

## **Polymer Science 2017**



3<sup>rd</sup> International Conference on

## **POLYMER SCIENCE AND ENGINEERING**

October 02-03, 2017 Chicago, USA

**e-Posters**

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# POLYMER SCIENCE AND ENGINEERING

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## Room temperature tunable ferromagnetism in solution grown mesoscopic conjugated polymer rings

**Arnab Das**

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Conventionally, ferromagnetic materials are restricted to metallic regime such as iron and nickel. Although syntheses in the literature have been attempted to induce ferromagnetism in organic polymers, most require sufficiently low temperature, have very low magnetic strength, and no tunability, inhibiting practical applications. This research proposed a novel generalized methodology to create tunable ferromagnetic conjugated organic polymers at room temperature without aid of magnetic metals. Room temperature existence of bipolarons in conductive polymers and the Peierls instability in mesoscopic rings of doped conjugated polymers were hypothesized as rationale for ferromagnetic behavior. Novel one-pot solution based oxidative templating method was employed to form doped mesoscopic conjugated polymer rings/cylinders, evidenced in Atomic Force Microscopy (AFM) and Scanning Electron Microscopy/Energy Dispersive Spectroscopy (SEM/EDS) images. Vibrating Sample Magnetometry (VSM) data for low radii (mean ~39 nm) polyaniline ring demonstrated hysteresis loop like baseline iron nanoparticles, indicating ferromagnetic signature. With increasing ring size (~300 nm) hysteresis loop shrunk and magnetic strength reduced, completely diminishing for larger ring size (~25  $\mu$ m). Chemical shift from liquid Nuclear Magnetic Resonance (NMR) corroborated VSM data, demonstrating tunability of magnetic strength with varying ring size by controlling oxidative templating. Saturated DC susceptibility from Physical Property Measurement System (PPMS) measurement was averaged to be 0.421 emu/g for low radii polyaniline ring, the highest ever magnetic strength achieved for organic magnets.

### Biography

Arnab Das is currently a research student mostly focusing on developing advanced organic magnetic materials. Earlier, he has developed a generalized methodology of inducing paramagnetic behavior in bio-compatible polymeric materials. He also developed a novel synthesis process to generate purely polymeric nanoparticles to detect oxidative stress induced free radicals in human body. He has been recognized nationally and internationally for his research (ISEF- 2015, 2016, 2017). In 2014, as a national level winner of Broadcom Masters, he had the opportunity to meet president Obama at the White House.

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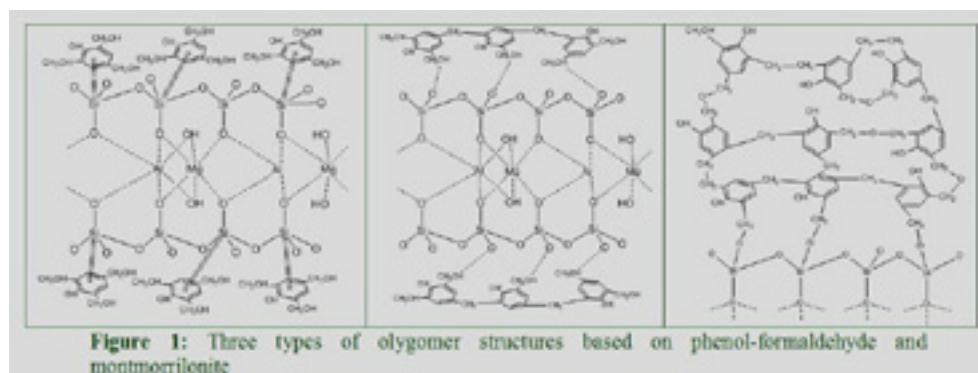
## POLYMER SCIENCE AND ENGINEERING

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**The synthesis and structure of oligomers based on phenol-formaldehyde resins and montmorillonite, the influence of concentration and acidity on their structures**

**Denys O Savchenko, Eugene O. Paschenko, Andrey N. Chernenko, Olga V. Lazhevskaya, Vyacheslav. V. Bichihin and Nikolay N. Nekoval**  
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**I**ntroduction: Montmorillonite is one of the fillers for polymers that are studied now. It attracts scientists due to the following reasons: 1) improvement of polymeric materials properties due to filler introducing 2) particularities of montmorillonite behavior in polymer melts and solutions 3) abundance and availability of the mineral. Introduction of montmorillonite into polymers and oligomers may improve their mechanical properties, heat-resistance, gas selectivity (for membranes), compatibility of polymers, and accelerate relaxation process and reduce water absorption. Polymeric composite materials based on montmorillonite can be applied for electrochemical sensors, drug delivery systems, packaging materials, sorbents, etc. However there are no literature data about application of such polymeric composite materials as binders for grinding tools. In addition, there is no enough information about structure peculiarities of oligomers based on phenol-formaldehyde, containing montmorillonite. Objectives of this work were: 1) to make the synthesis of oligomers based on phenol-formaldehyde and montmorillonite, 2) to study oligomer structures and the influence of concentration of montmorillonite and alkali on them, 3) to provide a substantiate preposition about a chemical reaction mechanism of oligomer formation. Experimental part: the synthesis of oligomers was conducted in seven steps: 1) the water was added to montmorillonite, 2) phenol-formaldehyde was dissolved in alkaline medium and a catalyst was added to it, 3) both mixtures were heated and stirred during 30 days, 4) montmorillonite sorbed the water was added in portions to the phenol-formaldehyde solution 5) the obtained system was heated and stirred as well 6) during heating and stirring the residue of oligomer has formed 7) oligomer was filtered and dried. The structure of oligomer was studied with IR-spectra. Findings: Oligomers based on phenol-formaldehyde, containing silica-alumina layers of montmorillonite were synthesized. Synthesized oligomers were of three structure types: 1) aromatic rings of phenol-formaldehyde are coordinated around silica atoms of silica-alumina layers 2) metoxy and hydroxyl groups are coordinated around silica-oxide groups of above mentioned layers 3) phenol-formaldehyde chains are chemically bound with such layers via Si-O-C bonds.

**Biography**

Denys Savchenko is a passionate chemical researcher. He studies development of materials for grinding tools. In 2014 he got PhD in Material Sciences. His research is dedicated to the study of the polymer structure and improvement of heat-resistance and mechanical properties of materials based on polymers.

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## Strength and ductility characteristics of polymer-modified CSA cement concrete

**Myoungsu Shin**

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This study investigated the age-dependent strength and ductility characteristics of calcium sulfoaluminate (CSA) cement systems modified by an acrylic redispersible polymer powder. The effects of the polymer on the compressive strength and microstructure were examined from an early age of 2 h to 90 days. The macro- and microstructural characteristics of the hardened mortars and cement pastes were characterized by compressive strength tests, mercury intrusion porosimetry (MIP), powder X-ray diffraction (XRD), and scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS). The test results suggested that a higher dose of polymer powder not only delayed setting, hydration, and strength development, but also refined the pore structure of the cement systems suitable for achieving superior ductility. We believe that our study makes a significant contribution to the literature because it contributes to reducing the energy consumption and associated CO<sub>2</sub> emission from cement production, specifically by providing information that can be used to enhance the mechanical characteristics of CSA cement systems.

### Biography

Myoungsu Shin holds a B.S. (1994) and M.S. (1998) from Seoul National University and a Ph.D. (2004) from the University of Illinois at Urbana-Champaign. He has been on the faculty of the School of Urban and Environmental Engineering at UNIST since March 2010. Dr. Shin was previously an Assistant Professor at Morehead State University in Kentucky from 2004 to 2006. He is a licensed Professional Engineer in the U.S. with about four years of practical engineering experience at Rosenwasser Grossman Consulting Engineers in New York, NY. Prof. Shin is a member of many national and international, technical and administrative committees, including ACI-ASCE Committees 352 (Joints and Connections), 421 (R/C Slabs), and ACI Committee 374 (Performance-Based Seismic Design). His primary research interests include seismic design, modeling, and assessment of civil infrastructures, design optimization of tall buildings, high performance sustainable materials (e.g. fiber-reinforced, self-healing, sulfur composites), and non-destructive evaluation technologies.

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**Accepted Abstracts**

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## Molecular dynamics simulation studies of structure and dynamics of poly(acrylic) acid in semidilute concentration regime

Abhishek Kumar Gupta and Upendra Natarajan

Indian Institute of Technology Madras, India

A detailed fully atomistic molecular dynamics (MD) simulation study was carried out with the aid of explicit specification of solvent molecules on poly(acrylic) acid (PAA) in salt free aqueous solution from dilute to semidilute concentration region at different degree of ionization (f) values viz.  $f = 0.2, 0.4, 0.7$  and  $1.0$ . The structural properties viz. Radius of gyration ( $R_g$ ), end-to-end distance ( $R$ ), hydrogen bonding (interchain, intrachain and intermolecular), intermolecular structure, bound water ratio, scattering structure factor, interchain distance, interchain contacts and dihedral angle distribution have been elucidated. The dynamic properties viz. hydrogen-bond dynamics and self diffusion coefficient of PAA and counterions have been reported and compared with experimental and model studies. The results have revealed that, conformation size ( $R_g$  and  $R$ ) decreases with increase in polymer volume fraction ( $\phi_P$ ) which is in qualitative agreement with the experimental studies where, ionized PAA particle length decreases with increase in PAA concentration in the semidilute region. Moreover, this behavior is in agreement with the model studies that, demonstrated a decrease in conformational  $R_g$  with polymer concentration. The number of interchain and intrachain H- bonds show an increase with increase in  $\phi_P$ . The self diffusion coefficient of PAA and sodium counterions showed a non-monotonic and monotonic decrease with increase in  $\phi_P$  which, is in good agreement with the bead – spring polyelectrolyte model studies under fully ionized conditions. The details of analysis of properties will be presented.

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## On linear instability of flows of an incompressible polymeric fluid with a strong discontinuity

**Andrey Yu Goldin<sup>1</sup>, Andrey I Marinov<sup>1</sup> and Alexander M Blokhin<sup>2</sup>**<sup>1</sup>Novosibirsk State University, Russia<sup>2</sup>Sobolev Institute of Mathematics, Russia

**Statement of the problem:** Nowadays there are a lot of models which describe the behavior of flows of polymeric fluids. But, some important properties such as stability or instability of solutions for these models have been studied insufficiently. Particularly, we consider the so-called Vinogradov-Pokrovskii model using the mesoscopic approach to the mathematical modelling of polymers. The stability of a polymeric fluid at rest and the stability of a strong discontinuity are analyzed. Two different ways of realization of the state of rest are discussed: the state of rest of one fluid in a flat infinite channel and the state of rest of two fluids with different parameters separated by a strong discontinuity. Also some results on the stability of a strong discontinuity in an infinite medium with the possibility of overflowing have been obtained. **Methodology:** The standard Lyapunov's method is used for studying stability and instability. We derive the linearized equations of the initial system of partial differential equations. The linearization is performed with respect to the state of rest. Then, special solutions are found. Algebraic conditions for the eigenvalues, which are responsible for the time growth, can be determined by cumbersome calculations. **Results:** The state of rest of one fluid in a flat channel is stable to small perturbations whereas time-growing solutions are constructed and, so, instability is shown for the case of two fluids with a strong discontinuity in an infinite medium with overflowing.

**Conclusion & Significance:** Nowadays polymeric materials have an important role in different fields of industry and technologies. In attempts to understand their behavior we can propose and study a lot of mathematical models. Then some main properties such as stability of flows and discontinuities can be studied. According to this information modern devices and technologies based on polymeric materials can be created or improved

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**Organoclay – Polyester nanocomposites: Structure-property relationship between organic additives to the clay and mechanical properties of the composites****Atindra D Shukla<sup>1</sup>, Kinjal J Shah<sup>2</sup>, Dinesh O Shah<sup>1</sup> and Toyoko Imae<sup>2</sup>**<sup>1</sup>Dharmsinh Desai University, India<sup>2</sup>National Taiwan University of Science and Technology, Taiwan

The organoclays with variety of quaternary ammonium substituents (QAS) were successfully synthesized and studied for their hydrophilic/hydrophobic behavior. These organic surfactants get accommodated in the inter-layer galleries of clay via cation exchange process. Modified clays were used as filler in unsaturated polyester (UPE) resin to yield organoclay nano-composites with altered mechanical properties. The organoclay-BQASMMT18 (octadecyldimethylbenzy-lammonium bromide modified montmorillonite) with only 3 wt% in the UPE enhanced tensile strength, tensile modulus, flexural strength and elongation at break by the order of 4.6, 2.4, 2 and 2.4, respectively, compared to the same properties of pristine UPE. The tensile strength and hardness of the UPE-organoclay nanocomposites was increased with increase in organoclay content in the nanocomposites. However, the tensile and flexural strength decreased with increased loading of BQASMMT18 from 3% to 5 wt% due to increased non-uniformity in dispersibility of organoclay in polymer matrix. Moreover, dispersibility of hydrophobic organoclays in UPE nanocomposite is higher when compared to that of hydrophilic and pristine clay. In summary, the hydrophilic or hydrophobic character of the organically modified clay significantly affected its dispersion in the polymer matrix, which in turn affected the mechanical properties of the resultant nanocomposites.

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## **Self-assembly and sequential processing for morphology control over organic photovoltaics and chemical doping of conjugated polymers**

**Benjamin J Schwartz**

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One of the key issues with improving the efficiency of conjugated polymer-based photovoltaics is controlling the nm-scale morphology of the two active components. Typically, efficiency is optimized by trial-and-error: component weight ratios, solvent additives, post-processing thermal annealing, etc. are all used to attempt to obtain the desired bulk heterojunction (BHJ) interpenetrating network. In this talk, I discuss some of my group's recent work aimed at using alternate, more reproducible methods for controlling BHJ morphology. Our results include the use of new amphiphilic semiconducting polymers and fullerenes that spontaneously self-assemble into co-axial cylindrical micelles in solution, and thus provide a built-in connected network when cast into gels that form thin films. Photoexcitation of the polymer in these systems produces separated charges on sub-ps time scales, and the separated charges are stable for weeks to months in air-free environments. We also show that sequential processing of the polymer and fullerene components can provide an exquisite degree of control of the nm-scale morphology of a BHJ, and that the degree of crystallinity of the polymer controls both the amount of intercalated fullerene and the geometry of the interpenetrating network. Finally, we demonstrate that sequential processing also can be used to infiltrate molecular dopants into films of conjugated polymers, providing improved film quality and allowing access to the physics of the mobile carriers in doped polymers that were previously unavailable.

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**Rheological and structural changes of polymerized whey protein after heat treatment****Cuina Wang<sup>1</sup> and Mingruo Guo<sup>2</sup>**<sup>1</sup>Jilin University, China<sup>2</sup>University of Vermont, USA

**R**heological property and structure changes of whey proteins as functions of pH (6-8), heating time (5-30 min) and temperature (70-95°C), and protein level (6-11%) were systematically investigated. Flow behavior at first day and shelf life of 7 days as function of shear rate were measured by a Rheometer. The structure changes were determined by FTIR and UV-CD spectrometer. The shear viscosity profiles of all heated dispersions were similar. Heating time and pH had more pronounced impacts on viscosity stability than other factors. Compared with native sample, all heated samples showed increased  $\alpha$ -helix content. pH and heating time had more significant impact on the structure changes on polymerized whey protein.  $\alpha$ -Helix content increased with increased temperature. Large aggregates were observed at whey protein samples heated at high temperature above 85°C. As protein concentration increased, bands at higher region become darker.

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## **Preparation and properties of NR based ebonite rubber suitable for use as engineering material**

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<sup>3</sup>Rubber Research Institute, Nigeria

**T**he preparation of various samples of ebonite vulcanizates and their physico-mechanical properties have been investigated using standard methods. This work explores the production of ebonite dust, production of ebonite vulcanizates and investigation of the characterization of the ebonite. Five different ebonite materials – labeled A, B, C, D, and E with sulphur content in parts per hundred grams of rubber (Phr) of 32, 34, 36, 38 and 40 respectively were produced. The physico-mechanical properties carried out were tensile strength, hardness and abrasion resistance. The tensile strength (MPa) for sample A, B, C, D and E were 5.6, 3.5, 4.7, 1.7 and 2.0 respectively while the abrasion(%mass loss) were 8.49, 4.24, 2.59, 1.08 and 1.05 respectively and the hardness(IRHD) being 63, 64, 65, 70 and 82. The results show that the preparation of ebonite from natural rubber as a base polymer is feasible considering the results of characterization obtained.

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**Composites by doum fiber and bakelite matrix: Mechanical and thermal studies****Hala Bensalah<sup>1</sup>, Hind Chakchak<sup>2</sup> and Kamal Gueraoui<sup>1</sup>**<sup>1</sup>Mohammed V-Rabat University, Morocco<sup>2</sup>Centre National pour la Recherche Scientifique et Technique (CNRST) UATRS, Morocco

In this study, we figured Phenolic resin (Bakelite). Based composites strengthened with chemically treated doum fiber at different packing from 10 to 40 wt. that were prepared by compression molding procedure that showed that These composites are characterized particularly by mechanical and thermal properties presenting some kind of smoothness in their comportment that were measured by some flow tests and cup .as a result, we found that Increasing fiber's weight percentage in these composites was the solution for the Improvement of their properties. For example, adding chemical drum fibers [20 wt. %] is able to increase the flexural properties significantly without losing strain values. For the thermal conductivities of composite illustrations were measured by homemade system. Besides, we found gradual decrease in thermal conductivity for an incensement in fiber content. Plus, dynamic mechanical analysis has shown the effect of tension, regularity and fiber charging as in the rheological properties of the composites.

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**Development of nano filled PP-PC blends for electrical wiring accessories for the underdeveloped countries****JP Sheth, UN Puntambekar and Satish Chetwani**  
ERDA, India

**N**ano Clay and Nano Calcium Carbonate particulates were synthesized using the wet chemical process. The crystallite size of the Nano powders was determined using XRD. The particle size distribution of the Nano fillers in the polymer matrix was determined using the SEM analysis. Chemistry and purity of the samples was determined using EDS analysis. These Nano powders were incorporated into PP-PC blend in proportions of 1, 3 and 5 wt% Mixing was carried out using a Brabender plasticoder followed by fabrication of Nano composites using hot press method. These Nano composites were tested for electrical and mechanical properties. The results were compared with the unfilled polymer and the properties were found to exhibit significant improvement suggesting application of these Nano composites in a variety of electrical applications such as wiring accessories like plugs, switch body, basal plates, fan regulator bodies etc.

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**Polyurethane composite based force controlled micro sensors for biomedical applications****Kishor Kumar Sadasivuni and John-John Cabibihan Deanna**  
Qatar University, Qatar

**P**olymers and its nanocomposites keep on serving as a basic solution for the developing electronic technologies. Their wider applicable ranges were through consumer electronics, photovoltaics, e-clothing, robotics and biotechnology. The requirement of electronically active systems composed of biomaterials has utmost significance. The present work uses polyurethane filled polymer nanocomposites for designing a flexible force sensor useful in biomedical applications. The device sensitivity and specificity are analyzed by varying different environmental conditions. It is observed that reproducible and constant signals are observed upon force. The sensor mechanism involves in the polymer network capacitance and resistance change. The interface of zinc oxide is checked for the effective interactions existing and the morphology of the composites are analyzed in detail to know the nanostructural architects. We have also analyzed the sensing effect with biomedical implants to grasp. Finally, the investigated sensitivity of the developed eco-friendly, low-cost sensor of reduced size demonstrates its capability to resolve many of the technological problems facing on sensing devices for biomedical applications. This sensor can be used in robotic systems for minimally invasive surgeries (MIS), precise surgeries, and their corresponding technologies.

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## Effects of rice straw-based polyol on the thermophysical properties of rigid polyurethane foam

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**Statement of the Problem:** Vegetable oils and lignocellulosic biomass are two major types of bio-based resources gaining interest for bio-based polyols for polyurethane (PU) production. However, the consumption of huge amounts of vegetable oils could result in a shortage of vegetable oils and will cause the increase in food prices. Therefore, lignocellulosic biomass is seen as a better alternative raw material for PU production. Various kinds of lignocellulosic biomass, have been used for the production of bio-based PU foams but the use of lignocellulosic rice straw is not yet explored. Thus, the study aims to develop a PU rigid foam from rice straw-based polyol and investigate the effect of isocyanate index on the thermophysical properties of the foam.

**Methodology & Theoretical Orientation:** PU foams were prepared by reacting isocyanates in varying indices with polyols containing 15% of rice straw-based polyol and 85% petroleum-based polyol and their thermal conductivity, density and compressive strength were determined.

**Findings:** PU foams with no biopolyol replacement has superior thermal and mechanical properties over the PU foams with biopolyol replacement. However, those with biopolyol replacement were significant less dense compared to the commercial formulation. This could indicate possible application in industries where lightweight materials is important. Thermal characterization of the foam samples at different isocyanate indices indicate that increasing the isocyanate content improves insulation property of the PU as evident with the decreasing conductivity. This is also true with compressive strength. The index is directly proportional to the compressive strength. Density, on the other hand, is directly proportional to the isocyanate content.

**Conclusion & Significance:** Successful development of PU rigid foam products using biomass-based polyols obtained from a renewable feed stock rice straw offers a practical and economic procedure for potential scale-up and commercialization.

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## Co (non) solvency or the puzzle of polymer properties in mixed good or poor solvents

**Kurt Kremer**

Max Planck Institute for Polymer Research, Germany

The relation between atomistic structure, architecture, molecular weight and material properties is of basic concern of modern soft matter science. Here computer simulations on different levels of resolution play an increasingly important role. To progress further adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution and thus pave the way to open systems simulations. Typical examples where such approaches are helpful are studies of stimuli responsive polymers, also called smart polymers. Here especially the so called co-solvency and co-non-solvency are puzzling examples of unusual polymer solvation behavior i.e. that of polymers in mixed solvents. Particularly PNIPAM in water alcohol mixtures reveals an interesting coil-globule-coil transition. This conformational transition cannot be explained within the classical Flory-Huggins picture, which is the standard mean field theory for polymer solutions and mixtures. The results point towards a general design of 'smart stimuli responsive polymers' and will be explored in detail. In the opposite case of a polymer in two poor solvents, e.g. PMMA in water and alcohol, a weak swelling is observed in mixed solvents. While appearing like just an inverse phenomenon of co-non-solvency, it turns out that here a delicate balance of depletion effects can be identified as the origin of the phenomenon.

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## Graphene/Transition metal dichalcogenite 2D materials for the development of ternary blend based polymer solar cells

**Kusum Kumari**

National Institute of Technology Warangal, India

Solar cells are among the most promising technologies for renewable clean energy. However, conventional silicon-based solar cells are too expensive for everyday use. Organic Photovoltaic(OPV) devices have shown great promise due to the advantages of low cost, flexibility, light-weight, easy processing etc. The current state of- the-art laboratory efficiency is 10-11%. These improvements are mainly attributed to the development of new materials and device engineering, including non-fullerene acceptor, morphology control, interfacial engineering. Despite those achievements, many issues remain (e.g., efficiency, lifetime, stability, etc.) that need to be addressed before OPVs are practically utilized. Recently, ternary polymer solar cell(PSC) blends have been explored as a strategy to improve OPV performance; however, this approach has been demonstrated only for polymer–fullerene solar cells with organic ternary additives and has not yet addressed stability issues. Here, we will present the PSCs comprising ternary blends of semiconducting polymers, PCBM acceptor, and 2D materials Graphene Oxide(GO)/ Transition Metal Dichalcogenite(TMD) as third component additives. These 2D materials such as GO and TMD nanosheets have recently been explored in OPV owing to their high carrier mobilities, high chemical stability, and exceptional charge transport properties. We found that the addition of GO and TMD nanosheets in polymer-fullerene blends improves performance and photo stability of such OPV devices. This is attributed to the fact that third component additive GO nanosheets reduces recombination by increasing the separation of holes and electrons between donor and acceptor via cascade charge transfer mechanism, and also aids the efficient charge transport through the blend matrix as they contribute to high carrier mobilities. Besides, the addition of TMD nanosheets as additives provides extra advantage of complementary optical absorption in the visible and infrared. Therefore, the utilization of GO and TMD nanosheets as ternary additives in OPV creates new opportunities for the development of OPVs.

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## Discovery of static shear-elasticity in liquids & melts

**Laurence Noirez, Patrick Baroni and Philipp Kahl**

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**O**n the basis of a Maxwell gas model (1867), it has long been suspected that liquids and polymer melts exhibit (shear) elasticity at sufficiently high solicitation frequencies (MHz or GHz) only. Recent experimental improvements indicate that liquids exhibit also shear elasticity at very low frequency (0.1 to 10Hz). This finding is of utmost importance, since it means that liquids are no fully viscous, but possess a weak but finite elastic threshold below which they are solids. The elastic property has been identified at sub-millimeter scale, both on simple liquids and complex fluids (polymer melts, molecular glass formers, Van der Waals liquids, ionic liquids, H-bond liquids) pointing out the generic characteristic of this neglected property that invalidates the single molecular approach of the viscoelasticity. We present the first experiments identifying static shear elasticity in the bulk from unentangled to entangled polymer melts. In particular, we show how the low frequency shear elasticity and the usual viscoelastic response are related. The low frequency shear elasticity involves collective processes and has profound implications on how the melt flows, on flow and surface instabilities, thermodynamics, fluidic transport mechanisms enables to foresee new effects as the cold production or the spectacular conversion of a liquid melt in a strain-driven optical harmonic oscillator.

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## Electrically conductive graphene/polymer nanocomposites

**M. Zafar Iqbal<sup>1</sup>, Ahmed A. Abdalla<sup>2</sup> and Matthew W. Liberatore<sup>3</sup>**

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<sup>3</sup> University of Toledo, USA

A unique combination of excellent electrical, thermal, and mechanical properties enable graphene as a multi-functional reinforcement for polymer nanocomposites. However, poor dispersion of graphene in non-polar polyolefins limits its applications as a universal filler. In this presentation, we discuss our research on improving the dispersion of graphene in polyolefins to produce electrically conductive nanocomposites. Highly non-polar nature of polyethylene (PE) was altered by blending it with a polar polymer, called oxidized polyethylene (OPE). Blends of PE with OPE were synthesized via solution blending method. Inclusion of OPE in PE produced miscible blends, but the miscibility decreased with increasing OPE loading. Meanwhile, the Young's modulus of blends increased with increasing OPE concentration, attributed to decreased long period order in PE and increased crystallinity. In addition, the miscibility of OPE in PE substantially reduced the viscosity of blends. Electrically conductive nanocomposites were manufactured by incorporating graphene in PE/OPE blends via solution blending. The rheological and electrical percolations increased substantially to 0.3 and 0.13 vol% in blend/graphene nanocomposites compared to 1.0 and 0.3 vol% in PE/graphene nanocomposites. Improved dispersion of graphene in blends was attributed to increased graphene/polymer interactions, leading to high aspect ratio of the dispersed graphene. A universal Brownian dispersion mechanism for graphene was concluded similar to that of carbon nanotubes, following the Doi-Edwards theory. Furthermore, the improved dispersion of graphene correlated with the formation of surface fractals in blend/graphene nanocomposites, whereas the poor dispersion of graphene in PE led to the formation of only mass fractals.

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## A rational molecular design of an efficient visible-light organic photoredox catalyst for light driven controlled radical polymerization

**Min Sang Kwon**

Ulsan National Institute of Science and Technology (UNIST), Korea

**V**isible light photoredox catalysis, formerly inaccessible redox-neutral reaction scaffolds, has enabled significant development of radical chemistry in organic and polymer synthesis. So far, most progress in this field has been made with transition metal complexes, yet several aspects of current transition-metal photoredox catalysis still remain important challenges. Although organic photoredox catalysis has been recently investigated as an attractive alternative of transition metal catalysis, only limited class of organic dyes has been employed as organic catalysts. In this presentation, I will discuss about a rational molecular design for an efficient visible-light organic photoredox catalysts with the broad diversity in structure and properties. Also, I will talk about their synthetic applications for light-driven controlled radical polymerization.

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## Flexible polyurethane blown with nanoclay as footwear component

**Moumita Mukherjee<sup>1</sup>, Saraswathy GnanaSundaram<sup>1</sup>, Sujata Mandal<sup>2</sup> and Bhabendra Nath Dasa<sup>1</sup>**

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Recently, PU foams composite of solid-gas material intrigued significant interest due to its wide applications. Conventionally polyurethane foam is prepared by adding two types of blowing agent, physical blowing agent (low boiling point solvent) and chemical blowing agent (water). In the present work, for the first time a series of flexible polyurethanes are developed by addition increasing amount of nanoclay (have been developed in our lab) 0.5-3% as a chemical blowing agent. The inter layer -OH group of the developed filler react with the -NCO terminated pre-polymer of PU to generate flexible polyurethane foam. The developed polyurethane contained exfoliated nanoclay structure cross linked with the native PU which is further confirmed by FESEM analysis. As a result it shows that the addition of nanoclay has been increased the flexibility. The physical, morphological and thermal properties of the developed PU foams have been studied to find suitability in shoe sole. The polyurethane foam prepared using the developed compositions are flexible and light-weight while maintaining other physical properties like hardness, density, abrasion resistance and tensile strength in advisable range for shoe sole application.

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# POLYMER SCIENCE AND ENGINEERING

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## Composites in machine tools & Work-holding

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With the growing need to build faster, efficient and economic machines, light weight and fatigue control are key considerations in the engineering of rotating machine elements. As the main concern for machining is higher air cutting times or idle times which is due to the weight of the structures constraining the quick acceleration and deceleration cycles. Also while concentrating on light weight machine elements, we also need to consider their high damping and static stiffness requirements to ensure the engineered geometries, required rates of production and acceptable surface finish are achieved economically. Composite materials, by the virtue of their high stiffness to weight ratio can meet the above objectives by reducing the impact of inertia if used for the structural components in machine tools. Work-holding components in the machine tools play a very crucial role in achieving the required part accuracies. Different conventional material combinations and geometric optimization are already in place to explore the possibility of machining the most complex components with high levels of accuracy. Moving ahead by exploiting the low weight and low cost properties of composites and the flexibility it provides for manufacturing, the possibility of having more efficient machine tools and work-holding systems will be discussed. Conclusion: By understanding the feasibility of material combinations and new degrees of freedom in the manufacturing involved, the feasibility of moving towards strong and economic engineered solutions with the initial probable trials to be made will be shown.

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## POLYMER SCIENCE AND ENGINEERING

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**Double-decked model of the flow of polymeric incompressible fluid past a flat wedge****Roman Semenko and Alexander Blokhin**

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As known, polymeric fluids consists of very large molecules (macromolecules) which causes remarkable properties of these fluids. Polymer melts has a non-linear viscoelastic behavior so a number of rheological model was developed to describe its motion. One of the most popular type includes mesostructural (or statistical) models. They are based on molecular structure of the substance and considers the processes of intermolecular interactions. This approach allows the one to study the connection between macroscopical and microscopical scales. Usually mesostructural models uses reptation theory which consider long linear entangled macromolecules. Often macromolecule is modeled as set of beads connected by springs which represents an elastic forces. We will use mesostructural model which is the modified Vinogradov-Pokrovskii model.. It considers friction between beads of a macromolecule as a tensor which is connected to the anisotropy of a shear flow. This anisotropy tensor is determined by size and shape of macromolecules. If the flow of polymermelts has non-zero velocity gradients then macro-molecules deforms along the flow which makes a media anisotropic. Our goal is to study the behavior of polymeric fluid for classical type of flows which is the flow past the flat infinite wedge. It is well-known that stationary solutions for supersonic flow of fluid past the wedge has surface of strong discontinuity of a shock wave type. We are looking for the similar type of the flow for polymeric fluids using modified Vinogradov Pokrovskii model. We showed classical scheme of stationary flow past the wedge has to be modified for polymeric fluid by adding extra surfaces of strong discontinuities (we have called this type of flow as a double-decked model).

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# POLYMER SCIENCE AND ENGINEERING

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## Response surface method optimization of rice straw-liquefaction using crude glycerol for rigid polyurethane foam application

**Rosal Jane G Ruda, Kriztine M. Icalina, Arnold A. Lubguban and Cañaveral**  
Mindanao State University, Philippines

**Statement of the Problem:** Polyurethane is a versatile class of polymer produced from the condensation polymerization of isocyanates and polyol, a hydroxyl-rich compound. Its application can be found in adhesives, sealants, coatings, flexible and rigid foams. However, polyol is traditionally sourced from petroleum raw materials. With increasing environmental and sustainability problems, lignocellulosic biomass is a potential alternative source due to its abundance, biodegradability and its hydroxyl component. In the Philippines, 11.3 M tons of rice straw is produced annually which when burned, produces air pollutants such as carbon dioxide, nitrogen oxide and sulfur dioxide. Rice straw can be liquefied using an atmospheric liquefaction process with the use of a catalyst. Researchers reported that varying liquefaction parameters can significantly alter the properties of a polyol<sup>3</sup>. The purpose of the study is to produce rice straw-based polyol with a low acid number, high OH number, low viscosity and high liquefaction ratio which is suitable for rigid foam applications.

**Methodology & Theoretical Orientation:** A one-pot liquefaction process was used to liquefy rice straw with the use of sulfuric acid as catalyst and crude glycerol as liquefaction solvent. Response surface methodology was used to optimize four factors: acid loading, biomass loading, reaction time and reaction temperature based on four responses: acid number, OH number, liquefaction ratio, and viscosity.

**Findings:** Statistical analysis showed that all four factors have a significant effect on polyol properties. Increasing the acid loading was shown to significantly increase residual acid while higher reaction times lead to a decrease in liquefaction efficiency. Polyols with optimum properties were produced at a reaction time of 180-300 minutes, acid loading of 1-2%, reaction temperature of 170-180°C, and a biomass loading of 10-15%.

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## POLYMER SCIENCE AND ENGINEERING

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**Fabrication of novel acrylic-based hydrogel for controlled release of organic and inorganic fertilizers****Rubab Zohra<sup>1</sup>, Muhammad Aslam Malana<sup>2</sup> and Shehnila<sup>3</sup>**<sup>1</sup>Forman Christian College (A Chartered University) Lahore, Pakistan<sup>2,3</sup>Bahauddin Zakaria University Multan, Pakistan

A novel terpolymeric hydrogel system composed of methacrylate (MA), vinylacetate (VA) and acrylic acid (AA) chemically crosslinked with Diethylene Glycol Dimethacrylate (DEGDMA) was studied for its application in the field of controlled release fertilizers. Two inorganic agrochemicals, ammonium nitrate (AN), potassium nitrate (PN) and one organic fertilizer, urea were selected as test chemicals to study the efficiency of the hydrogel. The copolymeric hydrogels were characterized through Fourier transform infrared (FTIR), Differential scanning calorimeter/ thermal gravimetric analyses (DSC/TGA) and Scanning electron microscopy (SEM). During swelling studies, it was found that the media penetration velocity and equilibrium media content changed adversely with the crosslink density. The pH of loading medium shifted the swelling mechanism from Fickian ( $n < 0.5$ ) to non-Fickian ( $n > 0.5$ ) behavior. The crosslink density also decreased the Molecular weight between cross links,  $M_c$ , and mesh size,  $\xi$ . The percentage loading capacity of hydrogel was found to be higher for inorganic chemicals (70 % for PN and 71.1% for AN) than that of Urea with loading percentage of 42.56-61.5. Extensive release studies of Urea indicated that the cumulative release of Urea could be controlled by changing its initial concentration in the loading medium and the acrylic acid component in the hydrogel. The release of Urea was also studied in soil solution and it was found that the ions present in the release medium highly affect the cumulative release amount of the fertilizer slowing down its release rate as compared to that in the deionized water. Moreover, mostly the hydrogels exhibited a non-Fickian type release behavior with the diffusion exponent ( $n$ ) having value greater than 0.5.. The promising response these hydrogels to the external pH, a reasonable agrochemical loading capability, optimum release capacity, first order release kinetics and favorable swelling behavior indicate that these hydrogel systems may be used, not only, as good controlled release fertilizer (CRF) but may also be helpful to enhance the water absorption capacity of soil alongwith avoiding soil erosion phenomenon in the best possible way.

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# POLYMER SCIENCE AND ENGINEERING

October 02-03, 2017 Chicago, USA

## **Engineering at the nanoscale: A strategy for developing high performance functional polymer materials**

**Sabu Thomas**

Mahatma Gandhi University, India

The talk will concentrate on various approaches being used to engineer materials at the nanoscale for various applications in future technologies. In particular, the case of clay, carbon nanostructures (e.g. nanotubes, graphene), metal oxides, bio-nanomaterials (cellulose, starch and chitin) will be used to highlight the challenges and progress. Several polymer systems will be considered such as rubbers, thermoplastics, thermos-setts and their blends for the fabrication of functional polymer nanocomposites. The interfacial activity of nanomaterials in compatibilising binary polymer blends will also be discussed. Various self assembled architectures of hybrid nanostructures can be made using relatively simple processes. Some of these structures offer excellent opportunity to probe novel nanoscale behavior and can impart unusual macroscopic end properties. I will talk about various applications of these materials, taking into account their multifunctional properties. Some of the promising applications of clay, metal oxides, nano cellulose, chitin, carbon nanomaterials and their hybrids will be reviewed. Finally the effect of dewetting up on solvent rinsing on nano scale thin films will also be discussed.

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**pH responsive polymer brushes grafted from the surface of intravaginal rings for reversible switch on/off on-demand drug delivery****Sedigheh Nazaripour<sup>1</sup>, Sadegh Ghanbar<sup>2</sup>, Yufei Chen<sup>2</sup>, Emmanuel A Ho<sup>2</sup> and Song Liu<sup>2</sup>**<sup>1</sup>Polycast International Ltd., Canada<sup>2</sup>University of Manitoba, Canada

**A** new pH sensitive reservoir type polyurethane intravaginal ring (PU IVR) was developed for on-demand drug delivery using a novel and versatile method. A combination of surface-initiated activator regenerated by electron transfer atom transfer radical polymerization (SI- ARGET-ATRP) and alkyne-azide click reaction was applied to graft pH responsiveness polymer brushes from the surface of PU IVR to achieve a rapid switchable release at specific pH environments. First, poly (propargyl acrylate) (PPA) brushes were grafted at the surface of PU IVR segments via. SI-ARGET-ATRP to get the alkynyl handle terminated PU: PPA-PU. Secondly, pH sensitive monomers were bonded onto the surface of PPA-PU via. alkyne-azide clic reaction. X-ray photoelectron spectroscopy (XPS) and Attenuated total reflectance Fourier transform infrared (ATR-FTIR) confirmed that polymer brushes were successfully grafted from the PU surface. The pH- responsive behaviour of untreated PU IVR segments and functionalized segments with pH-responsive polymer brushes were studied in PBS buffer solution at pH 4 and pH 7 over a minimum of 5 cycles using hydroxychloroquine (HCQ) as a model drug. The untreated PU IVR did not show any pH responsiveness upon pH changes. On the other hand, modified PU IVRs showed pH responsiveness upon changes in pH values. Release studies demonstrated that the “through pore mechanism” controls release of HCQ from pH sensitive reservoir-type IVR drug delivery systems. PU IVR grafted with anionic functional groups showed more release at acidic pH than basic pH. However, when cationic polymer brushes were grafted from the surface of PU IVR, more release was observed at basic pH than acidic pH.

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## POLYMER SCIENCE AND ENGINEERING

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**Bioactive polymer of plant origin – Prospective therapeutic agent****Vakhtang Barbakadze**  
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The caffeic acid-derived polyether, namely poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl) ethylene] or poly[3-(3,4-dihydroxyphenyl) glyceric acid] (PDPGA) was isolated and identified in the water-soluble, high-molecular weight fractions obtained from extracts of different species of Boraginaceae family. According to data of <sup>13</sup>C, <sup>1</sup>H NMR, APT, 2D <sup>1</sup>H/<sup>13</sup>C HSQC, 1D NOE and 2D DOSY experiments the polyoxyethylene chain is the backbone of the polymer molecule. 3,4-Dihydroxyphenyl and carboxyl groups are regular substituents at two carbon atoms in the chain. The repeating unit of this regular polymer is 3-(3, 4-dihydroxyphenyl) glyceric acid residue. Most of the carboxylic groups of PDPGA from *Anchusa italicica* and *Symphytum grandiflorum* unlike the polymer of *S. asperum*, *S. caucasicum* and *S. officinale* are methylated. The 2D DOSY experiment gave the similar diffusion coefficient for the methylated and non-methylated signals of PDPGA. Both sets of signals fell in the same horizontal. This would imply a similar molecular weight for methylated and non-methylated polymers. Then basic monomeric moiety of this polymer, 3-(3, 4-dihydroxyphenyl) glyceric acid (DPGA) was synthesized via Sharpless asymmetric dihydroxylation of *trans*-caffeic acid derivatives using an osmium catalyst. Besides, it is well known that epoxides are valuable synthons in organic synthesis and have been introduced into pharmaceutical applications. Subsequently, the building block for the production of derivatives of PDPGA, methyl 3-(3,4-dimethoxyphenyl)glycidate was synthesized based on the Darzen reaction or by oxidation of *trans*-caffeic acid with oxone in order to produce in future derivatives of synthetic analogue of natural polymer through ring-opening polymerization of 2,3-disubstituted oxirane. PDPGA is endowed with intriguing pharmacological properties as anti-complementary, antioxidant, anti-inflammatory, burn and wound healing and anticancer properties. *S. caucasicum* PDPGA and DPGA exerted anti-cancer efficacy *in vitro* and *in vivo*. However, our results showed that anticancer efficacy of PDPGA is more effective compared to its synthetic monomer. Overall, this study identifies *S. caucasicum* PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

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# POLYMER SCIENCE AND ENGINEERING

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## Preparation of chlorinated poly(propylene carbonate) and its properties

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Carbon dioxide is an inexhaustible inexpensive chemical raw material, and it has been recently noted to fix carbon dioxide into a chemical material on a large scale. Since Inoue synthesized aliphatic polycarbonates having high molecular weight by using the copolymerization of carbon dioxide and an epoxy compound in 1969,<sup>1</sup> the study on the copolymerization of carbon dioxide and epoxy compounds has been continuously deepened and developed.<sup>2</sup> Nowadays, it become a research focus in the field of polymer sciences to synthesize polymer materials by using carbon dioxide as the raw material. For an example, poly(propylene carbonate) (PPC) as a typical biodegradable material is an alternating copolymer of carbon dioxide and propylene oxide,<sup>3</sup> and has been put into the stage of industrial production. Recently, PPC was chlorinated in our laboratory by a gas-solid phase reaction(Figure 1).<sup>4</sup> Ion chromatography and NMR tests showed that chlorine atoms were successfully introduced onto the PPC polymer chains. We named this new chlorinated polymer as chlorinated poly(propylene carbonate) (CPPC). It was worth noted that the chlorination reaction is quite warm at 60°C without any solvent and catalyzer, which is easily and simply realized for industrial production. It was found that the CPPC processed many more distinguished properties in solubility, wettability, adhesive, and gas barrier et al comparing to the PPC. For examples, the bonding strength of the CPPC as adhesive was nearly four times higher than that of the PPC on wood, stainless steel and glass by thermal bonding at 180°C. The oxygen permeability coefficient of the CPPC exhibits a decrease of 33% comparing to the PPC. Moreover, the CPPC kept good biodegradability. These results indicated that the CPPC could be widely used in coating, adhesive, barrier materials, and so on, which could greatly promote the development of PPC industry. This work was financially supported by the National Natural Science Foundation of China for General Program (51673195).

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## Leveraging the power of manufacturing data to perfect your production process

**Willem Sundblad**

Oden Technologies, USA

Every plastics manufacturer dreams about having perfect transparency into their processes to continuously improve production efficiency and quality. Using data is the key to optimizing recipes, quality, and capacity to ensure factories stay competitive. The problem is that data tends to live and die in the equipment, without being recorded or utilized anywhere. Acquisition requires months of hard-wiring your factory into PCs on top of burdensome installation costs. The resulting data is raw, inconsistent, and hard to translate into insights. The latest technological advancements we take for granted in the rest of our lives—rising processing power, decreasing computing cost, abundant wireless connectivity, and limitless cloud storage—is finally available to make your existing machines truly digital. Now you can collect and analyze data from all your existing machines and sensors simply by attaching small transmitters to serial ports. Monitor all the metrics you value, together, in real time. Increase the efficiency and value of your existing extrusion lines. No lengthy IT projects, hardwired networks, or new equipment required. Willem Sundblad will give an update on the current Industry 4.0 landscape, where the market is heading, and what concrete solutions looks like for plastics manufacturers in addition to giving a demo of how machine learning algorithms can and are being used throughout the industry.

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**Characterization of ethylene norbornene copolymer aged: Impact of norbornene content on the stability thermal and oxidative****Wowro Sonia Rosine Lago<sup>1,2</sup>, Caroline Aymes-Chodur<sup>1</sup>, Ange Privat Ahoussou<sup>2</sup> and Najet Yagoubi<sup>1</sup>**<sup>1</sup>Université Paris, France<sup>2</sup>Université Félix Houphouët Boigny of Cocody, Côte d'Ivoire

This study is an overall theme on the study of material ageing induced by ionizing radiation, photodegradation and the heat, that mimicking sterilization and storage ageing of medical devices. It is therefore, performed on different grade of ethylene and norbornene (ENC). These copolymers have interesting physicochemical properties for pharmaceutical and medical applications, due to their transparency similar to glass, good chemical resistance and low permeability to gas and water. The results presented here put in evidenced the modifications of the physico-chemical properties of aged ENCs, using experimental techniques such as FTIR (Fourier Transformed Infrared spectroscopy), UV spectroscopy, DSC (Differential Scanning Calorimetry), TGA (Thermogravimetry Analysis) . ENC stability is influenced by several parameters including the rate of norbornene present in the structure. Nevertheless, the effect of treatment (ionizing radiation, heat or photodegradation) used as a sterilization process, and also the treatment by photodegradation, used as a storage process, has a real impact on the oxidation induction time to oxidation of ENCs. It is also highlighted in this study, the presence of oxidations compounds that can act as oxidation protector. It would be interesting now to identify them to determine their specific toxicity.

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