradation of  $\gamma$ -irradiated polyolefins in composting and microbial culture environments at both; low and high  $\gamma$ -radiation doses. It was found that the biodegradation increases with the increasing the dose of  $\gamma$ -irradiation and time of incubation in compost. A similar study was carried out by using different  $\gamma$ -dose rates (600 and 780 kGy/h<sup>-1</sup>). It was found that the biodegradation increases with the decreasing dose rate of  $\gamma$ -radiation source. It was concluded from the previous studies that the pretreatment of  $\gamma$ -irradiation can accelerate the biodegradation of neat polymer matrix in biotic conditions significantly. Films of isotactic polypropylene, high density polyethylene and ethylene-propylene (EP) copolymer were irradiated under  $\gamma$ -radiation with doses of 0, 10, 25, 50, 75 and 100 kGy. Two different <sup>60</sup>Co sources were used with dose rate 600 and 780 Gy h<sup>-1</sup>. Neat and irradiated samples were incubated in compost and fungal culture environments. The changes in functional groups, surface morphology and intrinsic viscosity in polymer chains were characterized by FT-IR spectroscopy, SEM and viscometric measurements, respectively. It was observed that both  $\gamma$ -degradation and biodegradation processes depend on the dose rate of  $\gamma$ -source and irradiation dose. The correlation between biodegradation time and different doses was obtained. The previous studies based on using the sewage, food, paper wastes for preparing the biological compost and the radioactive wastes as a source of gamma radiation. The possibility of this idea was discussed to be a valuable solution to treat the

medical plastics wastes which cannot recycle. This idea may also solve the accumulation problem of the different wastes.

**Key Words:** Polyolefins,  $\gamma$ -irradiation dose,  $\gamma$ -dose rate, Biodegradation, Composting and Fungal Culture.



## Processing and Characterization of Epoxy- Graphite nanocomposites

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### Abstract

In this paper, the composites were prepared by mixing epoxy resin and graphite in varying proportions by weight of resin. Aliphatic amine was used as an accelerator to improve the interfacial adhesion between the graphite filler and matrix. The experimental study relating to the morphological and mechanical properties of graphite filled epoxy composites was carried out. The study revealed that the properties of the composites mainly depended on dispersion condition of filler particles, particle size and aggregate structure. The epoxy graphite composites showed improved tensile modulus and Young's modulus in bending properties with increasing filler content.

Keywords: Graphite nanoparticles, epoxy resin, XRD, SEM, Mechanical properties

## Health Monitoring In Core Of Poly(Epoxy)/Glass Fibre Composites With Conductive Polymer Nanocomposite Piezo-Resistive Sensors

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### Abstract

Polymer composites are developing faster than ever in the transportation field due to the strong demand for materials with high performance/weight ratio [1]. Nevertheless, one of the brakes for this development is the lack of predictability of their damage under severe conditions such as crash or fatigue. Nanotechnology has brought about new prospects to monitor composites' health in order to anticipate their dramatic destruction and thus to improve their reliability. In case of glass fibre reinforced plastics (GFRP), all components being electrically insulating, it is possible to structure a conductive network by percolating carbon nanotubes (CNT) in the polymer matrix [2] or in fibres' sizing [3] that can be used to sense crack initiation and propagation. Construction of novel smart piezo resistive sensors about 0.5- 1.5  $\mu\text{m}$  thick, directly on E-glass fibre surface by spray layer by layer (sLbL) technique has been described in this study. Different strategies of piezo-resistive sensing in GFRP are compared in terms of efficiency to follow mechanical solicitations and damages in both elastic and plastic domains. The electrical response of the smart CPC sensor to the accumulated damage combined with the acoustic emission (AE) technique and microscopy are utilized to sense damage initiation and propagation in laminated composites.

**Keywords:** GFRP; Health; Monitoring; CPC; Conductive Polymer nanoComposites; CNT; piezo-resistive; Acoustic Emission

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## Highly Crystalline Nanostructured Comb Polymer of Perylenebisimide by Directed Self-Assembly

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### Abstract

Well defined nanostructured polymeric supramolecular assemblies were formed when an unsymmetric perylenebisimide substituted with ethylhexyl chains on one end and functionalized with 3-pentadecylphenol at the other termini (PDP-UPBI) was complexed with poly (4-vinylpyridine) (P4VP) via a non-covalent specific interaction such as hydrogen-bonding. The resulting P4VP(PDP-UPBI)<sub>n</sub> complexes were fully solution processable. The bulk structure and morphologies of the supramolecular film were studied using small angle (SAXS) and wide angle X-ray scattering (WAXS) which revealed the highly crystalline nature of the complex. Thin film morphology of the 1:1 complex analyzed using transmission electron microscopy (TEM) showed uniform lamellar structures in the domain range of 5 – 10 nm. In short, a simple and facile method to obtain spatially defined organization of n-type semiconductor perylenebisimide molecules using hydrogen bonding interactions with P4VP as the structural motif is showcased herein.

## AB-Diblock Polymeric Vesicles and their Encapsulation Capabilities

**Smita Kashyap and M. Jayakannan**

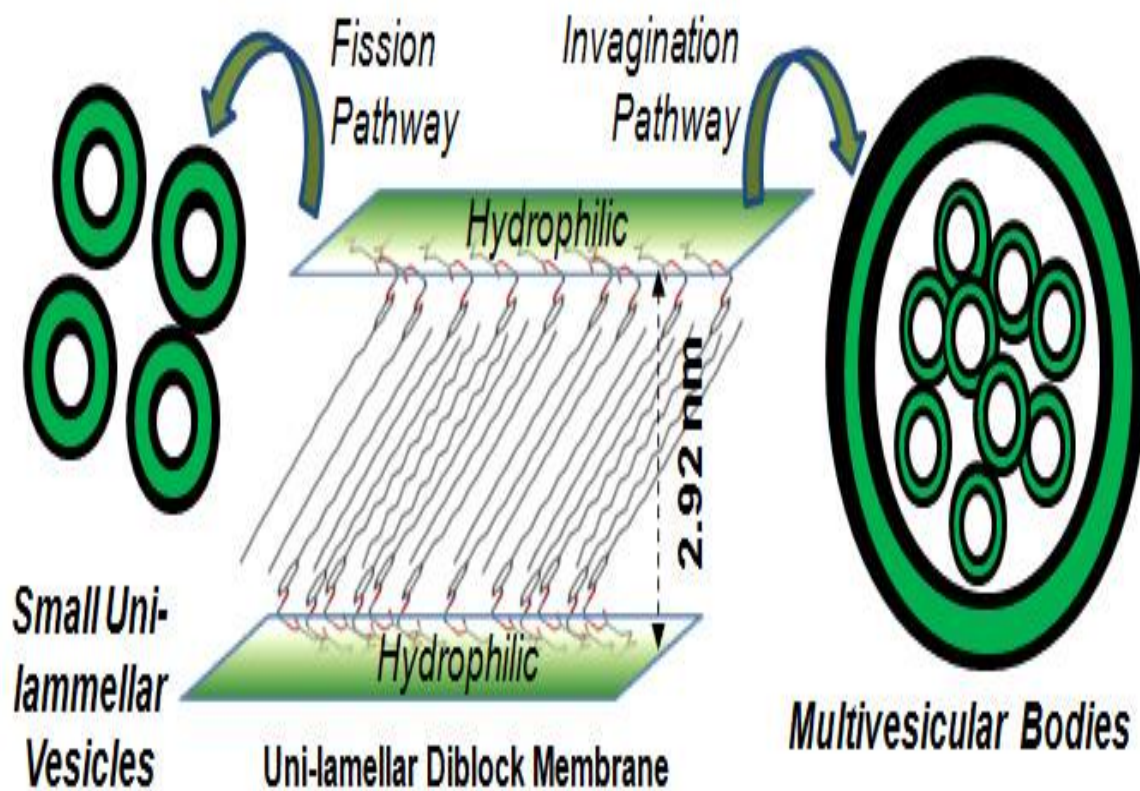
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### Abstract

In the regulation of several physiological processes under tightly controlled signaling pathways across the biological cell membranes multivesicular bodies (MVB)s are very important key-intermediates.<sup>1</sup> Synthetic A-B diblock sorting into multivesicular bodies (MVB)s, their fluorophore encapsulation pathways as well as their drug encapsulation capabilities are studied. Renewable resource based diblock having hydrophobic units and flexible hydrophilic polyethylene glycols (PEG) were custom designed for the above purpose.<sup>2</sup> The formation of uni-lamellar layer-like self-assemblies due to existence of strong inter-molecular interactions was proved by resolving single crystal structures. These amphiphilic AB diblocks produced small uni-lamellar vesicles (SUV)s or MVBs, by undergoing selective vesicular fission either by outward budding or inward invagination, respectively. Based on theoretical models, self-organization parameters such as relative volume ( $v_e$ ) and reduced area difference ( $\Delta a_e$ ) were determined and very good correlation with the experimental results was established for the synthetic-MVBs and SUVs. The mechanistic aspect of MVB formations was studied by encapsulating pyrene. In the pyrene dynamic excimer formation with respect to the sorting of diblock membrane into MVBs an unusual non-linear trend was observed. Strong inter-molecular interaction was found to be a critical deciding factor in synthetic diblock membrane to facilitate MVBs. The encapsulation capabilities of MVB and SUV were determined by encapsulating an anticancer drug, Camptothecin. MVBs found to be more efficient than SUV in encapsulating the drug. Hence, MVBs are potential vectors for drug delivery.



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## Conjugated Polymer-Lanthanide Hybrid Temperature Sensors

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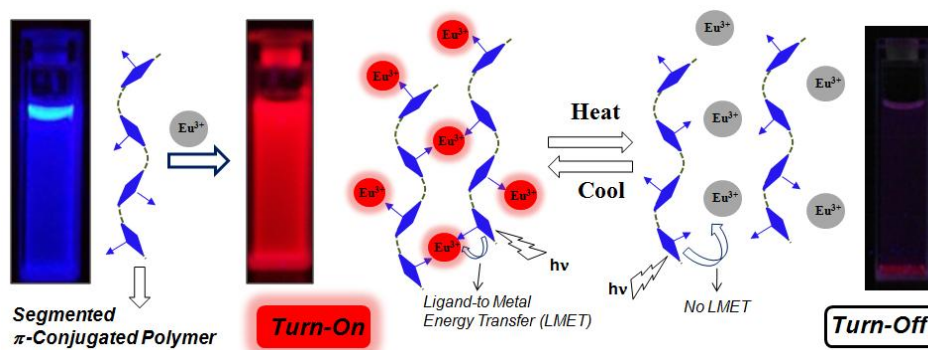
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### Abstract

Conducting Polymer-Lanthanide complexes have great attention due to their wide applications in the field of optoelectronics, sensors, etc. Developments of conducting (or conjugated) polymer-lanthanide hybrid materials are very attractive because new these candidates possess unique features such as mechanical stability of polymers and unique optical properties of the lanthanides.<sup>1,2</sup> Additionally, excited state energy levels of Ln<sup>3+</sup> ions were highly sensitive to the temperature and this property was exploited for temperature sensing applications in polymer-lanthanide hybrid materials in recent years. Here, we demonstrated  $\pi$ -conjugated polymer-Eu<sup>3+</sup> ion complexes as a new potential luminescent thermo-sensitive molecular probe.<sup>3</sup> Carboxylic functionalized segmented  $\pi$ -conjugated polymers having oligophenylenevinylene (OPV) chromophores in poly(ethyleneoxide) or polymethylene backbones were custom designed and utilized as efficient photosensitizer for Eu<sup>3+</sup> ion. Detailed photophysical studies and the luminescent decay dynamics revealed that these  $\pi$ -conjugated polymer-Eu<sup>3+</sup> ion complexes were highly sensitive to the temperature and behaved as completely reversible ‘turn-On’ or ‘turn-Off’ luminescent switches in solution and in solid state. The decay rate constants followed typical Arrhenius linear-trend over wide temperature range with almost identical activation energies. Both the nature as well as length of the segmented polymer chains which tied the OPV optical chromophores in the backbone determines the temperature range of the luminescent on-off process. The emission characteristics of the oligomer-Eu<sup>3+</sup> ion complex were found to be non sensitive to temperature which emphasized the superiority of polymeric backbone.



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## Synthesis and Characterization of Resole type Polymer Derived from 4-Hydroxychalcone

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### Abstract

This paper describes the synthesis of hydroxy chalcone starting from 4-hydroxybenzaldehyde and acetophenone using Claisen-Schmidt condensation. The compound is chemically characterized by infrared spectra and <sup>1</sup>H NMR spectral studies. Hydroxy chalcone was then reacted with formaldehyde solution under basic conditions to get resole type prepolymer which was subjected to thermal curing at 100<sup>0</sup>C to obtain the polymer. The formation of the polymer was characterized by IR technique. Thermogravimetry studies showed excellent stability for the synthesized polymer upto 300<sup>0</sup>C implying good fire retardance characteristics. DSC studies show that the cure temperature for the resin in the range of 90-120<sup>0</sup>C and crosslinking could be observed at wider temperature region.

*Keywords:* Hydroxychalcone; Pre-polymer, resole type polymer, Polymer characterization

# Poster Presentations

## ABA Type Tri-block Copolymers from Telechelic Polystyrene by Radical Initiation Process

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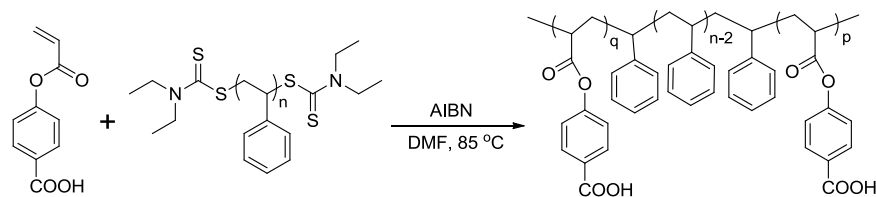
### Abstract

Synthesis of well-defined copolymers by novel pathways is our present research focus. The classical free radical polymerization is one of the best methods, which is compatible for all types of monomers and able to produce large scale polymers in industry. However, we could not obtain controlled macromolecular architecture and well defined block copolymers by classical radical polymerization. Moreover, the prepared homopolymers and copolymers should have broad range of polydispersity (PD) which affects badly the properties of the polymers. In the early 80s, Otsu discovered radical system (e.g., dithiocarbamate, disulfide) that exhibits some living characteristics. Subsequently, the controlled macromolecular architecture and living nature were achieved by living radical polymerization methods such as ATRP, NMP and RAFT methods. But each living radical polymerization method has its own limitations. Otsu et al succeeded in preparation of ABA type block copolymers by photo iniferter polymerization from telechelic polystyrene (*tel*-PS) as macroinitiator. This method is not applicable for various types of monomers, hazardous in using UV light and polymers get broad range of PD. In this presentation, we report syntheses and characterization of ABA type tri-block copolymers prepared from macroinitiator, *tel*-PS (B block) and acrylate based carboxylic acid functionalized monomers (A block) with radical initiation.

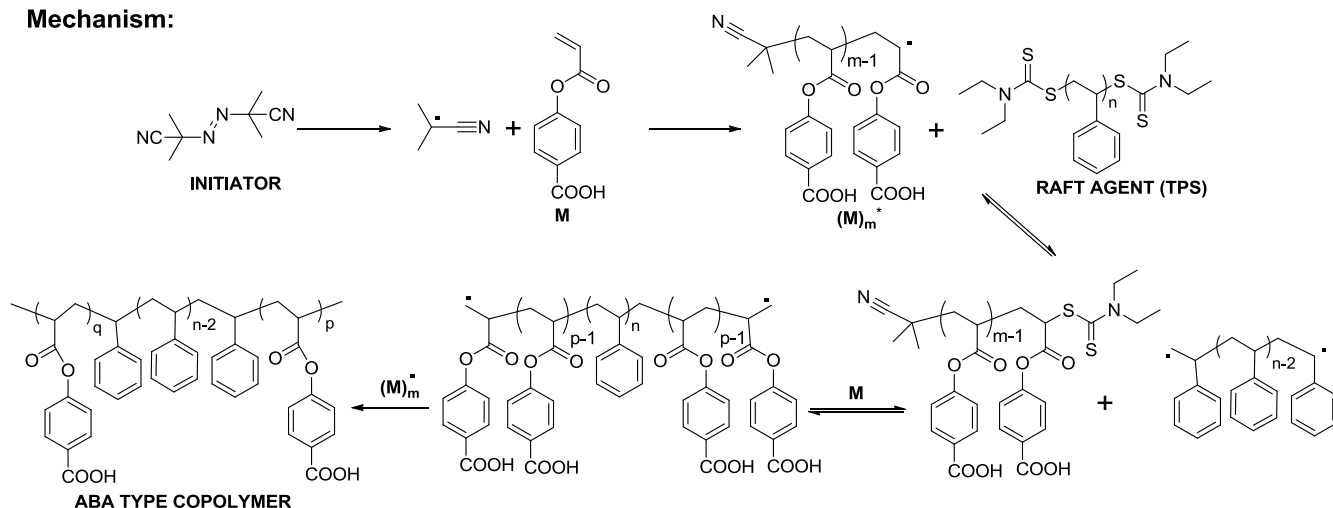
We have first time synthesized ABA type tri-block copolymers from *tel*-PS macroinitiator with acrylate monomers by the initiation of radical (mechanism involves in this process is reversible addition-fragmentation chain transfer (RAFT)) method. The monomer, *tel*-PS and ABA tri-block copolymer structures and mechanism are given in Figure 1. Homopolymers preparation from RAFT method was served as reference. The synthesized polymers were characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR, UV-vis, GPC for molecular weight and PD and thermal analyses (TGA and DSC). These polymers terminal ends were clearly identified in the  $^1\text{H}$  NMR spectra, which indicates the living nature. The  $\lambda_{\text{max}}$  values of the pendant azo groups of homopolymer and tri-block copolymer were exhibited at about 320nm, where as

functionalized COOH group pendant azo polymers showed at 335nm. The PD ( $M_w/M_n$ ) of the homopolymers and tri-block copolymers were in the range of 1.07 – 1.18 and 1.45 – 1.48, respectively. The polymers calculated molecular weights from  $^1\text{H}$  NMR were good agreement with the GPC values. There is no change in  $M_n$  values for homopolymers obtained from RAFT, iniferter and classical radical polymerizations, but polymer yield is higher in RAFT process. The monomer conversion and  $M_n$  values were independent of the polymerization temperature (80-120°C) by using RAFT process. The advantages of the initiation with radical to *tel*-PS on molecular weight control, degree of polymerization and equal activation of both the terminals of *tel*-PS will be discussed and compared to the photopolymerization method. The photopolymerized *trans*-4-pentylcyclohexyl ABA type copolymer polarizing optical microscopy textures and X-ray diffraction studies confirms that these exhibits smectic A phase. Furthermore, after magnetically forced alignment the samples exhibited similar optical texture but domain sizes of the LC phase were increased. The azo contain acrylate ABA type tri-block copolymers LC characteristics evaluations are under progress. We expect that carboxylic acid functionalized azo containing tri-block copolymers show LC nature and self-assemblies in specific solvent media and their annealed thin films with the help of pendant hydrogen bonds.

**Polymerization:**



**Mechanism:**



**Figure 1.** ABA type tri-block copolymer polymerization from radical initiation and mechanism.

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## Synthesis and Characterization of Poly(Ortho-Toluidine) and its Green Route Application For Oxidation of Aromatic Aldehyde into Carboxylic Acid

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### Abstract

In this paper, we have reported the synthesis of Poly(o-toluidine) by aqueous polymerization method using HClO<sub>4</sub> as dopant and ammonium persulphate as oxidizing agent with soft template acrylic acid. We successfully achieved the efficient and convenient catalytic oxidation of aldehyde to carboxylic acid by using Emeraldine salt form (oxidation states) of polyaniline. The polymers were characterized by UV-Visible, FTIR, SEM, XRD and conductivity measurements. A result shows that, UV-vis absorption spectra shows peaks at ~680-790nm with shoulder at 380-420 nm as characteristic peaks for the emeraldine salt (ES) phase of poly (o-toluidine). The FTIR spectra show a broad and intense band at ~2961-3000cm<sup>-1</sup> and ~1127-1185 cm<sup>-1</sup> that account for the formation of ES phase of the polymer. The X-ray diffraction spectrum shows a characteristic peak at 20-40°, 2θ range which reveals partial crystalline structure. The conductivity of the poly(o-toluidine) salt was found to be in the range of 0.37×10<sup>-3</sup> S/cm. SEM studies of poly(o-toluidine) doped with HClO<sub>4</sub> shows the continuous granular uniform morphology with sub micrometer evenly distributed particles of size ~50nm. Synthesized carboxylic acid derivatives were well characterized by <sup>1</sup>H-NMR, MS and FT-IR spectroscopy. The result were observed in good yields, role of catalyst was found to be very efficient, recyclable, eco-friendly, active, highly stable and requires low loading with easy workup procedure and it was easily recovered and regenerated for recycling.

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**Two Pack Polyurethanes Coatings Based on Renewable Source  
*Azadirachtaindicajuss* (Neem oil) Polyesteramidescured at Room Temperature**

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**Abstract**

Now days, the use of vegetable oils in the preparation of polymeric resin is gaining more importance due to renewability of oils, low cost and easily availability. In the literature vegetable seed oils such as linseed, castor, sunflower, soybean, coconut and cotton seed oils were used to prepare the polymeric resins. Vegetable oils used in past are in the form of alkyds, polyepoxies, polyurethane, polyesteramides and polyetheramides as sustainable resources. Although neem oil is present in ample amount, its application has not been focused for preparation of polymeric resin or in development of coatings. With this research work the novel attempt has been made to develop neem oil based two pack polyurethane coatings cured at room temperature. Polyesteramide is the route selected for development of polyurethanes resins from neemseed oil. In the present work the neem oil based polyesteramidewas prepared in two steps. In first step neem oil fatty amides (AIJFA) which was directly converted to polyesteramide. Spectral study of prepared resin was carried out by using FT-IR and NMR techniques. Polyesteramide further was utilized for preparation of PU coatings on mild steel plate by using varying percent of different diisocyanates like H-MDI, MDI and TDI. The coatings were tested by physico-mechanical and chemical/corrosion resistance tests. The coating properties like gloss, impact resistance, adhesion, flexibility and other mechanical properties were studied and found to be superior for anticorrosive industrial coating.

**Keywords:**Neem oil, anticorrosive, renewable source, polyurethane coatings.



## Sensor Applications of Norbornene Based Materials

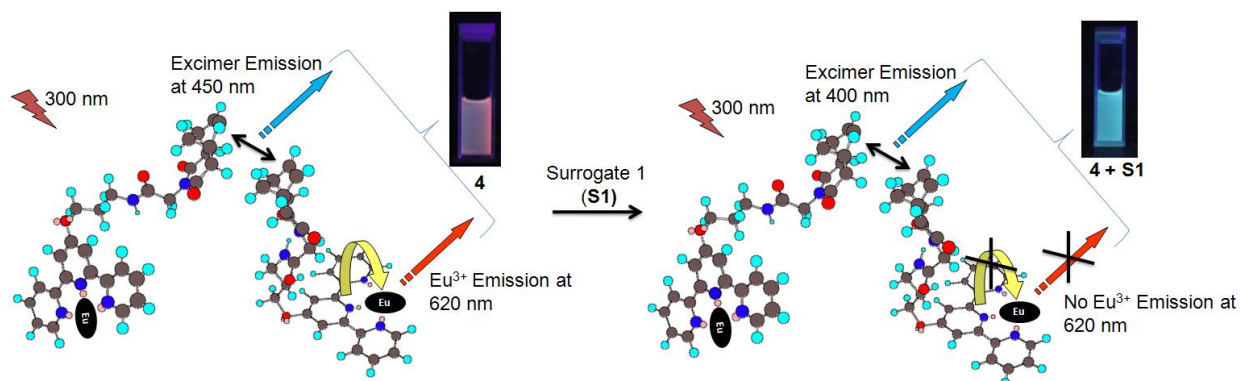
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### Abstract

We develop norbornene based sensors that have potential application in sensing area of heavy metals and nerve gas. The main threats to human health from heavy metals are associated with exposure to lead, cadmium, mercury and arsenic. To provide sensitive and selective sensor systems, fluorophores (e.g. Rhodamine, Hydroxyquinoline) with binding moieties are attached to norbornene backbone. It is found that hydroxyquinoline modified norbornene behaves as a fluorometric sensor molecule for  $\text{Cd}^{2+}$ , whereas rhodamine based norbornene acts as a dual sensor for  $\text{Hg}^{+2}$  and  $\text{Cu}^{+2}$ . Norbornene based monomers are polymerised by ROMP technique using Grubbs' Catalyst. Using UV & Fluorescence method, the sensing ability of the new molecules is confirmed.



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## Dopant Induced Sensitivity in Polyaniline for LPG Sensing

**Tanushree Sen, Navinchandra G. Shimpi and Satyendra Mishra\***

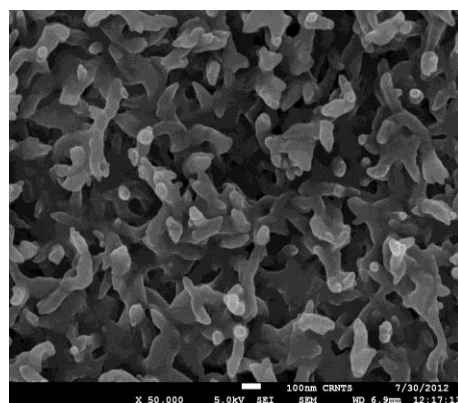
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### Abstract

The delocalized  $\pi$ -electron system in intrinsically conducting polymers (ICPs) is responsible for their electrical conductivity. Polyaniline, with its reversible doping/dedoping character and unique electronic properties, are frontrunners in the field of biosensors and electronic noses. Its interaction with analytes introduces changes in the physicochemical properties, resulting in an increase or a decrease of the density of charged species through polymer/analyte interaction. The dopant molecule in polyaniline not only facilitates charge mobility but also induces selectivity in the polymer towards sensing of different gaseous species. The present study is aimed at exploring the role of dopants in inducing selectivity, sensitivity & stability in polyaniline, and evaluating their application in room-temperature gas sensing. We have developed polyaniline doped with binary dopant. Polymerization of aniline in presence of the binary dopant was carried out at 30 °C. Polyaniline was obtained in the emeraldine salt form. The preferential directional growth of polyaniline doped with binary dopant lead to nanofibrillar morphology, as observed using the field emission scanning electron microscope (FE-SEM). This lends polyaniline a high active surface area for interaction with analytes. The quinoid and benzenoid ring structures in the polymer were identified using FTIR.



*Fig.1. FE-SEM micrograph of polyaniline doped with binary dopant (x 50,000)*

The absorption maxima of the polyaniline for  $\pi$  – polaron transitions could be seen at ~ 980 nm, which shows a highly extended conformation in its solvent, N-methyl pyrrolidone. Polyaniline doped with binary dopant was also found to possess good thermal stability, as evidenced by thermogravimetric analysis. A shift in temperature towards higher value was seen for dopant loss in the polymer, which

increased the range of the polymer's working temperature. The polyaniline/binary dopant system was found to be sensitive to LPG at room temperature.

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**Keywords:** polyaniline; nanofiber; binary dopant; sensing; LPG.

## **Effect of Inorganic Content on Shrinkage of Visible Light Cure Composites Prepared From Inorganic-Organic Hybrid Resins**

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### **Abstract**

Polymeric composites have been considered a material of major importance in restorative dentistry due to their esthetic properties. Commercially available light-cured composite resins are based on Bis GMA/UDMA/ both as resin medium. The use of existing dental composites based on conventional resins has limitations such as polymerization shrinkage, poor abrasion resistance, leaching of uncured organic monomers causing cytotoxic effects. The polymerization shrinkage persist in these composites creates contraction stresses in the resin composite restoration and internal stress and deformation in the surrounding tooth structure resulting in poor marginal adaptation, postoperative pain, and recurrent carries. Inorganic-organic hybrid resins are novel monomer matrix introduced into dental restoratives to diminish the polymerization shrinkage. With the current boom in nanotechnology, nanocomposites have received considerable attention thus the organic and inorganic components can combined at nanoscopic scale in these resins. Inorganic-organic hybrid resins contain a metal core and synthesized through sol-gel process to merge properties of organic polymers with properties of glass like materials to stimulate new properties. The abundance of polymerization opportunities in these materials allows it to cure without leaving monomers also it has the capacity to double the conversion of monomers. Therefore it has greater biocompatibility with the tissues and enhanced physical properties. Incorporation of essential elements in our body like calcium, magnesium and zinc in these inorganic-organic hybrid resins have low polymerization shrinkage and better hardness compared to Bis GMA which was reported earlier. It inspired to incorporate other essential elements like manganese, barium, strontium, zirconium in various concentrations into these resins. Manganese is essential for the metabolic activities in the body and the other elements are radiopaque in nature. Objective of the present study is to investigate effect of the above inorganic contents on polymerization shrinkage of visible light cure composites based on novel inorganic-organic hybrid resins.

## Designing Thiol Based Norbornene Materials for Sensing Metal Poisoning

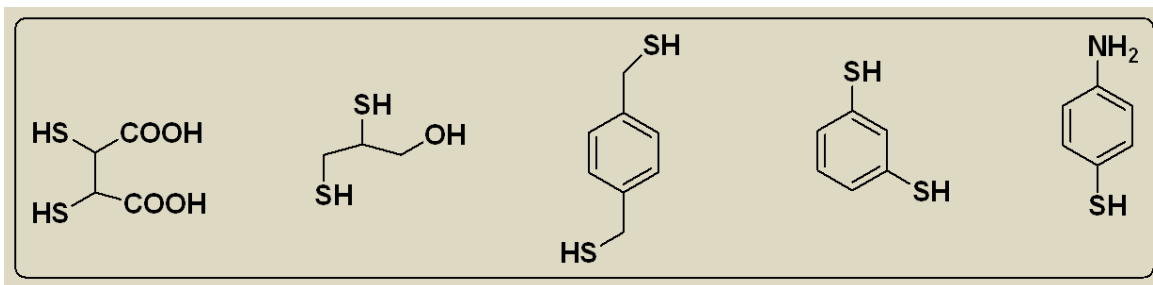
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### Abstract

Unique materials can be obtained with well-known polymeric properties from macromolecule architectures functionalized with electron rich moieties. The incorporation of metal-ligand interactions into macromolecules imparts them with potentially useful function. As both arsenic (III) and mercury (II) are having specific affinity towards thiol group, synthesis of thiol based copolymer via ROMP is employed for the application of sensing arsenic (III) and mercury (II) in drinking water. This novel polymer is throughly characterised by NMR, IR and gel permeation chromatography (GPC). Fluorescence and UV-Visible spectroscopy methods are used to monitor the sensing event of the newly designed polymer, both by fluorometrically as well as colorimetrically in it's very low concentration (standardized by WHO, 10µg/L).



[Thiolfunctionalized ligand expected to bind AS (III) and Hg(II)]

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# Norbornene Based Polymeric Nano-carrier for Anti-Tuberculosis Therapy

Shivshankar R. Mane and Raja Shunmugam\*

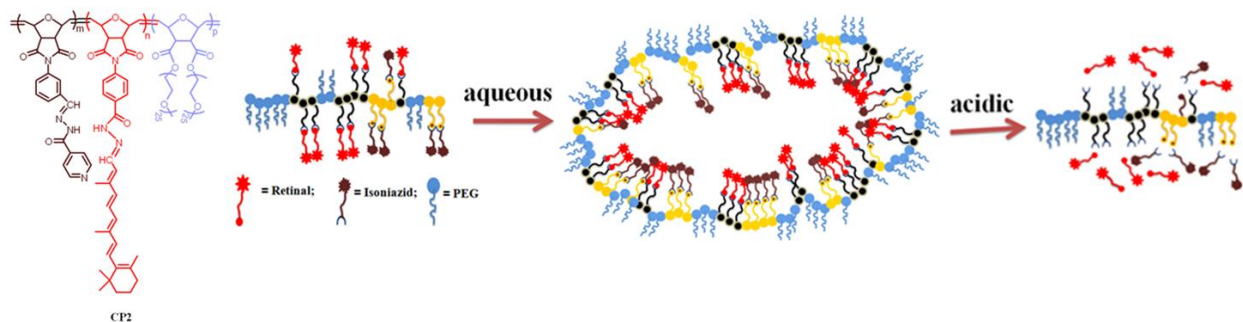
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## Abstract

The most important applications of polymers in modern pharmaceuticals are the development of advanced drug delivery systems, commonly known as controlled release drug delivery systems. Towards this application, Ring Opening Metathesis Polymerization (ROMP), a controlled/living polymerization technique is employed to make the polymeric nano-carriers. The detailed synthesis and characterization of the monomers and polymers using NMR, IR, UV and GPC techniques are discussed. These nano-carriers with hydrazone linker denote a promising reservoir with excellent performance for an efficient drug delivery system. An application of the newly synthesized copolymer in TB therapy is demonstrated. Moreover, the system also offers effective strategy and new modalities for the creation of TB therapy.



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## Self-assemblies of Segmented OPV-Polymers and their Donor-Acceptor System

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### Abstract

$\pi$ -Conjugated materials based on phenylenevinylene backbones have been extensively used as p-type materials in solar cells. The efficiency of such devices depends highly on the supramolecular organization donor and acceptor molecules, and, therefore, controlled and predictive self-organization of such  $\pi$ -conjugated materials at nano- and meso-scopic length scales has become one of the most challenging research areas in materials chemistry. Recently, we have reported supramolecular self-assembly approach for liquid crystalline  $\pi$ -conjugates in the solid state.<sup>1-3</sup> The present work reports design and development of novel segmented and rigid polymers based on bis-TCD substituted distryl benzene chromophores and study their molecular self assembly through FRET mechanistic pathways. Segmented polymers such as (poly-8 and Poly-12) were synthesized by incorporation of flexible octyl and dodecyl spacers between the TCD-substituted oligo(*p*-phenylenevinylene) segments. Molecular Aggregation in polymers was probed using solvent induced aggregation phenomenon. Photophysical analysis at different solvent compositions revealed that as the concentration of the poor solvent, like methanol, increases up to 20% (v/v), a large 50 nm red shift in emission spectrum and broadening of absorption band occurs in segmented polymer, whereas no such aggregation is observed in rigid m-PPV or corresponding oligomer. These polymers were then utilised to form Donor- acceptor arrays with electron deficient perylene bisimide moiety and their self organisation was traced by using FRET mechanistic pathways. These studies suggested that segmented polymers formed 10 times more stable D-A arrays than rigid polymers and the flexibility of the polymer backbone plays an important role in forming better D-A arrays which are useful for solar cell applications.





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## Site Specific Norbornene Based Prodrugs for Cancer Therapy

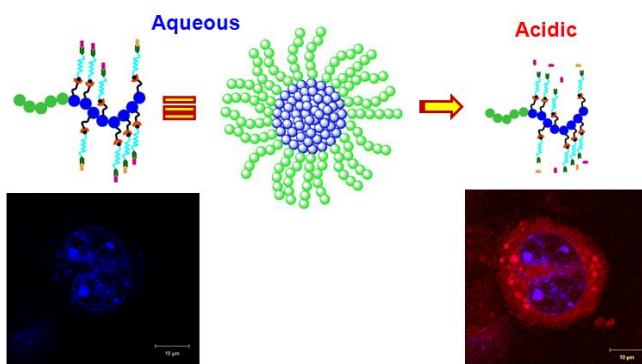
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### Abstract

Three new monomers namely cis-5-norbornene-6-(diethoxyphosphoryl)hexanote (mono **1**), norbornene grafted poly(ethyleneglycol)-folate(mono**2**), norbornene derived doxorubicin hydrazone linker (mono**3**) are synthesized. The synthesis and complete characterization of three monomers are clearly described. Their copolymerization by ring-opening metathesis polymerization (ROMP) to get the triblock copolymers **PHO-DOX-FOL**. Deprotection of phosphonic acid diethyl ester in **PHO-DOX-FOL** is carried by using trimethylsilyl bromide to get **PHOS-DOX-FOL**. Folic acid (FA) used as the receptor-targeted anti-cancer therapy, where the phosphorylhexanote is used for iron particle ( $\text{Fe}_2\text{O}_3$ ) attachment to evaluate for their tumor-targeting MRI contrast-agent. Doxorubicin hydrazone linker is used to release the drug exactly at the mild acidic conditions resembling the pH of the cancerous cells. FTIR, TGA are confirmed the iron particle ( $\text{Fe}_2\text{O}_3$ ) anchoring to the **PHOS-DOX-FOL**. Drug release profile suggests the importance of having the hydrazone linker that helps to release the drug exactly at the mild acidic conditions resembling the pH of the cancerous cells. It is also observed that the drug release from micelles of **PHOS-DOX-FOL** is significantly accelerated at mildly acid pH of 5.5 to 6.0 compared to physiological pH of 7.4, suggesting the pH-responsive feature of the drug delivery systems with hydrazone linkages.



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## Norborene Based Magnetic Copolymers for Imaging Applications

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### Abstract

Well-defined oxa-norbornene derived random copolymer and triblock copolymer having cobalt complex, doxorubicin and polyethylene glycol, have been synthesised using ring opening metathesis polymerisation (ROMP). All the polymers are characterized by <sup>1</sup>H NMR, IR, GPC and TGA techniques. The morphology of the copolymer nanocomposites are evaluated with DLS, TEM and AFM. The cobalt complex functionalization to the polymer is monitored by FTIR. To prove the paramagnetic nature of copolymer nanocomposites, SQUID experiment is performed at room temperature. Newly designed copolymers having paramagnetic nature are expected to be magnetic resonance imaging (MRI) agent.

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# Design and Development of Azoprodugs of Various Permutations and Combinations of 5-Aminosalicylic Acid and 4-Aminosalicylic Acid for Management of Inflammatory Bowel Disease *via* Colon-Specific Drug Delivery

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## Abstract

Ulcerative colitis (UC) and Crohn's disease (CD) collectively known as inflammatory bowel disease (IBD) is a chronic transmural inflammation of all or any part of the gastrointestinal tract (GIT), a chronic relapsing condition with a high morbidity and remains largely incurable. Four colon-specific mutual azoprodugs of 5-aminosalicylic acid (5-ASA) and 4-aminosalicylic acid (4-ASA) with each other in various permutations and combinations were synthesized for the management of IBD by reported procedures. The structures were confirmed by elemental and spectral analyses using IR, <sup>1</sup>H-NMR and mass spectroscopy. In vitro release was studied in rat fecal matter where 53% and 67.1% release of 5-ASA was achieved from produgs of 5-ASA with 4-ASA and prodrug of 5-ASA with 5-ASA respectively. 67% and 68% release of 4-ASA was achieved from azoprodrug of 4-ASA with 5-ASA and prodrug of 4-ASA with 4-ASA in rat fecal matter respectively. The produgs were stable at pH 1.2 and 7.4 in aqueous buffers. Pharmacological screening of the synthesized produgs was carried out in the chronically inflamed tissue of colon in trinitrobenzenesulfonicacid (TNBS)-induced experimental colitis model in rats. The produgs exhibited comparable ameliorating effect as that of sulfasalazine (SLZ). To evaluate and compare the safety profile of synthesized produgs with respect to 5-ASA-induced pancreatitis and sulfapyridine-induced hepatitis, the produgs were also assessed for their probable damaging effects on pancreas and liver with the help of histopathological analysis. From these particular findings, it can be concluded that the synthesized produgs exhibited improved safety profile than 5-ASA or SLZ. The results of ulcerogenic activity revealed that synthesized produgs showed substantial lowering of ulcer indices as compared to 4- or 5-ASA, which proves that like SLZ, the synthesized compounds were also capable of delivering 4- or 5-ASA specifically to colon without any release in upper GI tract.

## Synthesis, Hydrolysis Kinetics and Pharmacological Screening of Mutual Prodrug of Anthraquinone Derivative for Osteoarthritis

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### Abstract

Diacetylrhein, an anthraquinone derivative with interleukin-1-beta (IL-1 $\beta$ ) inhibitory activity reduces IL-1 $\beta$  induced matrix metalloproteinase (MMP)-13 production in osteoarthritis. L-glutamine is a conditionally essential amino acid as it is manufactured in body under extreme physical stress, possessing anti-inflammatory and wound healing effects. Therefore, mutual prodrug of diacetylrhein with L-glutamine was synthesized through a bioreversible amide linkage by a reported procedure. Structural confirmation was carried out by elemental analysis, IR,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR and Mass spectroscopy. *In vitro* release kinetics of this prodrug was thoroughly studied in aqueous buffers of different pH, stomach and small intestinal homogenates and 80% human plasma. *In vivo* release was studied in rat blood, urine and feces. The prodrug was stable in HCl buffer (pH 1.2) and stomach homogenates of rats. However; in phosphate buffer (pH 7.4) and in intestinal homogenates the prodrug exhibited 86.80% and 30.02% release of diacetylrhein respectively over a period of 8h following first order kinetics. In 80% human plasma (*in vitro*) and rat blood (*in vivo*) also 91.93% and 92.76% release of diacetylrhein was observed respectively. 3-8% of rhein, active metabolite of diacerein was observed in phosphate buffer (pH-7.4), intestinal homogenates and 80% human plasma after 5 h. The 24 h pooled samples of rat urine revealed presence of 6.24% intact prodrug, 5.14% of diacetylrhein and negligible amount of an unknown metabolite while rat feces pooled over a period of 24 h showed absence of diacetylrhein but presence of 6.78% of intact prodrug. The *in vivo* release kinetics of prodrug in rat clearly indicated activation of prodrug to be occurring in blood, being catalyzed by the weak alkaline pH of blood (7.4) in combination with amidases present therein. Prodrug was evaluated in collagenase-induced osteoarthritis in rats wherein the conjugate, physical mixture, individual diacetylrhein and L-glutamine were tested based on physical (body weight, knee diameter and tail flick hyperalgesia), hematological (Hb, RBC, WBC and ESR) and biochemical (CRP, SALP, SGOT and SGPT) parameters and prodrug showed significant results as compared to other treated groups. In conclusion, prodrug at the specified dose level of 6.93

mg/kg, p.o. (BID) showed weight gain, reduction in knee diameter and tail flick hyperalgesia and it could significantly normalize the hematological and biochemical abnormalities in collagenase-induced osteoarthritic rats. Further the histopathological studies confirmed superior antiarthritic effect of prodrug over plain diacetylrhein justifying the selection of L-glutamine as a promoiety in mutual prodrug design.

## Effect Of Organically Modified Natural Montmorillonite On Processing And Properties Of Poly(3-Hydroxybutyrate)

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### **Abstract**

Poly(3-hydroxybutyrate)/layered silicate nanocomposites have been prepared using melt mixing method. Since the interaction between the matrix and nanofillers are important for better end use applications, natural montmorillonite has been organically modified using hexadecyl ammonium bromide and PHB grafting. For a comparative account cloisite 30B, commercially modified nanoclay also has been used for nanocomposite preparation. Effects of organo modifiers on the intercalation/exfoliation process have been evaluated using morphological analysis, TEM, AFM and WAXD. Further, the performance characteristics as a function of dispersion of organo modified montmorillonite within the matrix polymer were studied through mechanical thermal and rheological characterizations.



## **Synergistic Effect of Multiwalled Carbon Nanotube and Layered Silicate on the Properties of Poly (propylene)**

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### **Abstract**

This work was aimed to synthesize and evaluate hybrid nanocomposite material based on Poly(propylene) (PP) matrix with multiwalled CNTs and clay particles. The hybrid nanocomposites were prepared through masterbatch route using melt intercalation phenomenon. The effect of processing parameter on the mechanical performance of the nanocomposites has also been studied in order to optimize it. The determination of fracture energy in order to analyse the toughness of the material was carried out. Also the creep recovery characteristics of the nanocomposite materials were analysed in detailed. The morphology of the fractured surface was investigated in order to see the effect of MWCNT on the fracture characteristic of PP/Clay nanocomposites. The Dispersion of the nanoparticles was investigated through transmission Electron Microscopy. The synergistic effect of MWCNT and clay was observed on performance of the PP/CNT/clay nanocomposites.

## Mechanical and Thermal Properties of Sisal Fiber Reinforced Epoxy/Unsaturated Polyester Blend Composites

Nagarjuna Reddy P, S Mohanty and S K Nayak

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### Abstract

In this work, the mechanical and thermal properties of the untreated and NaOH treated sisal fibers were reinforced with epoxy, unsaturated polyester (UP) and their blends. These composites were prepared through compression molding technique. The partial removal of wax, hemicelluloses, and lignin was confirmed through the FTIR spectroscopy. The Epoxy/Unsaturated polyester blends were prepared by mixing of epoxy resin (DGEBA) with 5, 10, 15 and 20% (by wt %) of unsaturated polyester using methyl ethyl ketone peroxide (MEKP) as catalyst, cobalt naphthenate as accelerator and Diethylenetriamine (DETA) as a curing agent.

The mechanical and thermal properties such as tensile, flexural, impact strength, heat deflection temperature (HDT), Dynamic mechanical analysis and thermogravimetric analysis were evaluated. Treated fiber reinforced unsaturated polyester toughened epoxy blend composites showed 61.82% of increase in tensile strength and 110.8% in impact strength while the untreated fiber reinforced blended unsaturated polyester toughened epoxy composites performed 26.8% increase in flexural strength. The SEM study was used to evaluate the surface changes of treated and untreated fibers and also to discuss the results originated from the evaluation of mechanical properties.

## **Preparation and Characterization of Low Temperature Oxygen Plasma Treated Sisal Fiber Reinforced Poly Lactic Acid Nanocomposites**

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### **Abstract**

Current study evaluates the effect of low temperature oxygen plasma treatments of sisal fiber (SF) on the mechanical, thermal and rheological characteristics of SF reinforced poly lactic acid (PLA) nanocomposites. Plasma treatments of long SF have been conducted at variable voltages and time inside a high vacuum oxygen plasma chamber. Further, immediately after the surface treatment, fibers have been chopped into 2-3 mm length and melt mixed with PLA and cloisite 30B nanoclay (C30B), under inert N<sub>2</sub> condition. Enhanced mechanical properties of the plasma treated SF reinforced nanocomposite reveals better interlocking among the matrix, SF and nanoclay by plasma treatment, than that of untreated SF reinforced nanocomposite. During the plasma exposure, ionized oxygen can oxidize the surface functionalities of SF (a lignocellulosic natural fiber) creates more polar site to promote improved interlocking network with the matrix PLA and C30B. Since the plasma treatment results in better interface within the nanocomposite, the thermal stability and thermal transition temperatures are also reported superior values during TGA and DSC analysis. The visco-elastic and rheological characterization also revealed a better application and processing window for PLA after the reinforcement of plasma treated SF.

## **Thermal Characteristics of Renewable Resource Based Polylactic Acid Nanocomposites: Effect of Layered Silicate Based Nucleating Agents**

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### **Abstract**

Total crystallinity is a major defining factor for physical characteristics of a polymeric system. Layered silicates are known nucleating agents within various polymer matrices, so as able to alter its performance characteristics. Current study evaluates the nucleation capacity of organically modified natural montmorillonite within PLA matrix using DSC analysis and also its effects on other thermal characteristics. To enhance the adhesion and basal spacing of natural montmorillonite with PLA, it has been activated using organic surfactant. To comprise a comparative account, commercially available organonano clays also have been utilized for nanocomposite preparation. Nucleation parameters were evaluated through isothermal cold crystallization kinetics study using Avrami plots. Lauritzen-Hoffmann theory was used to study the effect of organoclay reinforcement on crystallization regimes of PLA. Further the thermal stability and the reinforcing effect of nanoclays were studied using TGA, DMA and HDT tests.

## Effect of Fullerene on the Ylide Initiated Copolymerization of Methyl Acrylate and Styrene

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### Abstract

The kinetic parameters were calculated for studying copolymerization of methyl acrylate and styrene in dilatometer using, triphenylstibonium 1,2,3,4-tetraphenylcyclopentadienylide, in presence of fullerene (C<sub>60</sub>), under nitrogenous atmosphere, at 80 ± 0.2°C for 3 h. The expression for R<sub>p</sub> was found to be as,  $R_p \propto [\text{Ylide}]^{0.4} [\text{MA}]^{0.8} [\text{Sty}]^{1.2} [\text{Full}]^{-0.6}$ , suggesting non ideal kinetics for the copolymerization, due to the primary radical termination by the fullerene and degradative chain transfer effect of ylide. The copolymer(s) were treated with cyclohexane and acetonitrile, to remove the traces of homopolymers, if any, and finally percent conversion was determined. Negligible weight loss was observed. The synthesized copolymer(s) were characterized by FTIR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopic analysis. Fullerene acts as radical inhibitor in early steps, by reacting the free radicals, produced by initiator, and finally inserted into the copolymer(s) to produce fullerene containing polymeric materials.

## Photo-degradation and Stabilization Study of High Performance Polymer Membrane

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### Abstract

In this investigation we report the degradation and stability of polymer membrane (PBID) used in fuel cells as a proton exchange membrane. This membrane is made up of polybenzimidazole backbone with some structural modifications. The PBI based membranes are used at an elevated temperature of about 433 K to 473 K in the acidic as well as in oxidizing environments of fuel cells. These membranes are found to be very efficient in functioning, but the stability of chemical structure and composition with prolonged usage is scantily reported. To study the degradation and stability of membranes, accelerated degradation was done by photo irradiating these membranes using SEPAP 12 having four mercury vapour lamps as an ultraviolet source (wavelength above 300 nm).

Membrane samples were irradiated in UV chamber at 328 K and characterized at regular time intervals to detect signs of chemical degradation by using

advanced characterizing techniques like FTIR, XRD, DSC, TGA, SEM etc. These membranes were found to be stable at 328 K but tend to degrade with the UV irradiation. Also, with increase in the time of irradiation there was enough increase in the intensity in carbonyl and hydroxyl

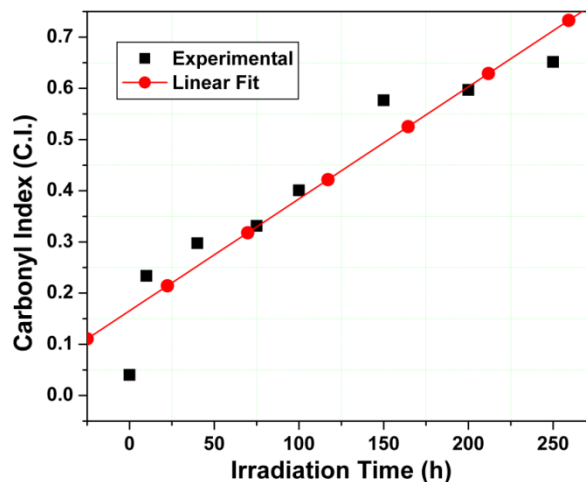


Figure-1 Zone of inhibition formed by azadirachta indica

region in FTIR spectrum, which shows that these membranes follow the mechanism of oxidative degradation.

**Key Words:** Membranes, degradation, irradiation, characterization, ultraviolet, oxidative.

**Acknowledgement:** OSK kindly acknowledges director, CSIR-NCL for providing infrastructure and UGC for Senior Research Fellowship.

## **Studies on the Thermal and Nanophase Properties of Modified MWCNT-Neoprene Nanocomposite**

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### **Abstract**

Polymer-MWCNT nanocomposites have attracted a great deal of attention for both scientific challenges and industrial applications because of their established improved mechanical properties, thermal stability, reduced gas permeability and other physicomechanical properties compared to neat polymer or conventional polymer composite. It is a well established fact that a few percent of MWCNT significantly enhanced various properties. Many presentine polymers have been used to prepare nanocomposites with MWCNT, but no work is documented in the open literature on neoprene elastomer filled with modified MWCNT.

Therefore, the present work is devoted to the preparation of Neoprene (CR)/Modified MWCNT by solution blending method and is expected to provide much better properties from the nano reinforcement of the filler under study. Thermogravematric analysis has been used to compare the decomposition trends of the CR/Modified MWCNT nanocomposites with the CR/MWCNT nanocomposite. MWCNT has been modified through the coating of polyhasphazene. The glass transition temperature ( $T_g$ ) of CR/Modified MWCNT composite has increased as compared with that of neat CR. The dynamic mechanical analyses of nanocomposites exhibit the increment in the storage modulus. Substantial improvements in most of the mechanical properties have also been observed in case of the nanocomposites. Morphological studies have been carried out with the help of scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM).



## Development of Multifunctional Micro/Nano Patterned Materials by Lithography Techniques

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### Abstract

Patterned structures or surfaces are of considerable importance in many areas of modern science and technology such as microelectronics, information storage, material science, chemistry, biotechnology and micro fluidics. For patterning the surfaces several lithographic techniques have been developed in the microelectronics industries including deep and extreme UV photolithography, electron beam writing and x-ray lithography. These techniques though elegant are costly in capital and operating costs, thus making them inaccessible, alternative simple and cost-effective techniques such as imprint lithography, soft lithography, etc. have been developed to broaden accessibility and diversify capability. We synthesized high quality patterned SiNWs by combining soft lithography and metal assisted chemical etching. Hierarchical assemblies of nanostructured building blocks on conducting substrates are significant for construction of functional devices. We also introduce a simple but unique strategy for the synthesis and patterned assembly of ZnO nanostructures within micro fluidic channels. The resulting micropatterned nanostructures exhibit excellent optical and antireflective properties. This structural hierarchy can reduce optical loss due to reflectance in photovoltaic cells and subsequently enhance energy conversion efficiency.

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## **Mechanical, Thermal and Morphological Studies on Polypropylene (PP) Reinforced with Glass fiber and Modified Montmorillonite Nanoclay**

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### **Abstract**

The present work aims to develop hybrid composite based on chopped glass fiber (GF) and modified montmorillonite (MMT) nanoclay in polypropylene (PP) matrix. The nanocomposites have been compounded using twin screw extruder. An attempt has been made to see the combined effect of chopped GF and modified MMT nanoclay on the mechanical properties e.g. tensile, flexural and impact of the hybrid PP/GF/MMT nanocomposite. The mechanical properties have increased with incorporation of GF and further improvement has taken place in case of hybrid PP/GF/MMT nanocomposite. Heat deflection temperature has also increased in the case of hybrid nanocomposite. The thermal stability of the developed nanocomposite has been carried out with the help of thermo- gravimetric analysis (TGA). The morphological properties of nanocomposite have been visualized by scanning electron microscopies (SEM), which demonstrate that the interfacial adhesion is appreciably good. This may be the reason for excellent mechanical properties and thermal stability of the developed nanocomposites.

Keywords: MMT, Glass fibre, Polypropylene, SEM, Nanocomposite

## Main Chain Liquid Crystalline polymer scaffolds containing azobenzene

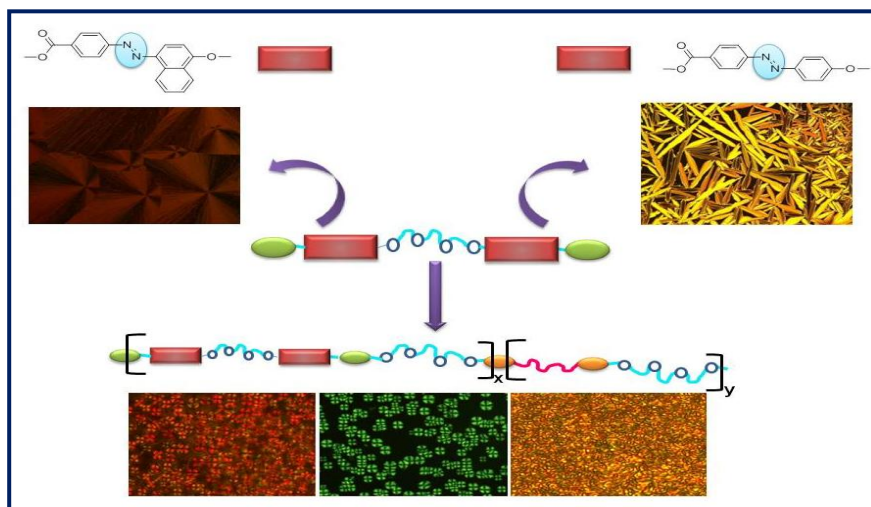
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### Abstract

Azobenzene is very interesting chromophore due to photoreponsive behaviour. It can photoisomerize trans to cis upon UV irradiation due to which it finds application in a variety of areas like optical data storage, molecular switches, display devices, non linear optical devices, photomechanical systems etc. here we did systematic studies on two homologues series of twin liquid crystalline (LC) molecules based on phenyl and naphthyl azobenzene (**PnP** and **NpnNp**) as well as segmented copolyesters based on them. The twin series had the structure azobenzene- oligooxyethylene - azobenzene where the ethyleneoxy length was varied from 2 to 6 units. Design of twin is very crucial which allow us to adopt a melt polycondensation route for synthesizing main chain liquid crystalline polymer. The LC properties of the twin series depended on the chemical structure of the azochromophore and also the length of the central oligooxyethylene segment. The **PnP** series exhibited smectic LC properties for  $n > \text{three}$  oligooxyethylene units. On the other hand, **NpnNp** series exhibited spherulitic phases only for the shortest member –**Np2Np**. One non-LC short spacer twin (**P2P**) and one LC long spacer twin (**P6P**) were incorporated as part of a main chain polyester composed of fully aliphatic segments of sebacate and di or tetraethylene glycol (DEG/TEG) units by melt polycondensation. The copolymer approach allows us to tune liquid crystalline property by varying twin spacer length and degree of segmentation.



## Development of Hydrophobic Coatings from Expanded Polystyrene

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### Abstract

A number of technologies are used for development of hydrophobic surfaces due to their numerous applications like self cleaning property, marine coating, anti-adhesive coating and aircraft. Biological hydrophobic multifunctional structure like lotus leaf, Gecko feet, Butterfly wing, Peacock feather, Fish scale, Rice leaf, Rose petal, Shark skin, Mosquito compound eyes are replicated by most of the researchers either by physical methods or chemical methods. Both physical and chemical methods involve formation of hydrophobic nano pillars that can lower the surface energy of substrate. Superhydrophobicity is characterized by high contact angle ( $WCA > 150^\circ$ ) with small angle of hysteresis. It is usually obtained by enhancement of surface roughness and modification with low surface energy materials. In order to get suitable water repellent surface, various methods like CVD (Chemical Vapor Deposition), sol-gel method, etching process, layer by layer assembling method, spraying, solution immersion, Lithography, spin coating, Electrochemical deposition process etc are adopted. However, recently researchers are exploring the possibility of developing materials like fluorocarbon, silicones, organic and inorganic materials for hydrophobic surface.

This paper focuses on the study of the wettability property of waste expanded polystyrene which is extensively used for thermal insulation, acoustic insulation, moisture resistance, lifetime durability and flame retardancy. Among various polymer produced in the world, expanded polystyrene is the biggest commodity polymer with total demand nearly 30 million tonnes per annum. Most of the used expanded polystyrene materials are not recycled cost effectively and they pose serious disposal issues. But the impact of waste polystyrene to environment has recently drawn a great deal of attention.

In this article the generated waste expanded polystyrene foams from thermal insulation was used as the possible candidate for investigating the hydrophobic properties. Varied concentration of waste graphite powders generated from battery industries where solution blended with waste polystyrene. These graphite

powders which exist in the form of layers due to weak vander-waals forces exfoliated. These exfoliated layers of graphite get dispersed in intercalated in the polystyrene matrix. The Sonication time of 30 mins and 1 wt. % graphite powder in polystyrene was found to be optimized formulation. Rheological properties of these formulations were extensively studied by using Brookfield viscometer to understand the coating parameters. Effect of varied thickness on superhydrophobicity was explored. Similarly surface roughness and surface morphology of each spin coated layer were studied by using atomic force microscopy (AFM) and scanning electron microscope (SEM) respectively. Water contact angle results of spin coated samples revealed that hydrophobicity was increased with increasing the percentage of graphite powder. Since maximum water contact angle of only  $110^{\circ}$  was obtained, it requires some further additives and study of surface morphology for enhancement of self-cleaning property and good slippery property of spin coated glass slide surface.

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## Smart Biopolymer “Bacterial Cellulose” as Antimicrobial Dressing Material

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**Abstract**

In the era of declining forests, global climate changes, continuing growth of industrialization; it is rational to consider the consequences of an alternative source of cellulose. A promising strategy to overcome this impediment involves the production of cellulose from microorganisms. Bacterial cellulose (BC) is an alternative for plant cellulose. Plant cellulose and bacterial cellulose have the same chemical structure, but differs with respect to its unique nanostructure and properties. BC has proven to be a remarkably versatile biomaterial and can be used in wide variety of applied scientific endeavors, such as paper products, electronics, acoustics, and biomedical devices. One of the most promising areas of BC application as biomaterials is the utilization as a temporary skin substitute in the therapy of difficult wounds, burns, and ulcers. However, BC itself has no antimicrobial activity to prevent wound infection. In present study production of BC and its application as novel wound-dressing materials has been explored by incorporation of silver nanoparticles and antibiotic.

**Key words:** Biomaterial, shaking culture, silver nanoparticles, antimicrobial activity

**Nanotechnology in Cancer Treatment**

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### **Abstract**

Nanotechnology is a multidisciplinary field, which covers a vast and diverse array of devices derived from engineering, biology, physics and chemistry. These devices include nanovectors for the targeted delivery of anticancer drugs and imaging contrast agents. Nanowires and nanocantilever arrays are among the leading approaches under development for the early detection of precancerous and malignant lesions from biological fluids. These and other nanodevices can provide essential breakthroughs in the fight against cancer.

**Graphene oxide modified quartz crystal microbalance (QCM) nanobiosensor  
for the rapid detection of *E.Coli***

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### Abstract

Graphene oxide (GO) contains a large and planar sp<sup>2</sup> hybridized carbon domain with a high specific surface area having enriched oxygen-containing groups; which render GO excellent biocompatibility, high conductivity, stability, capability of binding protein via chemical or physical interaction. GO film –based nanoplatform are currently under investigation for detection of biomolecules and analyte with high specificity and sensitivity. In this study, GO-films were fabricated using 1mg/ml and 0.1mg/ml concentration of GO onto 5MHz AT-cut quartz crystal surface of a quartz crystal microbalance (QCM) through drop coating method and both were characterized by Fourier Transform Infrared spectroscopy. The coated QCM surface was activated with 1-Ethyl-3-(3-dimethylaminopropyl) carbodimide- N-Hydroxysuccinimide (EDC-NHS) method for antibody immobilisation. The *E.coli* detection was done using anti  $\beta$ -gal antibody which recognized the particular micro-organism containing  $\beta$ -galactosidase; an enzyme that initiates lactose sugar breakdown. The binding events were determined by decreasing resonant frequency of the quartz crystal mounted onto the quartz crystal microbalance (QCM). The confirmation was made by studying the change in surface morphology using scanning electron microscopy (SEM), Electron Diffraction Spectroscopy (EDS). This QCM nanobiosensor based on graphene oxide nano-film fabricated and demonstrated for the rapid, sensitive and label free detection of *E.coli*; is a better technique to overcome the shortcoming of conventional QCM biosensors. The Graphene oxide nano-film based Quartz Crystal Microbalance (QCM) biosensor was developed and tested for the rapid detection of *E.coli*. The novelty of this work is to use graphene oxide; which is a single monomeric unit of Graphite, when fabricated over Au coated crystal surface forms a stable and ordered film. This thin film of graphene oxide on AT cut gold



coated quartz crystal appears to be thermally more stable at room temperature, and provide a better platform for attachment of antibodies through EDC-NHS complex in comparison of direct thiolated gold surface of QCM.

**Nano Silica Supported Lipid Bilayers (Protocells) As a Drug Vehicle for  
Cancer Therapy**

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### **Abstract**

Preparing an efficient drug delivery vehicle for cancer is always challenging. The present study was designed to develop and compare nanosilica containing nano liposomes, conventional liposome and PEG-liposome. The effort was made to study drug encapsulation efficiency and in vitro release of drug whether nanosilica -loaded nanovesicles could sustain the release of the drug by increasing residence time and thus, Vincristine sulphate could reduce its dose-related systemic toxicity. There were good encapsulation efficiency for nanosilica supported liposome 71% which is comparable to the conventional & PEG-liposome which was 74% & 78% respectively. The obtained vesicles were within 100- 150 nm. When the in vitro drug release was compared, it was found that the conventional liposomes released about 67% drug in 150 min, PEG-liposome released about 42% whereas the drug release was just 52% from the nanosilica encapsulated liposome in 150 min. The intermediate value of nanosilica supported liposome indicates the ability of stable and controlled release of drug, which prevents the rapidly bursting or release of drug and very slower release of drug. Thus, nanosilica supported liposome could be a better choice for delivery of cancer drug like Vincristine sulphate.

**Keywords:** mesoporous silica nanoparticle (MSN), liposomes, protocells, PEG-liposome.

## **Formulation and Characterization of Polylactide-Co-Glycolide (PLGA) Nanoparticles of Nateglinide and Its Bioavailability Study in Rabbits**

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### **Abstract**

The main objective of the present study is to develop sustained release nanoparticles for nateglinide an antidiabetic drug, used in the treatment of type-2 diabetes. The usual dosing regimen of drug in conventional dosage form is thrice a day due to its shorter half-life of 1.5 hours which requires frequent administration of 3 times a day. The PLGA-Nateglinide nanoparticles were formulated by nanoprecipitation method. Prior to the study, a compatibility study between PLGA and nateglinide was carried out by FT-IR and DSC studies to determine possible interactions between drug and polymer. Various formulation parameters such as drug to polymer ratio, effect of stirring rate, particle size determination, zeta potential, poly dispersity index, drug content, drug entrapment efficiency, *in vitro* release studies and oral bioavailability studies using rabbit model were systematically investigated. The average size of nanoparticles was found to be 135.7 nm with a polydispersity index of 0.285 and the zeta potential value of -4.91 mV. The *in vitro* release profile of drug from nanoparticles was found to be sustained over a period of 24 hours. The release of drug from the system followed first order kinetics obeying non-fickian diffusion. The *in vivo* bio distribution study indicated that the drug from nanoparticles is capable of exhibiting the sustained release over a period of time as compared to pure drug in suspension form. The developed nanoparticles formulation of nateglinide exhibited longer time to reach peak concentration ( $T_{max}$ ), prolonged elimination half-life ( $t_{1/2}$ ), improved oral bioavailability ( $AUC_{0-\infty}$ ) than drug in suspension form and appear to be more consistent in overall performance. This indicates that the drug from nanoparticles may be capable of reducing the dose intake, minimize the blood level oscillations, dose related adverse effects, cost and ultimately improve the patient compliance in the therapeutic management of diabetes mellitus.

**Keywords:** nateglinide, PLGA nanoparticles, nanoprecipitation, bioavailability study

## **Formulation of Poly lactide-Co-Glycolide Nanoparticles Incorporating Lenalidomide and Its Bio-Distribution Study in Rats**

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### Abstract

The main objective of the present study is to develop nanoparticulate drug delivery system of lenalidomide, an anti-cancer drug, used for the treatment of multiple myeloma. The half-life of lenalidomide is 1.8 hours, and results in poor bio-distribution in the target organ. So, the aim of the present study is to formulate a successful delivery system by reducing the dose intake and better drug utilisation and offer sustained release of drug to respective organs. The PLGA-lenalidomide nanoparticles were formulated by nanoprecipitation method. Prior to the study, a compatibility study between PLGA and lenalidomide was determined using FTIR. The various parameters such as effect of drug to polymer ratio, effect of stirring rate were systematically investigated. Nanoparticles have been used to enhance drug delivery to tumour cells with lower toxicity to healthy cells. The average size of nanoparticles was found to be 455.8 nm with a polydispersity index of 0.559 and the zeta potential value of 34.9 mV. The entrapment efficiency of drug was found to be in the range of 51.4-80.15%. The *in vitro* release profile of drug from nanoparticles was found to be sustained over a period of 24 hours. The release of drug from the system followed first order kinetics obeying non-fickian diffusion. The *in vivo* bio distribution study indicated that the drug from nanoparticles found to be increased in heart, lungs and kidneys and decreased drug distribution to liver. This indicates that the drug from nanoparticles exhibited better sustaining efficacy and may produce less hepatotoxicity as compared to drug in solution form.

Key words: Lenalidomide, PLGA nanoparticles, nanoprecipitation, bio distribution studies.

### **Egg albumin based non-woven nanofiber scaffolds for tissue engineering**

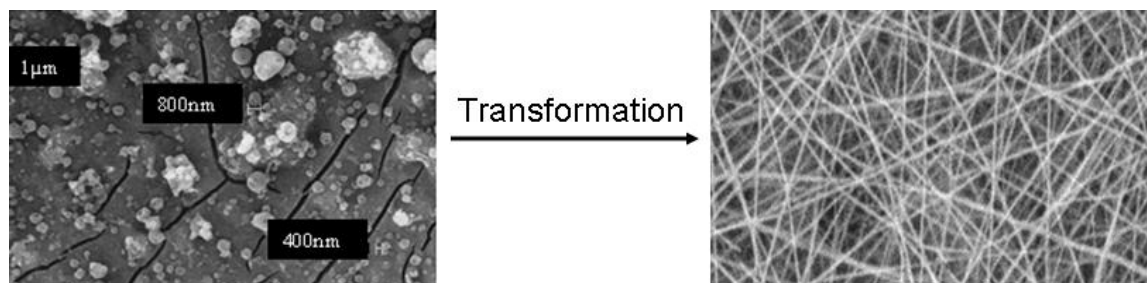
**Komal Pandey , Shubhang Agrawal , G. Vannurswamy, Irfan Khan and GVN Rathna \***

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### Abstract

The nanofiber scaffolds having the fiber diameter less than 1000 nanometers are more advantageous as compared to bulk scaffolds because of large surface area, better interaction with cells, tissue resemblance, enhanced hydrophilicity and biocompatibility. Poly-ε-caprolactone (PCL) is hydrophobic and biodegradable polyester with the ester linkages, which hydrolyse in physiological conditions in the human body and therefore used for biomedical applications. Polylactic acid or polylactide (PLA) is also a hydrophobic and thermoplastic polyester derived from various renewable resources, it is highly exploited for biomedical applications as it is biodegradable and biocompatible. Egg albumin (EA) is hydrophilic and highly functional globular protein with thermally crosslinkable disulfide linkages. Development of composites of PCL/PLA/EA nanofiber scaffolds will enable a new nanomaterial with improved properties for tissue engineering. In our study, we explored the development of non-woven nanofiber scaffolds of PCL/PLA/EA of various compositions. The morphology of the nanofibers was evaluated using environmental scanning electron microscopy (ESEM). The molecular weight of EA, polymer interactions, thermal and crystalline properties were analysed by gel electrophoresis (GL), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) and X-ray diffraction spectroscopy (XRD).



**Electro-sprayed egg albumin Electrospun nanofibers of PCL/PLA/EA**

## **Preparation and the study of Zinc Polyacrylate Cement: Dental Cement Behavior and properties**

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### **Abstract**

The solution polymerization method at 90<sup>0</sup>C was performed for the synthesis of Polyacrylic acid (PA) and the deactivated Zinc Oxide (ZnO) was obtained by heating at 1000<sup>0</sup>C and powdered. These powdered pre-materials were used for the development of the dental cement. The deactivated ZnO powder (approx. 75mm particle size) mixed with 40% aqueous polyacrylic acid with ratio of 1.5:1 (powder: liquid) to develop the polycarboxylate cement. The polyacrylic acid and polycarboxylate cement were characterized by TGA, DTA, FTIR, SEM and XRD studies. The viscosity average molecular mass of polyacrylic acid was determined for better result. The thermal stability of the polymer and the cement was evaluated by analyzing the TGA data. Which provides the various kinetic parameters like activation energy, Arrhenius (frequency) factor and entropy changes associated with the thermal decomposition of polyacrylic acid and polycarboxylate cement. It is inferred from the DTA and XRD data that incorporation of Zn<sup>2+</sup> ions (from ZnO) significantly enhanced the degree of crystallinity in the polycarboxylate cement. The setting time, compressive strength and diametral tensile strength of polycarboxylate cement was evaluated in this research article.

Keywords: Polyacrylic acid (PA), Zinc Oxide, Dental cement, TGA, DTA, FTIR, SEM and XRD

**Synthesis and Characterization of novel Poly(ether-ether-ketone)s from  
bisphenol containing ether- amide linkage**

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### Abstract

A new bisphenol containing ether-amide linkages, N, N'-Bis (4-hydroxyphenoxyphenylene) isophthalamide, IPCD (I) was synthesized and characterized by FT-IR, <sup>1</sup>H, <sup>13</sup>C NMR and Mass Spectrometry. A series of novel aromatic poly(ether-ether-ketone)s (PEEKs) was prepared by polymerization of difluorobenzophenone (DFB) with IPCD (I) and / or Bisphenol-A in different mole % proportions. These polymers were characterized by IR, viscosity measurement, solubility, TGA, DSC and XRD. The polymers had moderate to high molecular weights as evidenced by the inherent viscosities ( $\eta_{inh}$ ) in the range 0.51 – 0.69 dL/g. The polymers readily dissolved in N-methyl-2-pyrrolidone (NMP), N,N-dimethylacetamide (DMAc), N,N-dimethylformamide (DMF), m-cresol, pyridine and conc.H<sub>2</sub>SO<sub>4</sub>. Polymers did not show any weight loss below 325 °C and retained 25 to 50 % weight at 900 °C (Char yield) when investigated by TGA under nitrogen atmosphere demonstrating good thermal stability.

**Keywords:** N, N'-Bis (4-hydroxyphenoxyphenylene) isophthalamide, inherent viscosities, solubility, thermal properties

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## **Solution and Film Properties of Semi-rigid Rod Polyphenylenes and Polyphenylsulfones**

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### **Abstract**

Determination of the solution parameters of recently commercialized polyphenylene materials (PrimoSpire™) is of both scientific and commercial interest, to gain understanding of the molecular characteristics of the polymers and to assess their potential utility in film and coatings applications. Solution parameters of two grades of PrimoSpire™ (PR-120 and PR-250) and Radel R5100 NT (R5100) were investigated. The polymers were then blended in solutions of n-methyl pyrrolidone (NMP) and their miscibility and film formation properties evaluated. The radius of gyration ( $R_g$ ), second virial coefficient ( $A_2$ ), and weight-average molecular weight ( $M_w$ ) were determined by multi-angle laser light scattering (MALLS). The hydrodynamic radius ( $R_h$ ) was measured using dynamic light scattering (DLS). Solubility parameters and shape factors were estimated from these studies. Differential scanning calorimetry (DSC) was used to evaluate the miscibility characteristics of the blends, and measured  $T_g$ 's compared to those predicted by the Fox equation for miscible blends. Atomic force microscopy (AFM) was used to image morphology development of the film surfaces at both the air/solution and glass/solution interfaces. MALLS and DLS studies indicate the polymers assume a semi-rodlike conformation in solution. Blend miscibility is a function of polymer structure, solution processing and blend composition. Results from these evaluations and plans for future studies will be reviewed.

**Synthesis and Characterization of New Soluble Poly(amide-imide)s from bis-  
[(4'-aminobenzyl)-4-benzamide] ether**



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### Abstract

A novel aromatic diamine, bis-[(4'-aminobenzyl)-4-benzamide] ether (BABE) containing preformed amide, ether and methylene groups was synthesized and characterized by FT-IR, NMR (<sup>1</sup>H, <sup>13</sup>C, DEPT <sup>13</sup>C) and Mass spectrometry. A series of novel aromatic poly(amide-imide)s was prepared from BABE and different aromatic dianhydrides using two-step low temperature solution polycondensation method. All the poly(amide-imide)s were obtained in very good yields and were characterized by FT-IR Spectroscopy, viscosity measurements, solubility tests, differential scanning Calorimetry (DSC), thermogravimetric analysis (TGA) and X-ray diffraction (XRD). The inherent viscosities ( $\eta_{inh}$ ) of these poly(amide-imide)s were in the range 0.57-0.87 dL/g in DMAc at 30 ± 0.1 °C; indicating moderate to high molecular weight buildup. The poly(amide-imide)s showed solubility in aprotic polar solvents such as N-methyl-2-pyrrolidone (NMP), N,N-dimethylacetamide (DMAc), dimethyl sulphoxide (DMSO) and N,N-dimethylformamide (DMF) containing LiCl. The XRD results showed that the poly(amide-imide)s were partly crystalline. The glass transition temperature ( $T_g$ ) of these poly(amide-imide)s were in the range 251 to 274 °C. The thermogravimetric analysis of all polymers showed no weight loss below 322°C whereas the char yields at 900 °C were in the range 21 to 58 % indicating high thermal stabilities of these polymers. Thus these polymers meet high temperature resistant requirements and could find applications as special materials in aerospace, military and microelectronics industries. The structure–property correlation among these poly(amide-imide)s is discussed.

**Keywords:** Bis-[(4'-aminobenzyl)-4-benzamide] ether, inherent viscosity, XRD, thermal stability. \* To whom the correspondence to be addressed; Phone: (217)-2744772, 094210 42158; Fax: (217)-2744770.

**Effect of Oligomeric modified MMT clay on Mechanical Properties and Rheological Behavior of Poly (butylene terephthalate) / Organoclay Nanocomposites**

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**Abstract**

Polymer/clay nanocomposites have been extensively studied to enhance the properties of polymer by incorporation of small amount of clay, usually modified with organic cations, preferably containing long alkyl chains, which are exchanged with the inorganic cations in the clay gallery. In this work clay was modified with two different oligomeric surfactant viz: poly(styrene-co-vinylimidazole) and poly(styrene-co-4-vinyl pyridine) quarternized with benzyl chloride. The oligomeric modified clay contains 50% clay and 50% oilgomic surfactant. The oilgomic modified clay was used to prepare nanocomposites of PBT by melt blending. The resulting nanocomposites were evaluated for mechanical and rheological properties.

## Improving the Functionality of Biocomposite Scaffolds with Cellulose Nanocrystals

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### Abstract

The development of composite materials for bone tissue engineering has been strongly affected by both the advent and its consolidation of tissue engineering applications. Many composite materials based on natural and/or synthetic polymers have been fabricated and characterized for reconstruction of organs so that they can exhibit improved cytocompatibility with appropriate mechanical strength. Therefore, while designing a composite scaffold, certain factors must be taken into consideration such as consistency of mechanical properties with target site, high surface area to facilitate cell seeding and diffusion, and degradation stability according to rate of tissue formation within the body. Hence, green biocomposite scaffolds that blend natural and synthetic polymers can exploit the advantages of both types of polymers. In addition, biomaterial especially cellulose nanocrystals can improve the mechanical properties of the perspective bionanocomposite scaffolds. For this green chemistry point of view, ovalbumin (OVA) as natural polymer and polyvinyl alcohol (PVA) as biodegradable synthetic polymer were considered for fabricating the biocomposites, and for improving mechanical strength of biocomposites, sugarcane bagasse based cellulose nanocrystals were applied. Cellulose nanocrystals and as produced biocomposites scaffolds were characterized using scanning electron microscopy (SEM), atomic force microscopy (AFM), fourier transform infra-red (FTIR), X-ray diffraction (XRD), thermal properties (TGA-DTG-DTA). Thus, preliminary study demonstrates the further applicability of the materials for biocomposite scaffolds for tissue engineering applications.

**Keywords:** Cellulose nanocrystals; Biocomposites; OVA; Scaffolds; Tissue engineering.

# Hydrogen-Bonding Induced Assembly of Donor and Acceptor Chromophores: Self-Sorting vs. Mixing

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## Abstract

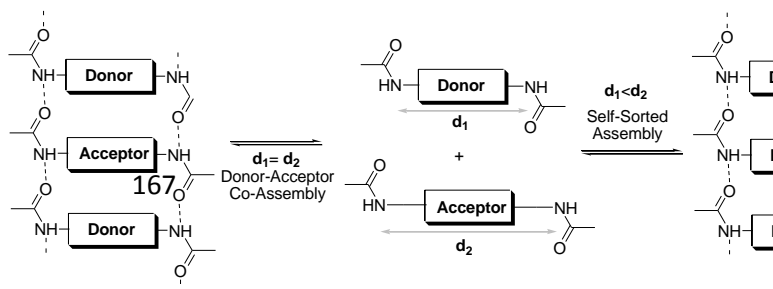
Supramolecular-assembly in donor (D) and acceptor (A) mixed system can be of two types; (i) orthogonal assembly (ii) D-A co-stacking. Suitable and generalized strategy for gaining control over the mode of self-assembly is important due to their implications in various opto-electronic devices. We

**Figure.1. Figure representing growth of carbonyl index in the  $1715\text{ cm}^{-1}$  region of FT-IR spectrum as a result of photo-irradiation with increasing hours**

realized that this can be achieved in bis-amide functionalized D and A  $\pi$ -systems by varying the *distances between the two amide functionalities* (Scheme 1). It is conceivable that if the distance matches for a particular D-A pair, alternate stacking will be favourable one. On the other hand if the distance does not match, self-sorted assembly will be the major one to gain the synergistic effect of inter-molecular H-bonding and  $\pi$ - $\pi$  interaction.

To test this hypothesis, we examined self-assembly among a bis-amide functionalized dialkoxynaphthalene (DAN)-derivative **DAN-1** with naphthalene-diimide (NDI)-derivatives **NDI-2** (Scheme 2). The number of methylene units between the chromophore and the amide functionality were adjusted in such a way that for (**DAN-1**+**NDI-2**) pair the distance between two amides were not equal.

Detailed spectroscopic studies in solution as a function of solvent and



**Scheme 1:** Schematic presentation of the proposed design for self-sorted

temperature indeed revealed self-sorted assembly and gelation for (**DAN-1** + **NDI-2**) pair and at no stage any signature of CT-interaction could be noticed. Appropriate control experiments were performed to demonstrate that if the distances were almost matched between the two amide groups in case of donor and acceptor chromophores then indeed CT-interaction induced self-assembly could be achieved. To gain better insight into the self-sorting phenomenon we synthesized the chiral-NDI derivative **NDI-1** in which the distance between the two amide bonds remain unchanged compared to that in **NDI-2**. In this case circular-dichroism (CD) studies revealed intense cotton effect due to self-assembly in non-polar solvent. Surprisingly when **NDI-1** was mixed with **DAN-1**, CD-bands were visible corresponding to both the chiral acceptor as well as the achiral donor chromophore. To explain this unprecedented observation, we synthesized **DAN-2** in which the peripheral groups consist of hydrophilic oligo-oxyethylene chains instead of hydrophobic chains as in **DAN-1**. Herein we found in the mixed D-A assembly CD-band was visible only corresponding to the acceptor absorbance. Details solvent and temperature variable CD-studies prompted us to conclude this as an example of chiral induction from the self-sorted chiral acceptor stack to the neighbouring donor-stack due to hydrophobic interaction. This in broader sense revealed there was no macroscopic phase separation among the molecularly self-sorted individual donor and acceptor stacks. In this presentation, detail photophysical studies related to self-assembly process of these donor-acceptor  $\pi$ -systems and its relevance in the context of broader applicability will be discussed.

**Keywords:** Self-assembly, H-Bonding, Donor-Acceptor, Self-sorting, Organogel, Charge-Transfer

**References:**

1. M. R. Molla, A. Das, and S. Ghosh, *Chem. Eur. J.* **2010**, *16*, 10084-10093.
2. M. R. Molla, A. Das, and S. Ghosh, *Chem. Commun.* **2011**, *47*, 8934-8936.

## **Glycolic acid-g-chitosan-Pt-Fe<sub>3</sub>O<sub>4</sub> nanoparticles nanohybrid scaffold for tissue engineering and drug delivery**

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### **Abstract**

This work presents the potential use of novel nanohybrid based on chitosan-g-glycolic acid and Pt-Fe<sub>3</sub>O<sub>4</sub> composite magnetic nanoparticles in drug delivery and tissue engineering applications. The Pt-Fe<sub>3</sub>O<sub>4</sub> hybrid magnetic nanoparticles are prepared by thermal decomposition of H<sub>2</sub>PtCl<sub>6</sub>.6H<sub>2</sub>O at high temperature. The prepared magnetic nanoparticles were characterised by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and Physical property measurement system (PPMS). In the next step, the drug loaded novel nanohybrid porous scaffold based on chitosan-g-glycolic acid and Pt-Fe<sub>3</sub>O<sub>4</sub> composite nanoparticle have been prepared by freeze drying of the grafted polymer solution. Drug loading and grafting of chitosan was characterised by Fourier transform infrared spectroscopy (FT-IR). The cell proliferation also shows that the prepared nanohybrids are biocompatible. The nanohybrid was found to be stable regardless of pH of the medium. Therefore, Pt-Fe<sub>3</sub>O<sub>4</sub> hybrid magnetic nanoparticles are viable additive for sustained drug delivery and it could be applied in the field of biomedical.

# Improved Mechanical and Photophysical Properties of Chitosan Incorporated Folic Acid Gel Possessing the Characteristics of Dye and Metal Ion Absorption

Priyadarshi Chakraborty, Bappaditya Roy, Partha Bairi and Arun K. Nandi\*

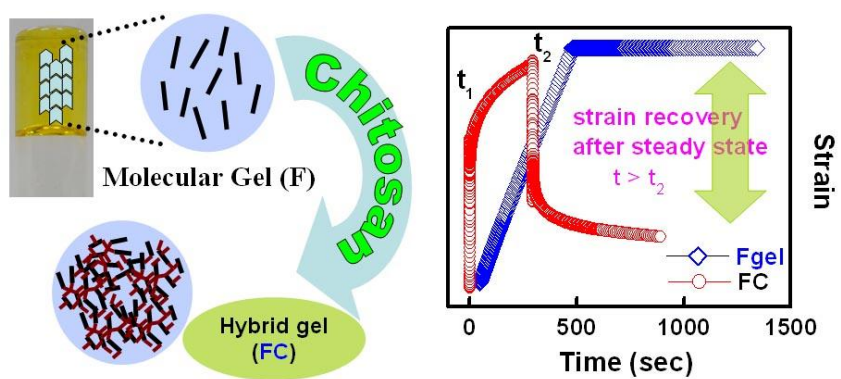
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## Abstract

The folic acid (**F**) gel, prepared in a 1:1 dimethyl sulfoxide (DMSO) - water mixture (v/v), at 0.2 % (w/v) concentration has nano-fibrous network morphology. FTIR spectra indicate the presence of the intermolecular H-bonding interaction in the gel. The folic acid-chitosan (**C**) hybrid (**FC**) gel appears as a yellow transparent semisolid mass consisting of nano-fibrous network with a higher density of branches. The fibrillar diameter of the **FC** hybrid gel is much lower than that of **F** gel. The FTIR band at  $3390\text{ cm}^{-1}$  of **F** gel shows a shift to  $3435\text{ cm}^{-1}$  in the **FC** hybrid gel indicating hydrogen bonding interaction between **C** and **F**. The fluorescence intensity of the **FC** hybrid gel is enhanced by 2.75 times than that of **F** gel. The shear viscosity of **FC** hybrid gel is 3 orders higher than that of the **F** gel and both the gels exhibit shear thickening at low shear rate ( $<10^{-3}\text{ s}^{-1}$ ) but above that, shear-thinning occurs. In the creep phase, for **FC** hybrid gel exhibits the strain recovery but the **F** gel does not. The complex modulus ( $G^*$ ) of both the systems initially exhibit sharp increase, followed by a slow increase with time (t) and  $dG^*/dt$  varies with **C** concentration in the **FC** hybrid gel showing a maximum. The WAXS pattern of the **FC** hybrid xerogel does not exhibit any crystalline peak suggesting that the additive (**C**) inhibits the crystallization of **F**. The dye absorption by the hybrid gel material is maximum for eosin yellow, however, methyl orange and methylene blue are absorbed to a lesser extent. The **FC** hybrid gel absorbs  $\text{Cu}^{2+}$ ,  $\text{Cr}^{3+}$  and  $\text{Co}^{2+}$  from their respective solutions.



Reference:

P. Chakraborty, B. Roy, P. Bairi, A. K. Nandi, *J. Mater. Chem.*, 2012, **22**, 20291-20298



## Highly Fluorescent Graphene Oxide-Poly(vinyl alcohol) Hybrid: An Effective Material For Specific Au<sup>3+</sup> Ion Sensor

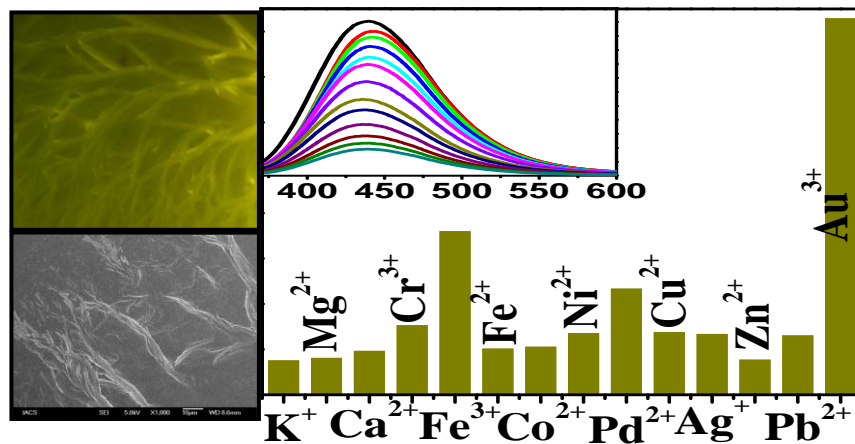
**Aniruddha Kundu, Rama K. Layek, Atanu Kuila and Arun K. Nandi\***

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### Abstract

We have developed a new highly fluorescent graphene oxide (GO) / poly(vinyl alcohol) (PVA) hybrid (GO-PVA) in acidic medium (pH 4). The hybrid is highly fluorescent due to passivation by H-bonding as evident from Raman and FTIR spectra. The fluorescent microscopic images of the hybrids exhibit fibrillar morphology and all of them emit highly intensified green light. FESEM micrographs also show fibrillar morphology which is produced due to the supramolecular organization of GO-PVA complex. The highly fluorescent GO-PVA1 hybrid has been used as a fascinating tool for selective sensing of Au (III) ions in aqueous media with a detectable limit of ~ 275 ppb. The sensitivity of Au (III) ion (300  $\mu$ M) in presence of 600  $\mu$ M concentrations of other ions and in presence of biologically analog mixture (D-glucose, D-Lysine, BSA, Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup>, Mg<sup>2+</sup>, Zn<sup>2+</sup>) (600 $\mu$ M each) suggest that the GO-PVA1 hybrid is an efficient sensor of Au (III) ions. The average lifetime of GO at pH 4 increases in the GO-PVA1 hybrid indicating the formation of a more stable excited state but the increase in lifetime value after addition of Au(III) salt solution to the hybrid solution indicates a dynamic quenching. The selectivity of sensing of Au (III) is attributed to higher value of its reduction potential than that of other metal ions and XPS data of GO-PVA1 hybrid with 300  $\mu$ M Au(III) substantiate the reduction of Au(III) to Au<sup>0</sup> due to the transfer of excitons from the hybrid facilitating the selective PL-quenching.



**Reference:**

A. Kundu, R. K. Layek, A. Kuila, and Arun K. Nandi; *ACS Appl. Mater. Interfaces*,  
**DOI:** 10.1021/am301467z

## Fluorophore-Labeled Poly(ethylene glycol)-Peptide-Poly(ethylene glycol) Biohybrid Block Copolymer: Synthesis and Aggregation

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### Abstract

At the present decade, there is a much interest in developing peptide based amphiphiles and block copolymers containing biomimetic peptide sequences due to its wide scale applications in bionanotechnology. In this work, we successfully synthesized a new kind of amphiphile consisting of poly(ethylene glycol)-peptide-poly(ethylene glycol) (PEG-pep-PEG) biohybrid having a hydrophobic fluorophore moiety via 'grafting to' technique. This hybrid contains the hydrophobic tripeptide with the attachment of fluorophore moiety conjugated to hydrophilic PEG of molar mass 2000, which serves as a simple model peptide based amphiphile. The hybrid is characterized by NMR, FTIR and CD spectroscopy. The micellar aggregation of the hybrid in water is confirmed from transmission electron microscopic (TEM), field emission scanning electron microscopic (FESEM) and dynamic light scattering (DLS) results. Association of hydrophobic aromatic phenylalanine residues of the biohybrid occurs due to its micellization, as revealed by circular dichroism (CD). A critical aggregation concentration associated with the formation of hydrophobic domains due to the aggregation of hybrid amphiphilic molecules is determined through fluorescence spectroscopy in presence of pyrene as a fluorescent probe.

## Nano Functionalized Biodegradable Corn Zein Protein Biopolymer

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### Abstract

Biodegradable corn zein protein (CZP) film with  $\text{TiO}_2@ \text{SiO}_2$  nanoparticles were prepared by solution casting technique. CZP solution with 1.5% of  $\text{TiO}_2@ \text{SiO}_2$  was subjected different levels sonication i.e. 0, 16, 80 and 160  $\mu\text{m}$  amplitude to improve the mechanical properties and uniform distribution of nano particles in the films prior to casting. Mechanical and microstructural properties of nano functionalized films were determined by tensile testing and TEM, respectively. The results presented in this study show the feasibility of using bio-nanocomposite technology to improve the properties of CZP biopolymer films. The influence of blending  $\text{TiO}_2@ \text{SiO}_2$  and sonication was systematically investigated. Films with nanoparticles showed better mechanical properties than films without nanoparticles but almost half reduction in elongation (tensile strain, %) was observed. Films without nanoparticle had lower tensile strength and higher percentage of elongation. Level of sonication and thickness of films has significant effect on tensile properties of CZP films with or without nanoparticles. TEM shows the distribution of  $\text{TiO}_2@ \text{SiO}_2$  in the films. CZP sheet and blown films were also prepared using extrusion. First, pellets were made by dry extrusion and then subjected to extrusion through slit die to produce sheet/film whereas, CZP dissolved in ethanol and precipitate extrusion failed to yield any results.

## Mechanical, Photophysical, Dye and Metal Ion Absorption Properties of Chitosan Reinforced Folic Acid Supramolecular gel

**Priyadarshi Chakraborty, Bappaditya Roy, Partha Bairi and Arun K. Nandi\***

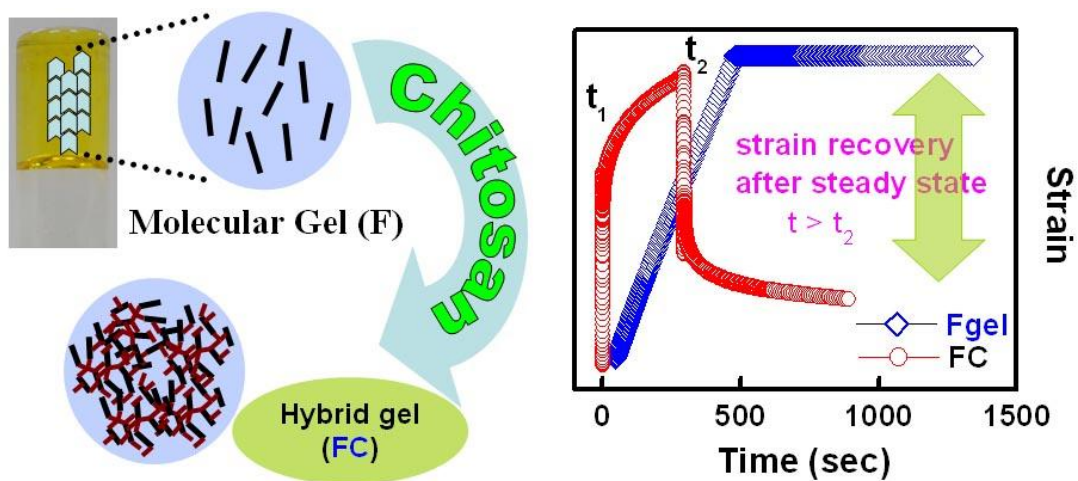
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### Abstract

The folic acid (**F**) gel, prepared in a 1:1 dimethyl sulfoxide (DMSO) - water mixture (*v/v*), at 0.2 % (*w/v*) concentration has nano-fibrous network morphology. FTIR spectra indicate the presence of the intermolecular H-bonding interaction in the gel. The folic acid-chitosan (**C**) hybrid (**FC**) gel appears as a yellow transparent semisolid mass consisting of nano-fibrous network with a higher density of branches. The fibrillar diameter of the **FC** hybrid gel is much lower than that of **F** gel. The FTIR band at 3390  $\text{cm}^{-1}$  of **F** gel shows a shift to 3435  $\text{cm}^{-1}$  in the **FC** hybrid gel indicating hydrogen bonding interaction between **C** and **F**. The fluorescence intensity of the **FC** hybrid gel is enhanced by 2.75 times than that of **F** gel. The shear viscosity of **FC** hybrid gel is 3 orders higher than that of the **F** gel and both the gels exhibit shear thickening at low shear rate ( $<10^{-3} \text{ s}^{-1}$ ) but above that, shear-thinning occurs. In the creep phase, for **FC** hybrid gel exhibits the strain recovery but the **F** gel does not. The complex modulus ( $G^*$ ) of both the systems initially exhibit sharp increase, followed by a slow increase with time (*t*) and  $dG^*/dt$  varies with **C** concentration in the **FC** hybrid gel showing a maximum. The WAXS pattern of the **FC** hybrid xerogel does not exhibit any crystalline peak suggesting that the additive (**C**) inhibits the crystallization of **F**. The dye absorption by the hybrid gel material is maximum for eosin yellow, however, methyl orange and methylene blue are absorbed to a lesser extent. The **FC** hybrid gel absorbs  $\text{Cu}^{2+}$ ,  $\text{Cr}^{3+}$  and  $\text{Co}^{2+}$  from their respective solutions.



Reference:

P. Chakraborty, B. Roy, P. Bairi, A. K. Nandi, *J. Mater. Chem.*, 2012, **22**, 20291-20298

## Reversible Addition Fragmentation Chain Transfer (RAFT) polymerization Of a Fluoroacrylate in Miniemulsion

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### Abstract

Fluoropolymers are high performance polymers, because of their unique mechanical, thermal, and surface properties. Controlled/living radical polymerization (CRP) of a fluoroacrylate was successfully carried out in miniemulsion by Reversible Addition-Fragmentation chain Transfer (RAFT) process. In this case 2,2,3,3,4,4,4-heptafluorobutyl acrylate (HFBA) was polymerized using a hydrophobic RAFT agent 2-cyanopropyl dodecyl trithiocarbonate (CPDTC). Being compatible with hydrophobic fluoroacrylates this RAFT agent offers very high conversion and good control over the molecular weight of the polymer. In this case the miniemulsion was stable without any co-stabilizer. The polymerization kinetics was studied for both KPS and AIBN initiated system as well as varying the concentration of ionic (SDS) and non ionic surfactant (Triton X-405). A linear decrease in reaction rate was observed with increase in surfactant concentration. The molecular weight ( $M_n$ ) and polydispersity index (PDI) were determined by GPC analysis. The particle size of the miniemulsion and its stability in terms of zeta potential were determined by dynamic light scattering (DLS) analysis. Transmission Electron Microscopy (TEM) analysis showed dispersion of nano-sized polymer particles in miniemulsion. TGA analysis showed that the polymer has excellent thermal stability.

**Keywords:** CRP, RAFT, miniemulsion, fluoroacrylate, SDS, TritonX-405

## Effect of Multiwall Carbon Nanotubes [MWCNTs] On the Properties of Polypropylene Random Copolymer

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### **Abstract**

Polymeric nanocomposites have been the subject of intense research interest over the past two decades in academia and industry, spawned by advances such as the discovery of spherical fullerenes and carbon nanotubes. As nano fillers are projected to provide advanced performance capabilities for engineering polymer applications, imparting the high strength and modulus obtained with traditional fillers without their negative side effects, such as reduced processability and impact strength. As compared to other nanofillers, carbon nanotubes (CNTs) have emerged as the most promising nanofiller for polymer composites due to its remarkable thermal/mechanical and electrical properties. Incorporation of CNTs in polymer matrices provides materials that could be used for many high performance engineering applications.

Therefore, present study was carried out to investigate the effect of multiwalled carbon nanotubes [MWCNTs] on the properties of polypropylene random copolymer (PPCP). MWCNTs were synthesized using chemical vapor deposition (CVD) method. PPCP nanocomposites based on MWCNTs were prepared using melt blending and their thermal, electrical, mechanical, rheological and morphological properties were evaluated.

*Keywords: PPCP-Multi-walled carbon nanotube Nanocomposites, Melt blending*



## Effect Of Nanoclay On The Properties Of Poly(Methyl Methacrylate)

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### Abstract

The present study deals with the preparation of PMMA/clay nanocomposites by bulk polymerization of MMA in presence of varying amounts of Cloisite 30B – an organically modified montmorillonite (OMMT) . The nanocomposites were characterized for their structural, thermal and morphological behaviour using wide angle X-ray diffraction (WAXD), dynamic mechanical analysis (DMA), thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The presence of nanofiller significantly enhances the thermal stability of PMMA [ as observed by TGA] and increase in glass transition temperature was observed by differential scanning calorimetry (DSC). The viscoelastic properties were measured as a function of temperature by using DMA. The storage moduli of all nanocomposites were found to be higher than pure PMMA. Overall, the best properties improvement of the nanocomposites was observed at clay loading of 0.5 wt %.

Keywords: PMMA, OMMT, Nanocomposites etc.

## Polyalicyclic Polyimides and Silica Gel Hybrids

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### Abstract

The preparation of polyimide-silica gel hybrids by the simultaneous *in situ* formation of polyimides during the hydrolysis-cum-condensation of tetramethoxy-silane (TMOS) is reported. The hydrolysis-cum-condensation of TMOS was effected in N,N-dimethylacetamide (DMAc) containing 5% ZnCl<sub>2</sub> and the seven-membered cyclic polyimide intermediate obtained by reacting each of the dianhydrides, i.e., bicyclo(2.2.2)oct-7-ene-2,3,5,6-tetracarboxylic dianhydride (BICODA), 5-(2,5-dioxotetrahydrofuryl)-3-methyl-3-cyclohexene-1,2-dicarboxylic anhydride (DTMCDA) and 4-(2,5-dioxotetrahydrofuran-3-yl)-1,2,3,4-tetrahydronaphthalene-1,2-dicarboxylic anhydride (DTTDA), with diisocyanates, i.e., isophorone diisocyanate (IPDI), toluene diisocyanate (TDI), hexamethylene diisocyanate (HMDI) and 4,4'-methylenebis(phenyl isocyanate) (MDI). Transparent hybrid films could be obtained by casting from their respective solutions. Pyrolysis of the hybrids (PIH-2, PIH-7 and PIH-8) at 600 °C for 24 h gave porous silica gels. Nitrogen adsorption-desorption isotherm studies on pyrolyzed silica gels (Gel-2, Gel-7 and Gel-8) revealed a pore radius (BJH method) of 1.8 nm, and surface areas (from BET plots) of 384 m<sup>2</sup> / g, 305 m<sup>2</sup> / g, and 298 m<sup>2</sup> / g, respectively. The mesoporous, bottle-shaped pores had a pore volume of 0.237 cm<sup>3</sup> / g, 0.277 cm<sup>3</sup> / g, and 0.297 cm<sup>3</sup> / g, respectively. Computer modeling studies indicated that the polyimide chains were fairly distended or folded and there was no agglomeration of chains.

## Antibacterial Fiber Materials for Defence Application

**Ramdayal, Balasubramanian K\*.**

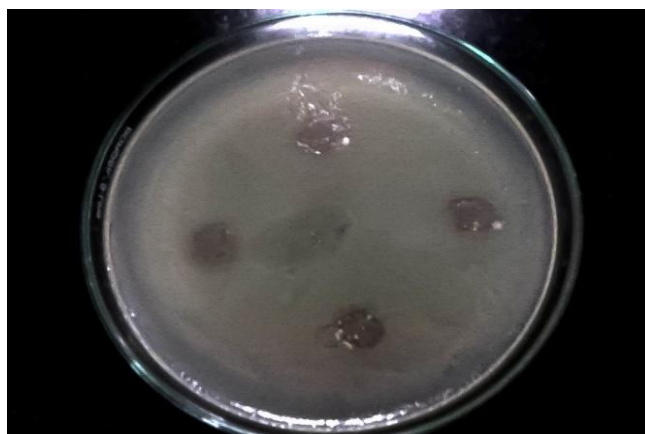
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### Abstract

Most textile materials currently used in military are conducive to cross-infections or the transmission of diseases caused by microorganisms. These infections are mainly caused by Gram positive *Staphylococcus aureus* (*S. aureus*), *Bacillus subtilis* (*B. subtilis*), and Gram negative *Pseudomonas aeruginosa* (*P. aeruginosa*) and *Escherichia coli* (*E. coli*). To avoid infections, antimicrobial properties can be imparted to textile material by incorporating functional agents in fibers and fabrics. Usually, antibacterial loading in micro/nanoparticle can be achieved by incorporating additives during the preparation of the particles or after the formation of the particles by incubating additives with fibers. The ability to fabricate a variety of antibacterial constructs with the different morphology such as films, gels, foams, patches and fibers contributes to a broad application spectrum of the biomaterials.

In this study, high molecular weight poly (vinyl alcohol) (PVA) fiber of the diameter 70-80  $\mu\text{m}$  were prepared by adding antibacterial additives like curcuma longa, mangiferaindica, azadirachta indica, Cu nano particles,  $\text{TiO}_2$  and  $\text{ZrO}_2$ . Known concentration of antibacterial additives was solution mixed and viscosity of the solution was tailored such that a fiber can be produced by nozzle. Simultaneously, inexpensive and biofriendly foaming agents like sodium chloride and sodium bi-carbonate etc were added to impart porosity on fiber for improving its efficacy of nano/micro additives for antibacterial properties. Beyond 2 Wt% loading of nano/micro additives like curcuma longa, mangiferaindica, azadirachta indica, Cu nano,  $\text{TiO}_2$  and  $\text{ZrO}_2$ , the melt strength of PVA was affected, which resulted in poor fibers. Agglomeration of the additives in the fiber was also noticed. Antibacterial assessments were carried out against *E. coli*, *S. aureus* and *P. aeruginosa*. Filter paper disk method was used to determine the area of zone of inhibition formed by fibers. The obtained result showed that azadirachta indica possessed larger zone of inhibition compared to other additives as shown in figure-1.



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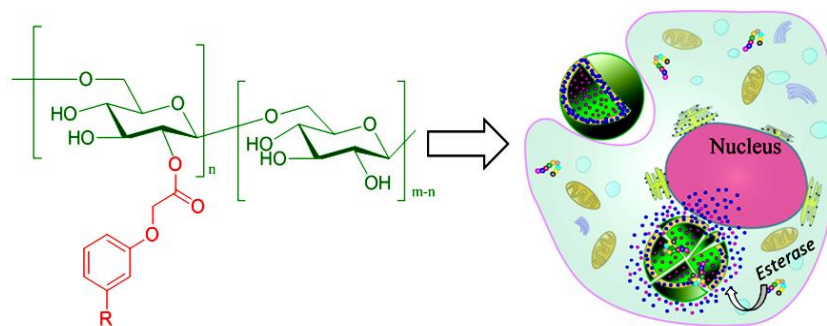
## Polysaccharide Vesicular Nanocarrier for Encapsulation and Delivery of Molecules into Cell

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### Abstract

In the last two decades polymeric vesicles (polymersome), have attracted rapidly growing interest based on their cell and virus mimicking dimension and potential application in the delivery of hydrophilic as well as hydrophobic anticancer drugs to tumor tissues <sup>1</sup>. The present work is emphasized to design dextran vesicular carriers using naturally available renewable resources based on cardanol, pentadecylphenol (PDP) and commercially available stearic acid as hydrophobic tails<sup>2</sup> The roles of the hydrophobic segments on the molecular self-organization of dextran into vesicular assemblies or nanoparticles were investigated using saturated and partially unsaturated units. The vesicular structure of the amphiphiles was confirmed by transmission electron microscopy (TEM) and scanning electron microscopy (SEM) and Atomic Force Microscopy (AFM), and Static Light Scattering (SLS) analysis. Dextran assemblies were found to be a unique dual carrier in which water soluble molecules (like Rhodamine-B, Rh-B) and polyaromatic anticancer drug (camptothecin, CPT) were selectively encapsulated in the hydrophilic interior and hydrophobic layer of the vesicles, respectively. The protection of active lactone form of CPT in the vesicular structure was proved using HPLC technique. The *in vitro* drug release experiments conducted at pH 7.4 PBS at 37° C revealed that Rh-B and CPT got released in a controlled manner. The aliphatic ester linkage connecting the hydrophobic tail with dextran was found susceptible to cleave by esterase under physiological conditions for fast releasing of CPT or Rh-B. Confocal microscopic images confirmed that both Rh-B and CPT-loaded vesicles was taken up by fibroblasts, better than Rh-B or CPT alone, showing a perinuclear localization in cells and CPT loaded vesicles were found to be 2.5 fold more effective in killing fibroblasts compared to that of CPT alone in PBS. The custom designed dextran vesicular provides new research opportunities for dual loading and delivering of hydrophilic and hydrophobic drug molecules.



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## Development of Dual Ester-urethane Melt polycondensation Approach for Small Molecules and Linear Polymers Based on Amino acids

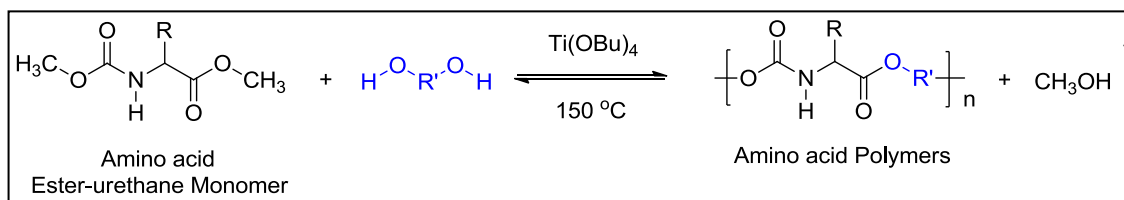
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### Abstract

Polymers synthesis based on amino acids (biological monomers) have been of great interest in the area of chemistry-biology interface due to their potential application in therapeutics, cosmetics, biodegradable and biocompatible engineering materials. Solvent-free melt polycondensation processes is one of the most widely employed eco-friendly technique for producing engineering thermoplastics such as polyesters, polycarbonates polyamides, etc.<sup>1-2</sup> In the present work, naturally abundant L-amino acids were converted into dual functional ester-urethane monomers by tailor made synthetic approach for developing the trans (ester-urethane) polycondensation route for A-A + B-B (A-Ester (or) urethane and B- alcohol) to synthesize linear polymers via melt route. Direct polycondensation of these amino acid monomers with commercial diols under melt condition produced moderate to high molecular weight linear poly (ester-urethane)s.<sup>3</sup> The specialty of these monomers by simply controlling the temperature we can easily tune the reactivity of ester or urethane group and the kinetics also can control depending on the use of the catalyst. The new dual ester-urethane condensation approach was demonstrated for variety of amino acids: glycine,  $\beta$ -alanine, L-alanine, L-leucine, L-valine and L-phenylalanine. The GPC analysis of linear polymers suggested the formation of polymers of  $M_w = 16,000$  to  $35,000$  respectively. The end group analysis via MALDI-TOF-MS confirmed that the monomers were thermally stable under the experimental condition. The new polymers were self-organized as  $\beta$ -sheet or poly proline type-II in aqueous or organic solvents. Thermal properties of polymers such as glass transition temperature and crystallinity could be readily varied using different L-amino acid monomers or diols in the feed. The thermal stability of the polymers was investigated by TGA and it was found that all the polymers were stable at around  $300^\circ\text{C}$ .



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## New Hyperbranched Polymers Based on Amino acids

Moumita Gupta and M.Jayakannan

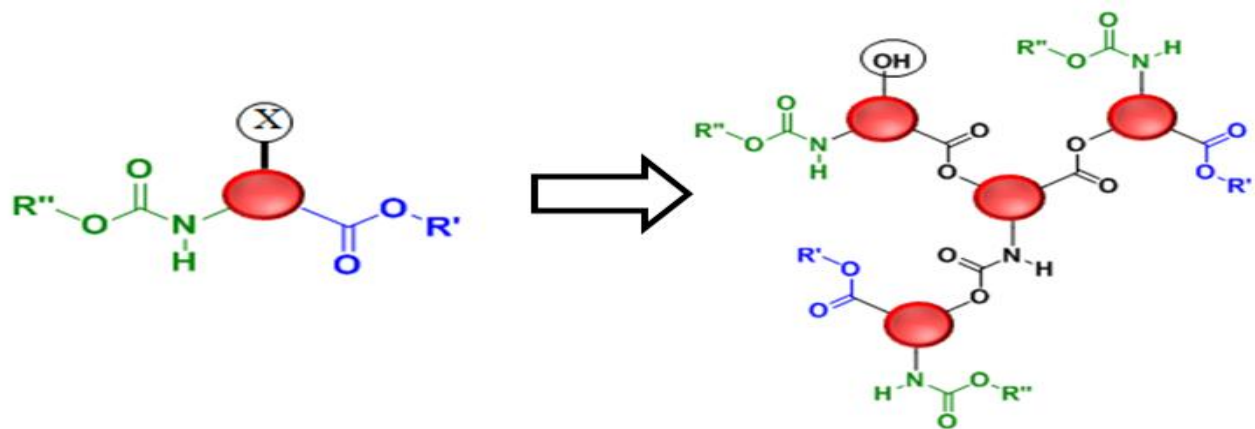
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### Abstract

Hyperbranched polymers are important class of macromolecular structures. These highly branched structures has a great interest in the area of chemistry-biology interface as they are well known for abundance of functional end groups at the periphery which could be useful of attaching and delivering desired drug molecules.<sup>1-2</sup> The present work is emphasized the synthesis of hyperbranched polymers via solvent free melt-condensation route from the AB<sub>2</sub> monomers based on naturally occurring amino acids (L-Serine and L-Tyrosine) as the starting materials.<sup>3</sup> A solvent free melt polymerisation based on dual ester-urethane condensation approach was developed for the above purpose. Amino acids were modified in to a suitable monomers via tailor made approach and subjected to melt at 150° C by using the Titanium-catalyst. The formation of the polymers and progress of polymerization reactions were monitored by NMR, MALDI-TOF and gel permeation chromatography (GPC). Moderate molecular weight of the polymers with the degree of branching in the range of 0.55-0.57 were obtained. MALDI-TOF mass analysis confirmed the formation of branched chains along with few cyclics. TGA analysis showed that thermal stability of the polymer is increased with formation of high molecular weight of the polymers and they are stable up to 200°C. The glass transition temperatures (T<sub>g</sub>) of the polymers showed in the range of -29.8 to 28.6°C from the DSC analysis. These hyperbranched structures are currently explored for drug delivery applications.



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## Development of Medical Textile Using Natural Dye against Staphylococcus Aureus

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### Abstract

The use of textile in medical field has a long tradition. Availability, prices and re-usability supported the use of textile materials. Natural textiles are mostly used for the medical purposes because It fulfills primary quality approaches like biocompatibility, flexibility, brethebility, skin friendly, stain repellency, anti-microbiality etc. Along with the technological development of bio-functional textiles their use in prevention of skin diseases has reached a new quality of interactivity between biological tissues and textiles.

In the present study we had used different natural dyes extracted from plants such as A.nilotica, M.philippensis, Q.infectoria, T.erecta, for dyeing the textile to improve their anti-microbial property. Dyed cotton fabric was characterized for different properties such as light fastness, rubbing fastness, washing fastness, perspiration fastness, L\*a\*b\* value, anti-microbial activity. Anti-microbial study of the dyed fabric shows that dyed fabric has better anti-microbial property than fabric as such. Study shows that dyes extracted from medicinal plants used to develop anti-microbial textiles. These dyes provide good color to the fabrics and kill the microorganism such as S.aureus.

**Vapor Sensing Application of Chitosan and Chitosan –co- Poly ( $\epsilon$ -caprolactone) Grafted Multiwalled Carbon Nanotube Transducers Assembled via Spray Layer-by-Layer Technique**

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**Abstract**

Recently, CNT-based sensors have attracted considerable attention. A combination of the well known characteristics of polymers (good stability, reproducibility, high number of active sites, strong adherence and homogeneity in electrochemical deposition) with those of CNTs leads to improved performance of the resulting sensing devices because of their complementary electrical, electrochemical and mechanical properties. Conducting polymer nanocomposite (CPC) electrodes have been one of the most preferred approaches for the preparation of electrochemical sensors for many years. [1] The unique abilities towards solvent vapor sensing of CPC have been a major focus of many researchers. The direct transduction of chemical information to an electrical signal associated with existing low power microelectronics and sensing technology has made it an attractive material. The versatility of CPCs comes from the wide range of combinations of conducting fillers with insulating polymer matrices.

CNTs promote electron transfer reactions of many compounds and their use as electrode modifiers leads to a decrease in over potential, a decrease in the electrode response time and an increase in the reaction rate of various electroactive substrates compared to conventional carbon electrodes.[2] The electroactivity of CNTs was attributed to the presence of reactive groups on their surface and defect-areas.[3] The advantages of using CNTs for electrode surface modification in the development of new designs for electrochemical sensors and biosensors was recently highlighted.[4] Nevertheless, the low solubility of CNTs in most solvents is a major challenge to their use as modifiers in the fabrication of chemical sensors and biosensors.

Composites of polymers and CNTs are generally synthesized by either chemical or electrochemical polymerization in the presence of CNTs. The polymer functionalization strategy is not only an effective

way of solubilizing CNTs in water, but is also particularly important for the preparation of polymeric carbon packaging, metal-ion adsorption, electrochemical sensors, novel drug delivery and gene composites. Furthermore, covalent techniques can be used to combine different polymers with CNTs to create new hybrid materials with desirable properties.

This study focused on the development of new CPC transducers taking benefit from the enhanced dispersibility and sensitivity due to grafted CNTs with chitosan and via the in-situ copolymerization of chitosan and poly( $\epsilon$ -caprolactone) (CNT-CS-PCL). The spray layer by layer technique is an important technique for developing the appropriate morphologies at both nano and micro scales, allowing control of the electrical properties of transducers for the detection of molecules that are only weakly adsorbed on a CNT surface, resulting in only a very weak change in resistance. Grafting various molecules or macromolecules with a different chemical nature to a CNT surface can provide a variety of transducers with different high selectivity. The synthesized materials (CNT-CS and CNT-CS-PCL) were characterized by Fourier transform infrared spectroscopy,  $^{13}\text{C}$  CP/MAS solid state nuclear magnetic resonance spectroscopy and thermogravimetric analysis. Both CNT-CS and CNT-CS-PCL transducers were analyzed for the response of volatile organic compounds and toluene vapors. The ranking of the relative resistance ( $A_r$ ) for both chitosan based transducers were as follows: toluene < chloroform < ethanol < methanol. The CNT transducer (CNT-CS) was correlated selectively with an exponential law to the inverse of Flory–Huggins interaction parameters,  $\chi_{12}$ .

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## Layer by Layer Chitosan Coated Multi-wall Carbon Nanotubes Smart Chemical Sensors

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### Abstract

The development of miniaturized portable chemical sensors that can detect toxic chemical analytes in real time is an essential issue in medical diagnostics, military security, environmental pollution, and other applications. In this respect, carbon nanotubes (CNT) and graphene have attracted great attention to be utilized as the active element of these detectors. CNT being a quasi-one-dimensional material comprises of only surface atoms. Chemical detectors based on CNT offer low power consumption mainly due to their large carrier mobilities and small size. CNT detectors also offer fast response and high sensitivity to the change in chemical molecules interacting with the surface. In present study, chitosan and carbon nanotube (CNT) are enclosed in smart passion via layer by layer coating of chitosan on CNT to develop conductive and functional material for volatile vapor molecules tracing. Transducers, fabricated via layer by layer spray process, were not only examined for different volatile vapor molecules such as water, methanol and toluene but also influence of vapor concentration in frame of Langmuir-Henry-Clustering (LHC) model have been invested. The layer by layer noncovalent CNT functionalization process open a new avenue for molecule tracing in a controlled way by tuning polymer layer thickness for advanced sensing application. In last, genral developments and properties of graphene based sensors will be presented.

**Keywords:** Vapor sensing; Carbon nanotube; Graphene; Chitosan; Layer by Layer Coating.

**Porous scaffolds based on Chitosan Intercalated in Montmorillonite:  
Enhanced functions of bone cells on polylactic acid-grafted chitosan for bone  
Tissue Engineering**

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**Abstract**

We describe here three dimensional biodegradable chitosan-grafted with poly-lactic acid/clay composite scaffold with improved bio-physical and mechanical properties compared to pure chitosan scaffolds for bone tissue engineering. Polylactic acid was surface grafted onto chitosan by a simple condensation reaction, followed by intercalation in montmorillonite clay. The resulting dispersion was subjected to lyophilization. The composite scaffolds were characterized by a highly porous structure with interconnected pores. Subsequently, a calcium chloride solution was further added to this solution to induce phase-separation induced porosity, where highly interconnected pores were observed. The nanocomposite scaffolds with grafted and intercalated CS exhibited greater compression modulus, slower biodegradation rate and reduced water uptake, but the water retention ability was similar to pure chitosan scaffolds. On the other hand, the scaffolds exhibited favorable biological response of bone cells with higher proliferation, and well spreading morphology as compare to pure chitosan scaffold. The study emphasizes grafted chitosan composite as a potential scaffold material for bone tissue regeneration.

## Peeling Model for Cell adhesion on Electrospun Polymer Nanofibres

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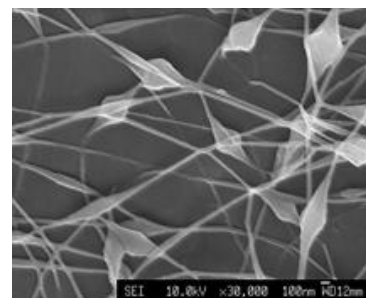
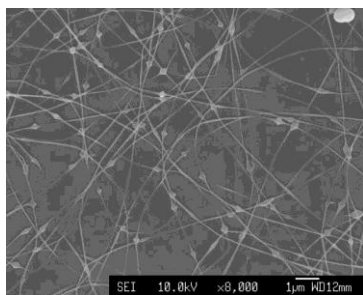
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### Abstract

Need of controlled drug delivery have gained much attention over the conventional dosage forms due to their improving therapeutic efficacy, reduced toxicity by delivering them at controlled rate. Recently electrospun fibres have found their major role in wide applications such as drug delivery systems, tissue engineering, vascular grafts for biomedical application. Electrospinning is a versatile technique employing electrostatic forces to produce polymer fibers, ranging in diameter from a few microns down to tens of nanometers. Drug delivery with polymer nanofibres is based on the principle that the dissolution rate of a particular drug increases with increasing surface area of both the drug and carrier. The main challenge in designing such a device for the release of low molecular weight hydrophilic antibiotics is to overcome the rapid discharge of the drug from the device. The electrospun wound dressing promises to solve this problem by changing the structure of the polymer. In the present work the feasibility of producing fibrous composite of polylactic acid with silver nitrate aqueous solution and hydroxyapatite using electrospinning technique was explored to understand the antibacterial property of the dressing. These non-woven fibres as in figure below were post processed and heat treated with UV radiation. This type of heat treatment was found to reduce the ionic silver to silver nanoparticles. Such a type of heat treatment was found to even improve the crystalline properties of hydroxyapatite and polylactic acid. The results of the antimicrobial tests showed that these fibres have maintained antibacterial properties against *Staphylococcus aureus* and *E.coli*.





It was noticed that there was no discoloration in the wound mat. To test the nature of biocompatibility of these fabrics, the electrospun mats were cultured with fibroblasts. The cultured cells were tested and evaluated for morphology. The results indicated that the cells attached and proliferated as continuous layers and maintained a healthy morphology. However, the task of tailoring any biomaterial with controlled structure and surface chemistry in order to encourage cell adhesion and tissue regeneration is highly challenging. In addition, once the biomaterial is implanted, no control is possible either over the biomaterial characteristics or the healing process. At this point, the modeling process takes over, thereby providing a means to modify the design of the biomaterial based on their response to cells adhesion, proliferation and differentiation and other factors. Present study is extended, to a mathematical model for a primary step in tissue regeneration - Cell Adhesion, using a 'One dimensional Peeling model'. Assuming linear and non-linear force profiles, the model is used to calculate the forces required to detach the cell, the nature of cell adhesion and the membrane contours of cell during adhesion.

## Synthesis of Novel Quaternary Ammonium Polymerizable Surfactants from Tertiary Amines, Long Chain Alkyl Maleic Hemiesters, and Epoxy Resins

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### Abstract

The quaternary ammonium polymerizable surfactants (QAPS) are known for their wide industrial applications. The QAPS with long alkyl chains has got biocidal property. Mostly the long alkyl chain is attached to the amine group making the QAPS to have its own limitations in biocidal effect. But, a new synthetic route has been disclosed where the long alkyl chain is linked to other functional groups which are then linked to the tertiary amines hence forming QAPS. These surfactants have well exposed quaternary ammonium groups making them much more lethal towards the microbes.

## Controlled Crystallite Orientation in ZnO thin films Prepared by Chemical Bath Deposition to DSSC

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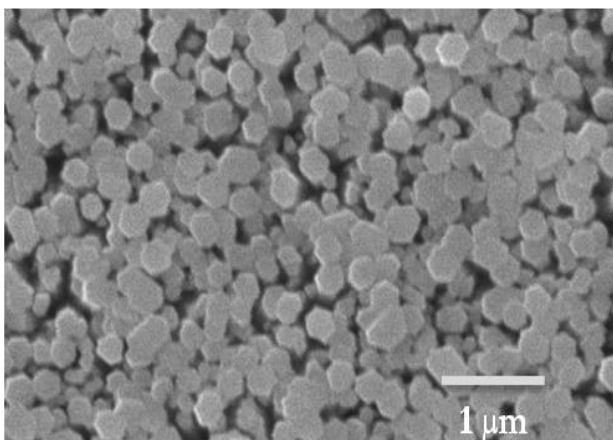
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### Abstract

Solar cells based on dye-sensitized ZnO are low-cost alternatives to conventional solid-state devices. The synthesis of one dimensional (1D) ZnO hexagonal nanorods onto indium-doped tin oxide (ITO)-coated glass substrates using a chemical bath deposition technique for dye-sensitized solar cell application is presented. The effect of annealing temperature and modified dye on performance of dye absorption of ZnO nano-rods electrode is investigated. X-ray diffraction study shows the wurtzite structure of ZnO film annealed samples. Surface morphology of ZnO nanorods is improved with annealing temperature. Our experimental finding suggests, the solar-to-electrical conversion efficiency in absorption of modified dye, exhibited the best properties for the dye-sensitized solar cells (DSSCs) when illuminated with 80mW/cm<sup>2</sup>. An M dye is employed to be the sensitizers for the ZnO NRs working electrode. A moderate fill factor is obtained in the M-sensitized cell which results in comparable efficiencies in ZnO-NRs DSSCs, The more abundant electron interfacial recombination occurs in the M-sensitized ZnO-NRs DSSC.



**Keywords:** *ZnO; Chemical growth; Structural analysis, surface morphology; Dye-sensitized solar cells.*

## Substrate Temperature Dependent Behavior of ZnO Thin Films Derived by Spray Pyrolysis

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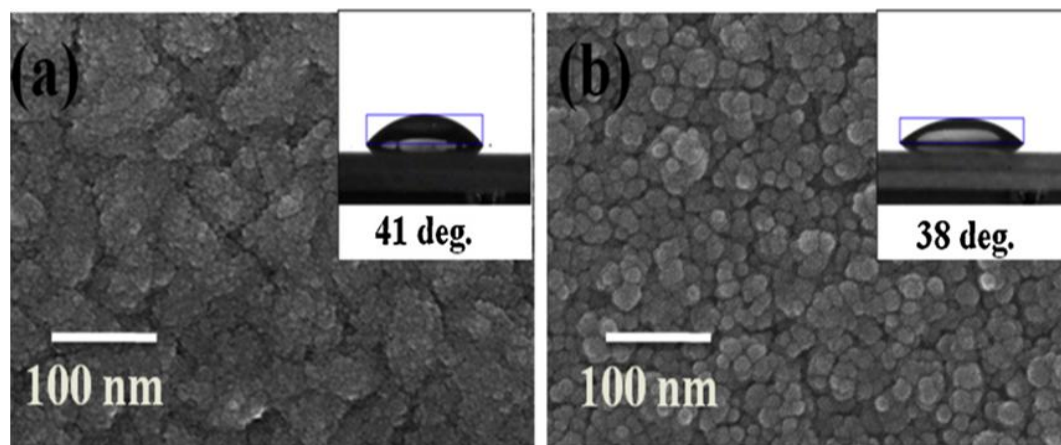
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### Abstract

Zinc oxide (ZnO) thin films have been deposited with various substrate temperatures by spray pyrolysis technique onto microscopic glass substrates. X-ray diffraction (XRD) results showed the random growth orientation of the crystallites and the presence of the wurtzite phase of ZnO. SEM images showed agglomerated nanocrystalline grains growth having average grain size of 40-50 nm. The x-ray photoelectron spectroscopy (XPS) measurements reveal the presence of Zn<sup>2+</sup> and chemisorbed oxygen in ZnO thin films. Atomic force micrograms (AFM) revealed a granular, polycrystalline morphology for the films. The grain size is found to increase as the substrate temperature increases. All films exhibit a transmittance of about 85% in the visible region. Electrical resistivity has been found to decrease; while the carrier concentration increases with substrate temperature.



**Keywords:** ZnO, Spray pyrolysis, Nanocrystalline, Optical properties, Electrical properties

## Formulation and Characterization of Poly (L-lactide-co- $\epsilon$ -caprolactone) (PLCL) loaded Gliclazide Biodegradable Nanoparticles as a Control Release Carrier

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### Abstract

A biodegradable nanoparticle has been used frequently as drug delivery carrier due to its better encapsulation capacity, sustained/ control release property and less toxicity. Gliclazide is a second generation of hypoglycemic sulfonylurea and acts selectively on pancreatic  $\beta$  cell to control diabetes mellitus. The objective of this study was to produce controlled release poly (L-lactide-co- $\epsilon$ -caprolactone) (PLCL) loaded Gliclazide nanoparticles using solvent evaporation - high pressure homogenization method. The method was optimized using design of experiments by employing a 3-factor, 3-level Design Expert (version 8.0.7.1) Statistical Design Software and was subjected to various characterization studies including Field Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM), X-ray diffraction (XRD), Encapsulation efficiency (%EE), Particle Size Distribution (PSD), etc. Formulated nanoparticles were also subjected to Fourier Transform Infrared Spectroscopy (FT-IR), Differential Scanning Calorimetry (DSC) for studying interaction between drug and polymer and the effect of lyophilization (Freeze Drying) on developed nanoparticles. The release profiles and encapsulation efficiencies are depended on the concentration of PLCL biodegradable polymer. These data demonstrated the efficacy of the biodegradable polymeric nanoparticles in controlling the Gliclazide drug release profile as novel drug delivery system.

**Keywords:** Poly (L-lactide-co- $\epsilon$ -caprolactone) (PLCL), Gliclazide, Biodegradable Nanoparticles, Lyophilization, High Pressure Homogenization

## Synthesis of Polystyrene Nanoparticles (nPS) and their Effect on Properties of Polyurethane Rubber

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### Abstract

Polystyrene nanoparticles (nPS) were prepared using ultrasonic assisted microemulsion technique. The size and shape of nPS were confirmed using transmission electron microscope (TEM) and recorded ~ 20 to 50 nm with spherical shape. Whereas, the presence of functional groups in the formation of nPS particles was confirmed using Fourier transform infrared spectroscopy (FTIR). The prepared nPS particles were used for the preparation of polyurethane composites. These composites were prepared on two roll mill and moulded on compression moulding machine so as to get a vulcanized sheet of 130x130x3 mm. The prepared composites of polyurethane: nPS were subjected to mechanical properties and thermal properties using universal testing machine (UTM) and thermogravimetric analyzer (TGA) respectively. Physical properties like hardness were studied using Durometer hardness tester (Shore A). Moreover the extent of dispersion nPS particles in polyurethane matrix was studied on field emission scanning electron microscope (FE-SEM) and atomic force microscope (AFM). The soft, glossy surface and fine size of nPS particles lead the uniform dispersion into the polyurethane matrix and show improvement in the above properties up to 2 wt %, while marginal decrement at 2.5 wt %. This decrease in the properties was due to the agglomeration of nPS by formation of electrostatic force of attraction at the time of mixing to the higher % of loading.

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## A Study on Copolymerization of N-Vinyl Pyrrolidone-Alt-Acrylic Acid

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### Abstract

A series of N vinyl pyrrolidone-alt-acrylic acid copolymers were synthesized using AIBN initiator using THF as solvent. The copolymers were characterized by FTIR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, DSC and TGA. Structure of the copolymer is determined by calculating the reactivity ratio. The reactivity ratio were calculated using F-R, K-T, EK-T methods and the values obtained were 0.24 ( $r_1$ ) and 0.136 ( $r_2$ ). It shows that the copolymer is alternating. The formation of alternating copolymer was processed by the formation of charge transfer complex. The glass transition temperature for the copolymer was observed at 126 °C and the polymer starts degrading at 219 °C.



## Synthesis of Novel Quaternary Ammonium Polymerizable Surfactants from Tertiary Amines, Long Chain Alkyl Maleic Hemiesters and Epoxy Resins

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### Abstract

The quaternary ammonium polymerizable surfactants (QAPS) are known for their wide industrial applications. The QAPS with long alkyl chains has got biocidal property. Mostly the long alkyl chain is attached to the amine group making the QAPS to have its own limitations in biocidal effect. But, a new synthetic route has been disclosed where the long alkyl chain is linked to other functional groups which are then linked to the tertiary amines hence forming QAPS. These surfactants have well exposed quaternary ammonium groups making them much more lethal towards the microbes. A series of quaternary ammonium polymerizable surfactants (QAPS) are synthesized. The synthesis involved three steps, where alcohols of various chain lengths are reacted with maleic anhydride forming respective hemiesters. Tertiary amines are reacted with epichlorohydrin to form glycidyltrialkylammonium cations. In the latter reaction the glycidyltrialkylammonium cations were reacted with hemiesters forming series of QAPS. The products were recrystallized three times from a mixture of ethanol and acetone. The surfactants thus obtained were white in color and has got good solubility in water. The products obtained were characterized at each and every step by IR. The final QAPS were characterized by FTIR, NMR and other analytical data. These surfactants has got good biomedical applications as the quaternary ammonium moiety is well exposed.

## Biodegradable Poly(L-Lactide-Co-Caprolactone) (PLCL) Copolymer Nanoparticles For Controlled Drug Delivery

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### Abstract

Biodegradable polymers especially poly(lactic acid) (PLA), poly(caprolactone) (PCL), poly(lactide-co-glycolide) (PLGA) and their diblock copolymers like PLA-Poly(ethylene glycol) (PEG), PCL-PEG and PLGA-PEG respectively are the areas of interest to research scientists since 1990s. The blending of polymer and drug to make biodegradable polymeric nanoparticles has sought profound applications in polymer, medical and pharmaceutical areas. PLA, PCL and their copolymers being hydrophobic in nature, they mostly entrap hydrophobic drugs. Nanoparticles being in size range of 100-500 nm cover a large area of organs increase the drug entrapment efficiency, help in reducing the dose of drug required, targeting of specific body tissues and controlling the release of drugs.

Cancer being a major disease of concern in present world, there is much focus on chemotherapeutic agents and their entrapment in polymeric nanoparticles. Magnolol is widely used as chemotherapeutic agent. It is also used in atherosclerosis, myocardial infarction and preventing platelet aggregation. Since chemotherapeutic agents suffer a major drawback of severe side-effects on oral administration and other conventional mode of administration, nanoparticle systems come to role.

The present study reveals the synthesis and characterization of PLCL copolymers with different compositions of lactide and caprolactone, characterization by FTIR spectra, drug entrapment efficiency, particle size and the release kinetics. The copolymers were characterized for FT-IR and <sup>1</sup>H NMR spectroscopy, differential scanning calorimetry (DSC) and gel permeation chromatography (GPC). The Magnolol loaded nanoparticles of PLCL copolymers were prepared

by nanoprecipitation method and characterized by particle size analysis, drug entrapment efficiency, FTIR, <sup>1</sup>H NMR spectra, scanning electron microscopy (SEM) and release kinetics. The best found formulation of nanoparticles prepared from the PLCL copolymers was further taken for release kinetics, particle size analysis and drug entrapment efficiency. It was found that nanoparticles were in specified size range, drug entrapment efficiency was good and release kinetics followed best fit model and the drug release kinetics vary significantly by varying the copolymer composition.

**Keywords:** Poly(lactic acid), Poly(L-lactide-co-caprolactone), Magnolol, nanoparticles, drug release kinetics

## Biodegradable Polymeric Nanoparticles for Controlled Drug Release

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### Abstract

Biodegradable polymers have been widely used in the biomedical and pharmaceutical field because of their biodegradable and biocompatible nature. They can be classified as synthetic and natural polymers. The synthetic polymers have more importance because of their ease of modification with different types of monomers and synthesis of polymers with similar properties. The most widely used and commonly studied class of biodegradable polymer is the polyesters and their copolymers. These polymers have been extensively used for controlled release of drug because of their resorbable nature.

Gemcitabine is a useful drug for treating different types of solid tumors. However, it suffers from major drawback of very short plasma half-life that causes degradation by enzyme and strong side effects when administered intravenously. In the past attempts have been made to protect the drug from degradation with the help of nanoparticles of PLA which promote the efficacy and reduce its side effects. However, nanoparticles based on PLA accumulate blood proteins on their surface during circulation through the body which results in removal of nanoparticles by immune cells before reaching to the tumor targets.

In the present work, Poly(L-lactic acid)(PLLA)-Poly(ethylene glycol) (m-PEG) a biodegradable amphiphilic copolymers were synthesized with different ratios of lactic acid and Poly(ethylene glycol) for controlled release of hydrophilic drug. The copolymers were characterized by solution viscosity, FTIR and <sup>1</sup>H NMR spectroscopy, gel permeation chromatography and thermal analysis. Gemcitabine, a first line drug was used as model drug useful for many solid tumors. The nanoparticles of PLLA-mPEG copolymers were prepared by using a modified nanoprecipitation technique and optimized with different drug and polymer concentration. The nanoparticles were characterized by particle size, particle size distribution and particle shape with the help of DLS and E-SEM. The drug release kinetics was studied by UV spectroscopy method. The results of this study showed that nanoparticles of biodegradable copolymer protects the drug from degradation and also provides controlled release hence reduces dosing frequency and side effects.

Key words : Biodegradable copolymer, gemcitabine, nanoprecipitation, controlled release

## Porous and Crosslinked Cellulose Beads for Toxic Metal Removal-Hg (II) Ions

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### Abstract

Heavy metal poisoning is one of the major threats to the ecosystem. Mercury which is a heavy metal poses threat to the ecosystem when it gets deposited in the environment. Mercury is one of the highly toxic and hazardous pollutants even in trace amounts and compared to other heavy metals, mercury even at low concentrations is highly neurotoxic. According to USEPA standards, mercury content in drinking water should not exceed 2.0ug/L and the permitted discharge level of mercury in waste water is 10.0ug/L. So it becomes necessary to remove it from the aqueous systems which has been a subject of interest for researchers for a long time now. In this study, we have synthesised highly porous and cross-linked cellulose beads magnetised with ferric oxide to remove Hg(II) ions from aqueous systems by the process of adsorption. These beads are prepared by solution polymerization using different solvents viz DMSO and N,N-Dimethyl Acetamide:Acetone. The beads were characterised using FTIR and SEM for functional group determination and surface morphology respectively.

Various parameters affecting adsorption such as pH of the solution, percentage of ferric oxide, dose, time and concentration of the Hg(II) ions were all investigated. Optimum pH for the maximum amount of uptake of Hg(II) ions is found to be pH 6.0. Among various w/w % of Fe<sub>2</sub>O<sub>3</sub> (1w/w% - 20w/w%), the beads with 5w/w% of Fe<sub>2</sub>O<sub>3</sub> were found to adsorb maximum amount of Hg(II) ions from aqueous solutions which can be correlated to the degree of dispersion of Fe<sub>2</sub>O<sub>3</sub> particles in the polymeric matrix. As the percentage of Fe<sub>2</sub>O<sub>3</sub> in the beads increased, adsorption also increased till 5w/w% and further increase in the percentage of Fe<sub>2</sub>O<sub>3</sub> had no effect on the adsorption since the degree of dispersion of Fe<sub>2</sub>O<sub>3</sub> in the polymeric solution was good upto 5 w/w% of Fe<sub>2</sub>O<sub>3</sub>. But beyond 5w/w% of Fe<sub>2</sub>O<sub>3</sub> it was observed that Fe<sub>2</sub>O<sub>3</sub> particles agglomerated. Also it was noticed that beyond 5w/w% of Fe<sub>2</sub>O<sub>3</sub> in the solution, the viscosity of the solution increased drastically. Time dependant study of intake of Hg(II) ions by polymeric beads from aqueous solutions of Hg(II) ions with different initial concentrations was

carried out and the concentration of Hg(II) ions was monitored spectrophotometrically using UV-Visible Spectrophotometer. Various isotherm models were tested among which Freundlich adsorption isotherm was found to be suitable. The process of adsorption followed pseudo second order kinetics.

Eventhough there is no much difference in the results using beads prepared with DMSO and N,N-Dimethyl Acetamide:Acetone as solvents, the ecofriendliness of the N,N-Dimethyl Acetamide:Acetone system makes it a better solvent to be used commercially. These beads which are formed from a natural material, Cellulose, can find good applications in removing Hg(II) ions from aqueous systems.

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## **Immobilization of Primary Amine Antimicrobial Mimics for the Determination of Bacterial Cell Death Efficacy**

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### **Abstract**

Antimicrobial peptide mimics, containing pendant primary amines, have been shown to present biocidal behaviors against a wide range of bacteria. In our recent work, poly(aminopropylmethacrylamide) (PAPMA) proves very efficient at eliminating both gram positive (*E. coli*) and gram negative (*B. subtilis*) bacteria. Additionally, PAPMA demonstrates minimal toxicity towards eukaryotic (erythrocyte and MCF-7) cells. As a continuation, PAPMA has been attached to silicon wafers in an effort to study the efficacy of immobilized antimicrobial peptide mimics. Specifically, PAMPA has been grafted to and from silicon substrates. Grafting various molecular weights of PAPMA, synthesized via RAFT polymerization, to the silicon surface was achieved via an azide-alkyne click reaction. Whereas, polymerizing PAPMA from the surface was achieved through AIBN surface initiated free radical polymerization. Each method results in different grafting densities and will provide model systems for understanding the optimal primary amine density required for effective bacterial cell death. Ellipsometry, contact angle, AFM and grazing angle IR will determine the thickness, wet ability, morphological character and compositional analysis, respectively, of each functionalized silicon wafer.

## Studies on Dispersion Behavior of Nano-Clay in Ultra High Molecular Weight HDPE and Its Effect on the Properties

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### Abstract

The paper describes the preparation and characterization of ultra high molecular weight polyethylene (UHMWPE)-nanoclay composites by melt compounding using a co-rotating twin screw extruder. Melt compounding was done in absence/ presence of varying amounts of compatibilisers (HDPE-g-MA, ULDPE-g-GMA) and Nylon. The effect of nanoclay, compatibiliser and Nylon contents on the morphological, thermal, mechanical and rheological properties was investigated. Mechanical properties such as tensile and flexural increased, but impact strength reduced with increase in nanoclay content. Morphology of the nanocomposites was studied using X-ray diffraction, transmission electron microscopy (TEM) and scanning electron microscopy (SEM). Intercalation as well as exfoliation was observed when nylon-clay master batch was blended with UHMWPE. On the other hand use of HDPE-g-MA and ULDPE-g-GMA did not help in the dispersion of nanoclay as d-spacing decreased after melt compounding. Thermal performance of nanocomposites was inspected using differential scanning calorimetry (DSC) and thermogravimetry (TGA). It was observed that % crystallinity decreased and maximum decomposition temperature increased upon adding nanoclay. Rheological behavior investigated using capillary rheometer showed an increase in shear viscosity in presence of nanoclay.

Keywords: UHMWPE, Nanoclay, Nylon, Nanocomposites,



## Applications of Co doped ZnO based PVA nanocomposite in Defence

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### Abstract

The paper describes synthesis and applications of Co doped ZnO based nanocomposite in defence. A short and effective method was used towards the synthesis of Co doped ZnO. It was further incorporated into PVA matrix to prepare the nanocomposite. Various studies were undertaken to evaluate its ballistic properties. To explore the mechanical properties of nanocomposites, different ratios (0.8-2 w/w %) of Co doped ZnO were incorporated in PVA matrix. It was observed that with the increment in ratio, the tensile strength increases from 60.3 MPa to 98 MPa. The E-Modulus was also found to increase with the increase in the doping concentration of nanomaterial in the polymer matrix. Further, we are studying the EMI shielding effects of the Co doped ZnO incorporated in PVA matrix. EMI is a specific kind of environmental pollution, which is drawing more attention recently, because of the utilization of electrical and electronic devices in military applications.

**Studies on the Effect of Reactive Extrusion of Linear Low Density Polyethylene (LLDPE) Using Peroxides On the Molecular Structure, Rheological and Thermal Properties**

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**Abstract**

The reactive extrusion of LLDPE with low levels of three different organic peroxides e.g.2,5-bis(tert-butylperoxy)-2,5-dimethylhexane, tert-butylperoxybenzoate, and dicumyl peroxide has been carried out to modify the molecular structure and rheological properties. The low levels of peroxides were used to introduce long chain branching and to avoid the crosslinking. The thermal behavior was characterized using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). TGA reveals no significant changes in the thermal degradation properties however DSC results show significant changes in the crystallization temperature, peak melting temperature and crystallinity after extrusion in the presence of peroxides. Short chain branching (SCB), branching distribution index (BDI) and lamellar thickness variations were estimated from DSC melting curves by fitting the curve. The rheological behavior was examined by MFI and capillary rheometer. Structural characterization was done using Fourier transform infrared spectrometer.

**Keywords:** Reactive extrusion, SCB, BDI, lamellar thickness variations, unsaturation

## Novel Functional Polymers via RAFT Polymerization and “Click Reaction”

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### Abstract

In recent years there have been great interest in the development of new functional polymeric materials for novel applications. Thermoreversible materials have applications in different smart and strategic application. This investigation reports the preparation of functional polymer having reactive furfuryl group as a pendent group. In this case the furfuryl methacrylate (FMA) was polymerized by Reversible Addition Fragmentation-chain Transfer (RAFT) technique using different RAFT reagents, like 4-cyano-4-(thiobenzoylthio) pentanoic acid (CTBPA), 4-cyano-4-[(dodecylsulfanylthiocarbonyl)sulfanyl]pentanoic acid (CDTSPA) and 4,4'-Azobis(4-cyanovaleric acid) (ABCVA ) as an initiator. This controlled radical polymerization (CRP) techniques was successfully used to prepare polymer with controlled molecular weight and narrow polydispersity index (PDI). The furfuryl group of poly (furfuryl methacrylate) (PFMA) was used to prepare thermoreversible cross-linked polymeric materials with suitable dienophile like 1,1'-(methylenedi-4,1phenylene) bismaleimide via Diels-Alder (DA) and retro-DA ‘Click Reaction’. At higher temperature this DA reaction can undergo rDA reaction leading to generation of the staring materials. The thermo-reversible properties of the cross-linked polymer were characterized by FT-IR and heating-cooling cycle in DSC analysis.

## **Influence of Lithium Tantalate Particles on the Thermal and Morphological Properties of PVDF/ PMMA Composite Film**

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### **Abstract**

The present investigation aims to prepare blend through solution blending process composed of PVDF and PMMA in polar aprotic solvent N-N, Dimethylformamide (DMF). PVDF/PMMA/Lithium Tantalate composite film has been fabricated by the incorporation of lithium tantalate at various loadings (10-40%) in 60/40 PVDF/PMMA blend with the aid of solution blending process. It has been earlier reported [1] that the dielectric properties such as dielectric constant, dielectric loss etc have significantly increased at 40% loading of lithium tantalate in PVDF/PMMA film. These films have been further characterized for their thermal and morphological properties with the aid of DSC, TGA and SEM respectively. The structure of composite film has been investigated by Wide Angle X- ray diffraction (WAXD) and Fourier Transform Infrared Spectroscopy (FTIR).

**Keywords:**-PVDF, PMMA, TGA, SEM, FTIR.

References:-

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## Effect of Nanoclay on Mechanical Properties of Poly Lactic Acid Modified PP/HDPE/EVA Blend

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### Abstract

This paper highlights the effect of addition of nano clay on PP/HDPE/EVA/PLA blend. Nanocomposite based on compatibilized polypropylene(PP)/ high density polyethylene (HDPE) with poly lactic acid (PLA) are prepared using an monomorphonite as a nano-filler and EVA is used as a compatibilizer for PP/HDPE(80/20) blend and to study the performance of nanocomposite in terms of mechanical and optical properties. The compositions are prepared by co-rotating twin screw extruder with post extrusion cast film. The screw speed of the extruder is maintained at 150 rpm. Mechanical properties like tensile strength, burst strength, tear strength, coefficient of friction are determined. Optical properties like haze and value of transmittance are also reported. The incorporation of nano clay has been varied from 0.5 Phr to 2 Phr in PP/HDPE/EVA/PLA (80/20/5/4) blend. It has been found that at 1.5 Phr loading of nano clay in PP/HDPE/EVA/PLA blend has shown highest tensile, burst and tear strength. Coefficient of friction of the film has found to be lowest at 1.5 Phr nano clay incorporated into the blend when compared with other compositions.

**Keywords:** Nanocomposite, Mechanical properties, Optical properties.

## Synthesis and Pharmacokinetic Profile of Mutual Prodrugs of Biphenylacetic Acid as Gastro-Sparing NSAIDs

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### **Abstract**

Fenbufen, a bioprecursor prodrug of biphenylacetic acid (BPA) has high incidences of inter-subject variation and poor bioavailability due to involvement of multiple metabolic pathways some of which are activating while others are inactivating. BPA is one of the active metabolites of fenbufen which is twice as potent as its precursor. The present work focuses on synthesis, *in vitro/ vivo* release kinetics of mutual prodrugs of biphenyl acetic acid with L-tryptophan (BPTP) and L- glutamine (BPGU). The prodrugs were synthesized by DCC coupling and characterized by IR and <sup>1</sup>H-NMR. Release profile for BPTP was studied in buffers (pH 1.2 and 7.4), simulating the pH of stomach and small intestine respectively. BPTP was stable in HCl buffer while 12.45 % BPA ( $t_{1/2}$ : 2272.13 min) was released in phosphate buffer. *In vivo* release studies in blood showed that BPTP bypassed absorption/hydrolysis in stomach while around 21% of BPA was furnished in small intestine during 2-6h. Release of 31.27 - 68.5 % BPA at 8h and 24h respectively indicated that the intact prodrug might have reached the colon where it was hydrolyzed by N- acyl amidase resulting in the release of BPA that might have entered into systemic circulation after absorption through colonic mucosa. Excretion pattern of BPTP in urine and feces was also studied where 0.3 -1.5 % BPA was furnished in 24h pooled samples of urine and feces respectively and 1.43 % intact BPTP was also present in 24h feces emphasizing its transport to colon.

# Supramolecular Assemblies Of 1,2,4,5-Cyclohexanetetracarboxylic Acid With Various Aza-Donor Compounds

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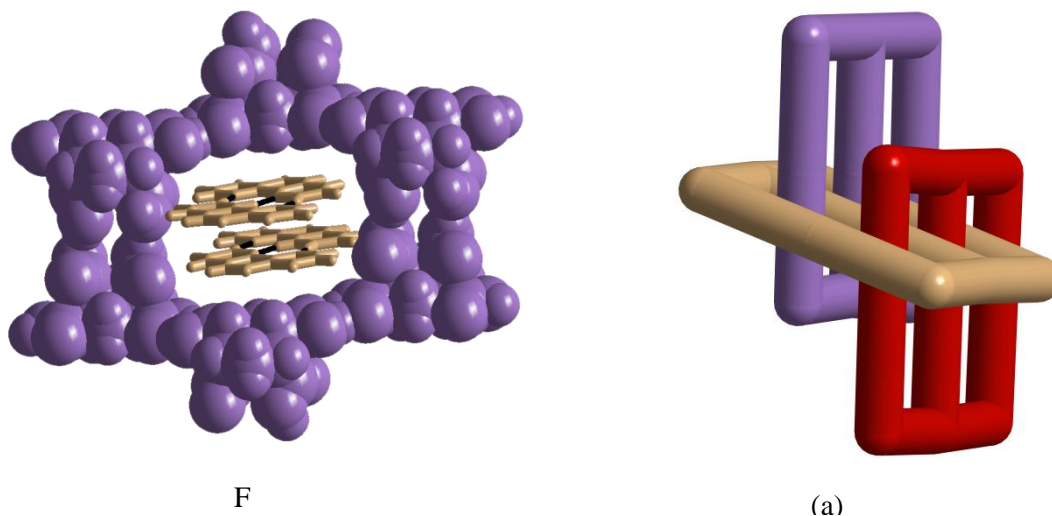
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## Abstract

A supermolecule is an organized entity that is created by the association of two or more chemical species held together by intermolecular forces such as hydrogen bonds, van der Waals forces, coordination bonds, halogen bonds, etc.<sup>1</sup> As the carboxylic acid moiety represents the most widely studied functional group within the realm of supramolecular synthesis, we have carried out co-crystallization of 1,2,4,5-cyclohexanetetracarboxylic acid(**1245CTC**) with various aza donor compounds like 4,4'-bipyridine, 2,2'-bipyridine, 1,2-*bis*(4-pyridyl)ethane, 1,2-*bis*(4-pyridyl)ethene, phenazine, 1,10-phenanthroline, 4,7-phenanthroline, etc., to study the affinity of the polycarboxylic acids in molecular recognition.<sup>2,3</sup> The complexes, thus, obtained have been characterized by single crystal X-ray diffraction method and the structural analysis reveal the formation of exotic supramolecular assemblies in the form of host-guest type networks, sheets, interpenetrated ladders, etc. Packing arrangement for the representative examples are shown in Figure 1. The structural features of these assemblies would be illustrated in detail in poster presentation.



**Figure 1:** Supramolecular assemblies formed by 1,2,4,5-cyclohexanetetracarboxylic acid with (a) 1,10-phenanthroline and (b) 4,4'-bipyridine (schematic representation).

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