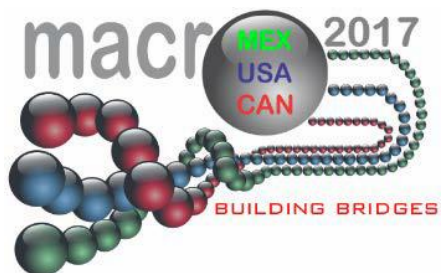


# *SOCIEDAD POLIMÉRICA DE MÉXICO*



Sociedad Polimérica  
de México, A.C.



*Los Cabos, Baja California Sur del 3 al 7  
de diciembre del 2017.*

*XXX Congreso Nacional de la S.P.M.*

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***Angel Licea Claverie, Iván Zapata  
González y Rubén González Núñez***

# **PATROCINADORES**



Proyecto 279522 apoyado por el CONACYT

# PREFACE



Dear participants of the 4th US-MÉXICO BINATIONAL SYMPOSIUM ON ADVANCES IN POLYMER SCIENCE “MACROMEX2017” and XXX National Meeting of the Mexican Polymer Society:

This is the fourth time that the Sociedad Polimérica de México A.C. (SPM) is pleased to co-organize with the Polymer Chemistry Division of the American Chemical Society (POLY-ACS), this meeting focused on increasing cooperation and scientific interaction among researchers in North America. This time we also include the participation of the Chemical Institute of Canada as co-organizers contributing to the success of this international meeting with the motto “Building Bridges”.

MACROMEX2017 takes place on December 3rd-7th of 2017 in the beautiful city of Los Cabos at the tip of the Baja Peninsula which harbors the impressive Sea of Cortez, named by Jacques Cousteau as “the Aquarium of the World”.

The conference includes participants from 9 countries, and includes 114 oral presentations and 124 posters, among them 4 plenary speakers and 33 Invited speakers from USA, Mexico, and Canada, together with other invited speakers and contributors from other countries including Chile, Spain, France, Germany, Portugal and Italy.

A rich variety of presentations related to different contemporary issues in polymer science and engineering are organized in the following symposia:

- 1.-Advances in Macromolecular Synthesis
- 2.-Reactions on Polymers: Crosslinking, Functionalization and Grafting

- 3.-Macromolecules and Nanotechnology
- 4.-Polymers for Biomedical Applications
- 5.-Functional Polymers for Advanced Technologies: Optoelectronics, Membranes and Energy
- 6.-Composites and Blends
- 7.-Polymer Engineering and Modeling
- 8.-Smart Polymers and Surfaces
- 9.-General Topics on Polymers

The Chairs of the meeting are Rigoberto Advincula (Case Western Reserve University, USA), Michael F. Cunningham (Queen's University, Canada) and Angel Licea-Claverie (Instituto Tecnológico de Tijuana, México).

The Organizing Committee of MACROMEX2017 is grateful to all contributors, plenary and invited speakers for sharing their knowledge and expertise in the conference and for contributing to the success of MACROMEX2017.

The Organizing Committee wishes also to express its thanks to all the sponsor institutions and companies, particularly to the National Council of Science and Technology of Mexico (CONACYT, grant 279522) and to the Polymer Division of the American Chemical Society (International Committee) for its generous financial support for the organization of the meeting.

**WELCOME TO MACROMEX 2017!**

Rigoberto Advincula, Michael F. Cunningham, and Angel Licea-Claverie

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## Plenary Presentation

## NANOSTRUCTURED FUNCTIONAL HYBRID MATERIALS BY ATRP

KRZYSZTOF MATYJASZEWSKI

Many advanced nanostructured functional materials were designed and prepared by ATRP (atom transfer radical polymerization). Copper-based ATRP catalytic systems with polydentate nitrogen ligands are among most efficient controlled/living radical polymerization systems. Recently, by applying new initiating/catalytic systems, Cu level in ATRP was reduced to a few ppm. Also metal-free ATRP was developed. ATRP of acrylates, methacrylates, styrenes, acrylamides, acrylonitrile and other vinyl monomers was employed for macromolecular engineering of polymers with precisely controlled molecular weights, low dispersities, designed shape, composition and functionality. Examples of well-defined copolymers and various hybrid materials and bioconjugates prepared with high precision will be presented. These polymers are used as components of various advanced materials such as health and beauty products, coatings, elastomers, adhesives, surfactants, dispersants, lubricants or sealants. Special emphasis will be on nanostructured multifunctional hybrid materials for application related to environment, energy and catalysis.



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Plenary Presentation

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**SYNTHESIS, APPLICATIONS AND RADICAL POLYMERIZATION KINETICS OF  
NOVEL DEGRADABLE MACROMONOMERS**

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ROBIN A HUTCHINSON, THOMAS R ROONEY

Short-chain polyester methacrylate macromonomers with alkyl, tertiary amine, carboxyl, and hydroxyl end-group functionalities are synthesized by ring-opening polymerization and subsequent modification. The functionality controlled in the synthesis is imparted onto the comb-polymer structures formed via radical polymerization, with an even greater diversity of materials is accessible through copolymerization. This presentation will provide an overview of the materials produced and their applications, which range from degradable cationic flocculants for oil sands tailings to nanoparticles with tunable biodegradability for drug delivery. Specialized techniques have been applied to study the polymerization behavior of the macromonomers, to facilitate the design and control of the resulting (co)polymer materials. The propagation rate coefficients ( $k_p$ ) determined by pulsed laser polymerization experiments for bulk poly(lactic acid ethyl ester methacrylate (PLANEMA) macromonomers with  $N=1$  and 5 average number of polyester units are not significantly different, but are elevated by 60% compared to methyl methacrylate. The results indicate that the nature of substituents several units beyond the methacrylic group does not decisively impact bulk  $k_p$  measurements. In addition, the effect of macromonomer length and end-group functionality on reactivity is studied by tracking monomer conversions and composition drift during batch radical copolymerization with styrene using an in situ NMR technique. The effects of end-group functionality and hydrogen bonding on relative reactivity are pronounced for monomeric analogues of the macromonomers. However, the polyester spacers significantly dilute these effects in macromonomer copolymerization. Instead, the chemical identity up to several units from the methacryloyl group is the most important indicator of macromonomer relative reactivity.



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## Plenary Presentation

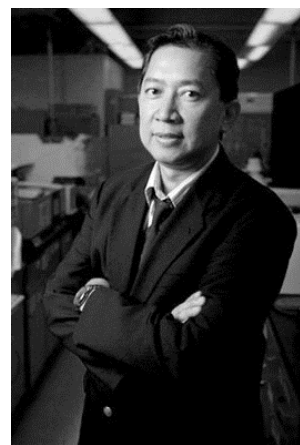
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### HIGH TIME FOR POLYMERS IN 3D PRINTING

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RIGOBERTO ADVINCULA

The advent of 3D printing has ushered a new direction in design complexity and advances in materials' structure-composition-property relationships. Advanced and Additive manufacturing means a departure from traditional modes of high-throughput methods, focusing on on-time, limited, complex, and high-performance materials and parts manufacturing. An important question is "what is the role of polymer materials in advancing the value chain of 3D Printing?" This talk will focus on some of the challenges, potential, and demands for polymer materials in 3D printing. The Advincula research group has done work on utilizing nanocomposites to improve on the thermo-mechanical properties of objects including their biocompatibility. The methods of SLA, SLS, FDM, VSP have amenable methods for utilizing resins, powders, filaments, and pastes respectively as representative polymer materials and formulations which can be optimized to produce the desired processing methods and parts properties. Graphene nanoparticles have been used to optimize the strength of these materials with inclusion in both thermoplastics and thermoset resins. SLS offers a method of direct blending of powders to result in specific processability in hybrid compositions, not easily accessible by blends or solutions. Lightweighting applications, biomedical applications, non-metallic substitution, and parts monolith fabrication (or reduce number of parts) are some of the potential benefits in the use of predominantly polymer materials in 3D printing.



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Plenary Presentation

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**SYNTHESIS OF NANOPARTICLES AND NANOCOMPOSITES BY NANOEMULSION  
AND SEMICONTINUOUS HETEROPHASE POLYMERIZATION PROCESSES**

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JORGE PUIG ARÉVALO

The polymerization of a series of alkyl methacrylates in nanoemulsions made by the Phase-Inversion Temperature (PIT) method is presented here. Results indicate that the nanoemulsion droplets act as templates for the formation of nanoparticles, since the particle size does not change during the polymerization. Kinetics mechanism and characteristics of the polymers obtained are reported. In addition, the semicontinuous heterophase polymerization (SHP), in which initially neat monomer(s) is dosed at a controlled addition rate to produce the nanoparticles, is examined. Addition rate controls particle size and polymer characteristics; in fact, as the monomer addition rate diminishes, smaller particles with smaller molar masses are produced. It is also reported the synthesis by SHP (i) of mesoporous nanoparticles for drug delivery, of conductive polypyrrol nanoparticles with better conductivity produced in smaller reaction times than those obtained by microemulsion polymerization, and (iii) of poly(acrylamide-co-N-isopropylacrylamide)/chitosane core/shell nanocomposites designed as controlled drug delivery carriers. The increase in molar ratio of acrylamide/N-isopropylacrylamide moves the volume phase transition (or collapsing) temperature of the polymer to values within the ranges of healthy and sick living mammals. Finally, with the semicontinuous inverse heterophase polymerization, where a water-soluble monomer is added at a controlled rate over an oleic phase containing only surfactant and initiator, poly(sodium acrylate) nanogels able to absorb water in more than 2000 times their weight were obtained.



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## Invited Presentations

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### POLY(ESTER-URETHANES) BEARING AMINO-ACIDS MOIETIES: SYNTHESIS, CHARACTERIZATION AND DRUG-DELIVERY BEHAVIOR

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ANTONIO MARTINEZ-RICHA, KARLA A. BARRERA-RIVERA

Synthetic biodegradable polymers can be used as materials for temporary scaffolds for tissue engineering purposes, as sutures, drug delivery devices, orthopedic fixation devices or temporary vascular grafts. These polymers need to possess the desired biocompatibility, suitable mechanical properties and predictable biodegradability. Biodegradable polyurethanes (PUs) are generally prepared by using easily hydrolyzable polyols, such as polycaprolactone diol (PCL), polyacrylic acid (PAA), polylactic acid (PLA), and polyglycolic acid (PGA), as soft segments. Biodegradable polymers also are commonly biocompatible, water soluble, low crystalline or having low melting point. Biodegradation of PCL films by pure strains of microorganisms isolated from industrial compost induces a weight loss of 95 wt% (with respect to the initial mass) after 200 h of incubation. It is expected that derivatives obtained by chain extension reactions of PCL also show similar biodegradable properties. One of the more important factors to consider for PCL chain extension reactions is the chemical nature of the polyester end groups. Diol derivatives ( $\square$ - $\square$ -telechelic diols) are specially targeted, due to the feasibility of the hydroxyl end-groups to react with different functional groups. In this work, synthesis and characterization of polyurethanes containing alpha-aminoacid moieties using a chemoenzymatic process is presented. The release profiles of different drugs at three different pHs will be discussed. In most of the cases studied, drug release was a two-stage process: an initial rapid release stage (burst; value calculated by visual observation from the change in the curve slope) followed by a second slower release stage.

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### POLYURETHANE BLENDS FOR SMALL CALIBER VASCULAR GRAFTS

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ARACELY LINNETTE MEZA VILLEGAS, CESAR ANTONIO PEREZ ARANDA, OMAR DE JESUS CASTILLO CRUZ, ROSSANA FARIDE VARGAS CORONADO, JUAN VALERIO CAUICH RODRIGUEZ

Polymer blends based on Tecoflex® and HMDI-PCL-arginine polyurethane (SPUR) were obtained by solvent casting and studied by FTIR and Raman spectroscopy, DSC, TGA, SEM and XRD. In addition, longitudinal and circumferential tensile properties were measured and compared with tensile properties of dumbbell specimens. Finally, the pressure burst strength was measured with a in-house equipment. In blends, FTIR showed the as the SPUR content increased, carbonyl absorption at 1726  $\text{cm}^{-1}$  also increased while the Raman shift of the same group was of lower intensity. Melting of PCL soft segment were detected by DSC in agreement with  $2\theta$  reflections at  $21.3^\circ$  and  $23.6^\circ$  assigned to SPUR as Tecoflex® was amorphous and only exhibited an endothermic transition at  $81.1^\circ\text{C}$ . In general, tensile modulus of blends was observed between Tecoflex® and SPUR except for 50%, 60% and 80% of SPUR which were lower than expected. In contrast, vascular graft modulus was higher for 40%, 50% and 80% of SPUR in the blend. The circumferential strength of blends was observed between 10 MPa (Tecoflex®) and 50 MPa (SPUR). Pressure burst strength was higher than



1000 mmHg for all blends but changes in deformation were only observed for pristine Tecoflex and blends with 20% of SPUR. By SEM, delamination of vascular graft was observed in blends as the amount of SPUR increased.

### ELECTROSPUN FIBROUS MEMBRANES CONTAINING DRUGS: RELATIONSHIP BETWEEN MOLECULAR INTERACTIONS AND RELEASE RATE

MARÍA MÓNICA CASTILLO-ORTEGA, ITZEL YANIRA LÓPEZ-PEÑA, DAMIAN FRANCISCO, PLASCENCIA-MARTÍNEZ, ARSENIO FÉLIX-NÚÑEZ

Coaxial electrospinning has been used in different materials, such as membranes composed of poly(vinyl pyrrolidone) and N,N-dimethylacetamide, biodegradable nanofibrous mats, polycaprolactone with incorporated protein, and others. Materials prepared by the electrospinning method have been used for different applications, such as drug delivery systems, and in general for biomedical applications. In previous articles we reported the preparation of fibrous membrane of cellulose acetate and the poly(vinylpyrrolidone) by the electrospinning method and release of amoxicillin from them. As well as, a comparative study of the fibrous composite membrane with amoxicillin, triclosan or epicatechin embedded, and their characterization, morphology, physical-chemical and mechanical properties using SEM, TEM, FTIR, thermal, mechanical as well as the evaluation of the release rate. In this work we present experimental results to evidence the relationship between molecular interactions and release rate.

### PHASE-SEPARATING BIOCONJUGATES AND THEIR APPLICATIONS IN REGENERATIVE MEDICINE

KRISTI KIICK

The incorporation of motifs from natural proteins, such as collagen and resilin, into bioconjugates offers important opportunities in designing biomaterials with useful stimuli-responsive behavior. Their conjugation to polymers affords biomaterials with diverse properties responsive to multiple biologically relevant triggers. Conjugates are able to form a range of structures that modulate cell behavior and influence the retention and release of cargo, offering substantial improvement in cargo activity. These materials can be designed with microstructural heterogeneity as well as into particles that are useful in a variety of drug delivery approaches. The materials exhibit high cytocompatibility, can be used to modulate signaling by vascular cells, and can rescue the radial compliance of skeletonized blood vessels.

### IMPACT OF MOLECULAR ARCHITECTURE OF PEGylated POLY(AMINO ACID)S ON THEIR BIORELEVANT PROPERTIES

DAVID ULKOSKI, JEFF SPARKS, MAJED MATAR, CARMEN SCHOLZ

The possibility to pre-determine and vary the molecular architecture of triblock copolymers is an advantageous feature. Under conditions of a living polymerization, PEGylated poly(amino acid)s, PAA,s were synthesized, using poly(ethylene glycol), PEG, as macroinitiator to and contain an ionic (poly(L-Lysine), p(L-Lys) or poly(L-glutamate), p(L-Glu),

and a hydrophobic (poly(L-Leucine), p(L-Leu), PAA-block). Copolymers were also synthesized with the PAA segment as random copolymer. The block length, i.e. ionic strength, and block position, i.e. the ionic block forms either the middle or the end-block, were varied and the resulting copolymers were investigated for their biorelevant properties. Block copolymers containing p(L-Lys) were specifically investigated for gene delivery applications, p(L-Glu) containing copolymers were considered for drug encapsulation. The p(L-Leu) segment initiates the self-assembly of the resulting nanoparticles, as well as polyplexes and provides stability. Biorelevant properties were investigated using mobility gel analyses, ribogreen assays, toxicity evaluations and cell transfection studies. Indomethacin and Doxorubicin were used as model drugs in encapsulation studies. Results revealed that polyplexes containing blocked PAA segments were more efficient and more stable in DNA condensation, protection and transfection than their counterparts with random PAA segments. The block position was relevant in transfection studies.

### PROTEIN ROLE IN THE INTERACTION OF PLASMA POLYMERS WITH BIOLOGICAL SYSTEMS

ROBERTO OLAYO

The chemistry and morphology of the surface are part of the main properties for biomaterials, the interaction with the biological system will define the capacity of interaction and many times if the material may be characterized as biocompatible. The surface of the material will interact with the proteins of the system and this will be the way to relate with cells, extracellular matrix, and in general with the biological system. Plasma polymerized polymers using pyrrole as monomer had shown good interaction in implants and as surface modification in scaffolds in tissue engineering, the chemical diversity of the surface allows for a good protein interaction. In the talk, different experiments will be discussed showing how this material interacts with proteins and how it allows to give several formulations that improve the biological interaction, the concept has been discussed in the nanomaterials literature as the protein corona, and it defines the real functionality of the material. Examples of implants, scaffolds, nanosystems and computer simulations of the possible interaction will be discussed.

### BIOMOLECULAR SYNTHESIS OF SSDNA: REACTION KINETICS, SELF-ASSEMBLY, AND APPLICATIONS

STEFAN ZAUSCHER

Polynucleotide block-co-polymers show rich micellization behavior in solution, and hold promise as surface-tethered brushes as novel functional materials for nano- and biotechnological applications. To date, however, the enzymatic synthesis of block-co-polynucleotides with high MW is still a challenge. Moreover, little is known about the design rules for the micellar morphologies that are formed by these polymers. Here, we report on our approaches to enzymatically synthesize polynucleotides in solution and their assembly into micelles and networks. Specifically, we provide a kinetic model and the design rules for the synthesis of multi-functional polynucleotides that can self-assemble into highly modular, micellar systems, with potential for drug delivery applications. Furthermore, we discuss the effect of unnatural nucleotides, incorporated into ssDNA, on DNA nuclease stability.

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## NEW FINDINGS ON POLYMER ELECTROSPUN SCAFFOLDS FOR THE CULTURE OF CELLS

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RICARDO VERA-GRAZIANO

Biomedical applications of polymer scaffolds based on poly(lactic acid), poli(caprolactone), poly(lactic-co-glycolic) acid, chitosan, collagen, gelatin, and fibroin have been studied. Structure-properties relations of electrospun polymer scaffolds for the culture of cells are discussed. Optimized electrospinning set-ups are used to prepare 2D and 3D scaffolds. The influence of electrospinning processing parameters on morphology, main physical, chemical and biological properties of the polymer scaffolds are studied by using different techniques (SEM, HRTEM, XPS, XRD, SAX, FTIR, NMR, DSC, TGA). Biocompatibility and cell viability and are also studied in-vitro and in-vivo. Biophysical characteristics of the scaffoldings look similar to those of living tissues for the culture of cells.

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## BIOLOGICAL FATE OF POLY LACTIC CO GLYCOLIC NANOCARRIERS: AGGREGATION/DEGRADATION IN VITRO AND IN VIVO

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SERGIO MOYA

Polymeric Nanocarriers (NCs) have emerged as a promising alternative to improve the therapeutic index of drugs by increasing their targeting capacity and accumulation in specific organs, tissues or cells while decreasing potential toxic and off-target side effects. However, the effective transition of the carriers into the clinical arena demands for a proper assessment of their interaction with biological fluids and cells, the kinetics of drug release, in vitro/in vivo degradation, and biological fate. Biocompatible and biodegradable poly lactic-co-glycolic acid (PLGA) NCs have pharmacological approval by the US Food and Drug Administration and the European Medicines Agency. PLGA NCs can be templated by emulsion or precipitation techniques and have a hydrophobic core suitable for the encapsulation of drugs with low aqueous solubility. We want to present different aspects of the fate in vitro and in vivo of PLGA NCs. Cellular uptake and intracellular degradation will be studied by combining Flow Cytometry, Confocal Laser Scanning Microscopy and Confocal Raman Microscopy. The bio distribution, organ accumulation and fate of radiolabelled poly lactic co glycolic NPs will be studied in animal models by means of Positron Emission Tomography (PET) and Single-Photon Emission Computerised Tomography (SPECT). NPs dose per organ will be evaluated. A dual radiolabelling strategy of nanoparticle core and coating will be presented using gamma emitters with non overlapping emission bands. After intravenous administration into rats, energy-discriminant (SPECT) resolves each radioisotope independently revealing different fates in vivo for the core and coating, which will be used to evaluate nanoparticle integrity in vivo.

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## Oral Presentations

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### LIPOSOME LOADED CHITOSAN HYDROGELS: A PROMISING WAY TO CONTROL THE BURST EFFECT IN DRUG RELEASE

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JACQUES DESBRIERES, MARCEL POPA, CATALINA PEPTU, BOGDAN CIOBANU, SIMONA BACAITA

Because of its favorable properties (non-toxicity, biodegradability, mucoadhesiveness) chitosan was studied as a biomaterial and as a pharmaceutical excipient in drug formulations. These formulations may be produced in a wide variety of forms including hydrogels or hydrogel based particles. In these formulations chitosan hydrogels are able to provide local delivery of loaded therapeutic agents but their delivery can be rapid and not easily time-controllable due to, particularly, the burst effect. This leads to a loss in drug efficiency and lifetime. To overcome the consequences of burst effect, systems involving liposomes incorporated into chitosan hydrogels may appear as a promising material in tissue engineering, regenerative medicine and drug loading systems. The use of liposomes entrapped within chitosan hydrogels allows a strong decrease of burst effect as well as a better control of release kinetics. The release kinetics mechanism was modelled; the mechanism of drug release is a complex Fickian diffusion, consisting of drug diffusion through the swollen hydrogel and/or water filled pores, being continuously fed by calcein loaded in liposomes. This knowledge will be a very interesting tool for designing new formulations for tissue engineering, regenerative medicine and drug delivery systems.

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### SEMI-INTERPENETRATING NETWORKS OF CARBOXYMETHYL-CHITOSAN WITH POLY(2-HYDROXYETHYL METHACRYLATE) FILLED WITH POLY(N-VINYL CAPROLACTAM) NANOGELS: BIOMATERIALS WITH POTENTIAL APPLICATION AS SKIN SUBSTITUTE

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OSCAR RUIZ-GALINDO, ANGEL LICEA-CLAVERIE, ARTURO ZIZUMBO-LÓPEZ

In the first step, chitosan (175 000 g/mol and deacetylation degree of 75%) was functionalized to yield a fully water soluble carboxymethyl chitosan (CMCS). 2-hydroxy ethyl methacrylate (HEMA) was crosslinked with ethyleneglycol-dimethacrylate (EGDMA) in the presence of CMCS by an UV radiation crosslinking method, to yield semi-interpenetrating networks. Different amounts on CMCS were dispersed in the monomer solution before synthesis, up to 1 W% of CMCS in relation to HEMA could be homogeneously dispersed. The inclusion of CMCS turned the relatively brittle PHEMA network (in the dry state) into a softer-elastic semi-interpenetrating network. The measured compression and tension moduli were closer to those found of human skin than those of PHEMA hydrogels without CMCS. Additionally, poly(N-vinylcaprolactam) (PNVCL) and poly(ethylene glycol) methacrylate (PEGMA) core shell nanogels were prepared by an already reported soapless emulsion polymerization method. These nanogels were prepared with a mass relation PNVCL:PEGMA of 50:50 and 55:45, also the synthesis of the nanogels was successfully scaled up five-fold to obtain enough amount on nanogels for their use as fillers. Finally, the semi-interpenetrating PHEMA-CMCS networks were filled with nanogels by repeating the same synthetic protocol by UV radiation described before, but mixing nanogels in the monomer solution. The semi-

interpenetrating hydrogel networks were filled with up to 0.5 W% of nanogels and show good dispersion in the hydrogel matrix. In relation to their mechanical properties, they are even softer as compared to the non-filled hydrogels and their percentage of deformation is closer to the deformation shown by human skin.

### **MATS BASED ON BIODEGRADABLE POLYESTERS AND ZINC OXIDE NANOPARTICLES ENGINEERED BY CENTRIFUGAL SPINNING WITH POTENTIAL USE AS BONE SCAFFOLDS**

VICTORIA PADILLA-GAINZA, HERIBERTO RODRÍGUEZ-TOBIAS, ROBERT GILKERSON, KAREN LOZANO, GRACIELA MORALES

Centrifugal spinning is a recent technique used for producing submicrometric fibers in a higher yield compared to the analogous technique denominated as electrospinning, therefore, the former is envisioned as a technology with high potential for the massive production of medical devices such as mats and scaffolds for tissue engineering. In this regard, this communication addresses the use of centrifugal spinning for the preparation of mats based on submicrometric poly(D,L-lactide) or poly(3-hydroxybutyrate) fibers embedded with zinc oxide nanoparticles. The centrifugal spinning process was optimized in order to obtain fibers with diameter lower than 1 micron, through the variation of polymer solution concentration and centrifugal rate. Considering the optimal conditions for the preparation of PLA or PHB fibers, zinc oxide nanoparticles were added to the precursory solution and subjected to centrifugal process. Electron microscopy (SEM and TEM) were used to determine the effect of the analyzed variables as well as the influence of ZnO content on final fibers morphology. Additionally, osteoblasts proliferation was performed to verify the potential use of the polyesters and polyesters/ZnO mats as scaffolds for bone regeneration.

### **DESIGN, SYNTHESIS AND CHARACTERIZATION OF A BIOPOLYMER AS A TREATMENT FOR CARTILAGE INJURIES**

JORGE ALFONSO TAVARES NEGRETE ARGELIA, ROSILLO DE LA TORRE, JOSÉ JORGE DELGADO GARCÍA, LAURA EDITH CASTELLANO TORRES, IRAIS AMARANTA QUINTERO ORTEGA

Cartilage extracellular matrix (CECM) is a natural scaffold composed mainly of water, collagen, and glycoproteoglycans that are secreted by chondrocytes. Daily activities such as mechanical overload, bad posture, incorrect sport performance and age promotes its degeneration. Chondrocytes death is the inherent consequence of the (CECM) degradation due to mechanical pressure. Therefore, if the specialized cells have not the ability to replicate they will be diminished, and when a critical point is reached the existing chondrocytes will be unable to synthesize enough CECM that allow them to survive and they will gradually disappear. Usually hydrogels formed by chitosan and other natural polymers such as collagen or hyaluronic acid are used to mimic the CECM and encourages its regeneration. A three polymer crosslinked hydrogel was synthesized with chitosan as the main chain, which will provide biocompatibility, antibacterial properties and structural strength; collagen was incorporated for enhancing the flexibility and tensile strength and hyaluronic acid (a glycoproteoglycan) was added for promoting cellular adhesion in the native cartilage, as a source of nutrient for chondrocytes and collagen precursor. The

synthesis of this biomaterial was done by the "Schiff" base and acetylation reaction, which take advantage of the amino and hydroxyl groups of the polymers, allowing crosslinking, which results in a biomaterial that mimics the physical and biological properties of the cartilage. The hydrogel was physicochemically characterized by a swelling behavior study, infrared, scanning electronic microscopy and shear and stress resistance. In vitro degradation evaluation was performed using human macrophages.

#### **PREPARATION OF PLA/ BIOGLASS 45S5 SCAFFOLDS VIA NONSOLVENT THERMALLY INDUCED PHASE SEPARATION (NTIPS) METHOD FOR APPLICATIONS IN BONE TISSUE ENGINEERING**

NORA JANETH LÚA-GÓMEZ, ENA ATHENEA AGUILAR-REYES, ROBIN DREW, CARLOS ALBERTO LEÓN-PATIÑO, PAULA WOOD-ADAMS

Scaffolds composed of biodegradable polymers and bioactive particles have been shown to possess the mechanical, biological and structural characteristics necessary for their application in the regeneration of bone tissue. In the present project, highly porous 3D PLA/Bioglass 45S5 structures were developed and the effect of Bioglass particles on the bioactivity, mechanical properties and morphology of the obtained scaffolds was evaluated. The synthesis of the scaffolds was carried out by the nonsolvent thermally induced phase separation (NTIPS) method. Polymeric solutions with various initial concentrations of polylactic acid (PLA) (13, 18 and 23 wt.%) and Bioglass 45S5 (5 and 10 wt.%) in dichloromethane were prepared. Phase separation in all systems resulted in highly porous (> 83%) semi-crystalline structures with interconnected macroporous of up to 120  $\mu\text{m}$ . The degree of crystallinity obtained was 53-59%. Compression tests were also carried out to determine the modulus and maximum strength at compression, the highest compression strength was recorded for 23% PLA scaffold with a value of 24.17 MPa. Finally, in vitro studies were performed on simulated body fluid (SBF) to evaluate the degradation and bioactivity of the scaffolds. The change in pH of the solution, as well as the weight loss and water absorption capacity of scaffolds at 3, 7, 14 and 28 days of incubation were monitored. Compression tests were performed after 28 days of immersion in SBF to evaluate the change in resistance. The formation of hydroxyapatite on the surface of the foams was observed by SEM and detected by FT-IR and XRD.

#### **SYNTHESIS AND PHYSICOCHEMICAL CHARACTERIZATION OF SILICON DIOXIDE NANOPARTICLES FOR ANTICONVULSANT DRUGS RELEASE.**

FRANCISCO JAVIER ROMERO ARGOTE, JOSE JORGE DELGADO GARCÍA, BIRZABITH MENDOZA NOVELO, IRAÍS AMARANTA QUINTERO ORTEGA, J. GABRIEL LUNA BÁRCENAS, ARGELIA ROSILLO DE LA TORRE

Nanoscale biomaterials used as drug carriers represent a potential strategy for transport and delivery of drugs in several pathologic conditions in which the drugs have limited access to the site of action. Silicon dioxide ( $\text{SiO}_2$ ) nanoparticles present a wide variety of properties such as chemical stability, biocompatibility, effective protection of molecules from enzymatic degradation, among others. In addition, these systems are especially suitable for transporting hydrophobic substances, a characteristic feature of many anticonvulsant drugs

(AD). The aim of this study was to synthesize, characterize, and evaluate SiO<sub>2</sub> nanoparticles as AD delivery system. Nanoparticles were synthesized by the Stöber method, which involves the hydrolysis and subsequent condensation of tetra-ethyl-orthosilicate (TEOS) in an ethanolic solution in the presence of a catalyst. For obtaining the nanomaterial with the necessary size, shape and porosity features, different parameters of the reaction conditions, such as, TEOS: ethanol: catalyst rate and reaction time, were evaluated. The nanoparticles were loaded with an AD by absorption. The nanomaterials were characterized physiochemically by infrared spectroscopy, scanning and transmission electron microscopy. The *in vitro* kinetics release evaluation was studied by UV-Vis spectrometry. The microscopy analysis verified the sphere-shaped morphology of loaded and unloaded nanoparticles and the *in vitro* release evaluation showed a two-phase behavior: first an initial burst discharge followed by a sustained AD release. These nanocarriers represent a potential strategy for transport hydrophobic drugs that have limited access to the site of action.

### GELLAN GUM DOUBLE NETWORK HYDROGELS FOR TISSUE ENGINEERING

FERNANDA ARAIZA-VERDUZCO, EUSTOLIA RODRIGUEZ-VELAZQUEZ, MANUEL ALATORRE-MEDA

Tissue Engineering (TE) is an emerging branch of medicine focused on the development of biocompatible materials, referred to as scaffolds, to restore, maintain or improve tissue functions. Double network (DN) hydrogels are novel interpenetrated networks that are attracting the interest of the scientific community as functional synthetic scaffolds. The main feature of DN hydrogels is that they present enhanced mechanical properties related to their inner structure. Additionally, if produced from natural polymers, they can also exhibit cytocompatible properties related to their friendly metabolism inside the body. This work explores the formation of DN hydrogels from gellan gum (GG) and its photosensitive methacrylated derivative GG-MA. The DN was synthesized upon mixing of both polymers, followed by the chemical crosslinking of GG-MA prompted by Irgacure and the ionic crosslinking of GG with CaCl<sub>2</sub>. The obtained DN was characterized by FT-IR, SEM, mechanical tests, and biodegradation assays, among others. FT-IR analyses demonstrated the occurrence of a Fermi resonance ascribed to the CO-Ca coupling resulting from the GG-CaCl<sub>2</sub> interaction. The SEM characterization showed the formation of large and interconnected pores. The mechanical tests proved the DN hydrogels as highly stable against deformation, resisting an applied load of 12.8 kPa, while the covalent and ionic single networks resisted 4.1 and 9.5 kPa, respectively (all applied loads were recorded at 22 %□). Finally, the biodegradation assays demonstrated that the DN hydrogels showed an outstanding stability against degradation with lysozyme. Taken together, the attained results depict the GG-based DN hydrogel as a potential candidate for tissue replacement.

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## ANALYSIS OF THE CONJUGATED DRUG-DELIVERY POLYMER, POLYGLUTAMATE-DOXORUBICIN BY THE LATEST ADVANCED MULTI-DETECTOR GPC SYSTEMS

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MARK POTHECARY, WEI SEN WONG, CARRIE SCHINDLER

In pharmaceutical research, targeting delivery location and release profile of drugs is a critical challenge. Polymers are playing an increasing role in drug delivery applications as targeted controlled-release mechanisms. One potential solution is to conjugate chemotherapy drugs such as Doxorubicin (Dox) with a delivery polymer such as polyglutamate (PG). Preferential uptake of PG-Dox conjugates by cancer cells and local degradation and drug release could more effectively target cancer cells over healthy cells. Gel-permeation chromatography (GPC) is widely used for measuring molecular weight (distribution) of natural and synthetic polymers. Historically, the elution volume of a sample was compared with that of known standards to estimate molecular weight. However, this so-called 'conventional calibration' will not give accurate molecular weights for conjugated polymers like PG-Dox. Static light scattering detectors measure the intensity of light scattered by a sample as it elutes from the column and therefore allow the direct measurement of the sample molecular weight independent of its elution volume. A viscosity detector can also be used to measure the parameter of intrinsic viscosity which can be combined with molecular weight data to calculate hydrodynamic radius. In combination, these data overcome the limitations of conventional measurements to measure accurate molecular weight, structural changes and drug loading. In this paper, we analysed PG, Dox, and two PG-Dox conjugates. Drug loading levels were accurately assessed and molecular weight and structural changes were also analysed. Regular use of multi-detector GPC measurements could support development and testing of these drug delivery candidates accelerating research in this area.

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## CORE-SHELL PLA/CARBOXYMETYL CELLULOSE NANOFIBERS CONTAINING CURCUMIN THROUGH COAXIAL ELECTROSPINNING

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GABRIELA LEÓN, GETHEMANI M. ESTRADA, EFREN MUÑOZ, JUAN MORALES, ROBERTO OLAYO

Coaxial electrospinning is an upcoming technology that has emerged from the conventional electrospinning process in order to realize the production of nanofibers of less spinnable materials with potential applications in the field of drug delivery, tissue engineering, and wound healing. The biocompatible and natural polymers as Poly Lactic Acid (PLA) and Carboxymethyl Cellulose (CMC) as a both core and shell materials may greatly enhance its scope in biomedical area. Curcumin (CUR) is a polyphenol and apart from its usage as a therapeutic agent, it is widely employed as a spice, food preservative, flavoring and coloring agent. Its common application for various diseases including cancer, cardiovascular and Alzheimer's disease, inflammatory and neurological disorders is owing to the outstanding biological functions such as antioxidant, anti-tumor, and anti-inflammatory activities. This study aims to develop the core-shell PLA nanofibers loaded with Curcumin (CUR) and coated with CMC obtained by coaxial electrospinning. In this work the profile release of CUR drug was studied, whose dosage mechanism is based on diffusion and the degradation of the CMC and PLA. Different concentrations of curcumin and PLA were evaluated. The chemical structure of the fibers was characterized by Fourier Transform Infrared Spectroscopy (FTIR), Raman, Scanning Electron Microscopy (SEM),



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Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and the dosing rates of curcumin were quantified by UV-Vis Spectroscopy.

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### COLLAGEN DERIVED BIOMATERIALS: IMPORTANCE OF THE CROSSLINKING BASED ON PROTECTED OLIGOURETHANES

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ESTEFANÍA G. VILLANUEVA, DANIEL PAREDES, JOSÉ L. MATA-MATA, ARTURO VEGA-CORONA, LAURA E. CASTELLANO, JORGE DELGADO, BIRZABITH MENDOZA-NOVELO

Coaxial electrospinning is an upcoming technology that has emerged from the conventional electrospinning process in order to realize the production of nanofibers of less spinnable materials with potential applications in the field of drug delivery, tissue engineering, and wound healing. The biocompatible and natural polymers as Poly Lactic Acid (PLA) and Carboxymethyl Cellulose (CMC) as a both core and shell materials may greatly enhance its scope in biomedical area. Curcumin (CUR) is a polyphenol and apart from its usage as a therapeutic agent, it is widely employed as a spice, food preservative, flavoring and coloring agent. Its common application for various diseases including cancer, cardiovascular and Alzheimer's disease, inflammatory and neurological disorders is owing to the outstanding biological functions such as antioxidant, anti-tumor, and anti-inflammatory activities. This study aims to develop the core-shell PLA nanofibers loaded with Curcumin (CUR) and coated with CMC obtained by coaxial electrospinning. In this work the profile release of CUR drug was studied, whose dosage mechanism is based on diffusion and the degradation of the CMC and PLA. Different concentrations of curcumin and PLA were evaluated. The chemical structure of the fibers was characterized by Fourier Transform Infrared Spectroscopy (FTIR), Raman, Scanning Electron Microscopy (SEM), Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and the dosing rates of curcumin were quantified by UV-Vis Spectroscopy.

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### INTEGRATION OF POLYPYRROLE SYNTHESIZED BY PLASMA SPINAL CORD INJURIES EVALUATED BY MAGNETIC RESONANCE IMAGING

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AXAYACATL MORALES-GUADARRAMA, GUILLERMO CRUZ, ROBERTO OLAYO, CAMILO RIOS, HERMELINDA SALGADO-CEBALLOS, JUAN MORALES, MA. GUADALUPE OLAYO, ARACELI DIAZ-RUIZ, OMAR FABELA-SÁNCHEZ

Central nervous system repair after spinal cord injury (SCI) remains the major challenge for any therapeutic strategy that seeks to restore adequate neurological function. An example of such strategies is the use of polymers synthesized by plasma derived from pyrrole (PPP<sub>y</sub>) and implanted in animal models (such as murine or rhesus monkeys) with SCI, which favor the protection of nerve tissue adjacent to the lesion and the functional recovery of models. Animal studies have contributed greatly to a better understanding of the pathophysiology of SCI, techniques such as histology or immunohistochemistry are commonly used to evaluate the effects of treatments with SCI, unfortunately it is necessary to sacrifice the subjects in different stages of therapy to obtain significant histological evidence. Magnetic resonance imaging (MRI) offers an *in vivo* approach to follow the evolution of SCI in a non-invasive way, allowing the same subject to be examined over time and to obtain

quantitative information correlated with treatment efficacy, in addition to the fact that each injury has a different behaviour and MRI can provide specific information for each case. In this study, MRI studies were performed to evaluate the behavior of SCI and the integration of PPPy over time in vivo, analyzing the lesion zone histoarchitecture of murine and rhesus monkeys.

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### PLA/SMMA/ACRYLIC-COMPATIBILIZER BLENDS: THERMAL, RHEOLOGICAL, AND MECHANICAL PROPERTIES FOR BIOMEDICAL APPLICATIONS

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LUIS SOLORIO, ALEJANDRO VEGA

PLA has revolutionized the biomedical thermoplastic industry by offering a new option of processing, design, and performance. With the incursion of shape polymer memory issue in this polymer age, PLA will play a crucial role in the next decades of medical devices. PLA Blends are usually followed to attain the properties needed to manufacture and to innovate those products that are for the welfare of the human health. Facing the mechanical challenges of the PLA, the present study presents and analyses the idea of producing new hydrophilic-hydrophobic PLA blends. PLA/SMMA/ACRYLIC-COMPATIBILIZER are characterized thermal, rheological, and mechanically, granting a new possibility of polymer composites to be considered in biomedical applications. Staying the main advantage of such blends by the cost-performance, partial biodegradability behavior and availability source worldwide. Under the loads reported in vitro, in vivo and through finite element, and by the simulation route, the material offers adequate mechanical properties to keep up the different biomechanical demands.

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### POLYSACCHARIDE-BASED SCAFFOLDS FOR CELL SEEDING AND ENCAPSULATION

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MANUEL ALATORRE-MEDA, EUSTOLIA RODRIGUEZ-VELÁZQUEZ

Tissue Engineering and Regenerative Medicine (TERM) are interdisciplinary biomedical fields that integrate biology, engineering, materials science, and medicine with the aim of developing biological substitutes to interact with living cells in order to restore, replace, maintain, or enhance tissue and organ functions. Most of the TERM strategies are based on the use of scaffolds that are seeded with cells obtained from the organ or tissue to be treated. The cells are expanded in vitro within the scaffold up until they reach a certain level of proliferation, and then the cell-laden scaffold is implanted in the patient at the desired site of action. The cellular component is responsible for the generation of the new tissue; meanwhile, the scaffold material provides a template to guide the cellular growth and mechanical stability. Polysaccharides are excellent materials for the synthesis of scaffolds. Among others, as extracted from natural sources, they are usually biocompatible and possess a significant ability to absorb water. Moreover, they can be conveniently modified by chemical means so as to display improved biological and physicochemical properties. The last but not the least, they are abundant in the natural Extracellular Matrix (ECM) and have a tremendous affinity for different endogenous macromolecules. Herein, we present an overview of the most significant results we have obtained in the last 5 years with respect to the synthesis and characterization of polysaccharide-based scaffolds for cell seeding and

encapsulation. Key features of the different systems such as the chemical, superficial, mechanical, and biological characteristics are fully discussed.

### MORPHOLOGY, BIOCOMPATIBILITY AND THERMOMECHANICAL PROPERTIES OF NYLON-CHITOSAN-KERATIN FILMS PRODUCED BY ELECTROSPINNING

LAURA EDITH ROJAS-MARTÍNEZ, CYNTHIA GRACIELA FLORES-HERNÁNDEZ, LUZ MARÍA LÓPEZ-MARÍN, CARLOS VELASCO-SANTOS ANA, LAURA MARTÍNEZ-HERNÁNDEZ

Polymer hybrids (natural- synthetic) combine the best of two or more materials to get some properties that are not found in only one. Nylon is a polymer known for its important mechanical properties, also polymers as chitosan and keratin are biopolymers known as biocompatibles. On the other hand, electrospinning is an important technique useful to develop nanofibers combining the mentioned polymers, avoiding high temperatures which could degrading the natural polymers. This research is focus to develop different polymer hybrids; nylon as support material of the biomolecules of chitosan and keratin. Three main systems in different concentrations are obtained by electrospinning: nylon-chitosan, nylon-keratin and nylon-chitosan-keratin. The electrospinning conditions are 20kV, 17 cm in distance, 2.5mL/h flow rate, time one hour. Nanofiber diameter is influenced by biopolymers. Thinnest fiber observed by Scanning Electron Microscopy (SEM) are produced with keratin and closed framework is also obtained by the influence of this biopolymer. However nylon-keratin films produce films with low storage modulus, measured by Dynamical Mechanical Analysis (DMA). Chitosan concentration in nylon increase the thermomechanical properties but the fiber are thicker than with keratin. The system that combine the properties of both biopolymers with nylon produce good thermomechanical properties and more closed framework than only with one biopolymer. Also biocompatibility measure by cell growth is improved slightly by keratin in comparison with chitosan. However, the polymer films results indicate that all samples are biocompatible including the samples with the three polymers. Thus, these results promise than these polymers could be useful in tissue engineering.

### POLYRHODAMINE: TOWARDS THE DESIGN OF A POLYANILINE MIMIC

COLLEEN SCOTT, RANGANATH WAHALATHANTRIGE DON, BRANDON BUTLER

Polyaniline (PANI) stands out as one of the most widely employed polymer, with commercial applications in printed circuit board manufacturing, antistatic and electrostatic dispersive (ESD) coatings, and corrosion protection. PANI also has great potential for applications in many other fields such as supercapacitors and batteries, electronic devices as hole-injection layers, solar cells, biosensors, and toxic metal recovery. Unfortunately, practical applications of PANI in these fields are limited by the material's electrochemical instability, and the lack of standard/optimized deposition methods. We present a new conducting polymer based on the rhodamine dye as a model system towards the development of a series of new conducting polymer to mimic PANI. Our model polymer (polyrhodamine, PRho) was prepared from a Buchwald/Hartwig synthesis of fluorescein ditriflate with p-phenylenediamine to give the polymer in good yield (80 %) and high molecular weight ( $M_n = 47000$ ). The polymer was shown to have good optoelectrical properties consistent with the

rhodamine dye and good chemical and electrical stability. The polymer can be cycled between acid (pH ~1) and base (pH ~12) solution without any noticeable change in the absorption spectrum. The cyclic voltammogram of a 100 cycle scan shows two redox peaks that were reversible even after 100 scan, with only a small change in the current for the second redox cycle. Amazingly, the polymer was found to have a conductivity of 5.27E-5 S/cm, which is in the range of semiconductors. This is the first report to our knowledge of a rhodamine backbone polymer with semiconducting properties.

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**COMPARISON BETWEEN HOMOPOLYMERS AND TRIBLOCKCOPOLYMERS. THE CASE OF HYDROXY TELECHELIC POLY(E-CAPROLACTONE) (HO-PCL-OH) AND POLY(E-CAPROLACTONE)-POLY(ETHYLENEGLYCOL)-POLY(E-CAPROLACTONE) (HO-PCL-PEG-PCL-OH) AND THEIR POLY(ESTER-ETHER-URETHANES) (PEUS)**

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JOSE EDUARDO BAEZ GARCIA, ANGEL MARCOS FERNANDEZ

A systematic study of two different types of hydroxy telechelic species derived from  $\alpha,\omega$ -hydroxy telechelic poly(e-caprolactone) (HO-PCL-OH) (homopolymer) and  $\alpha,\omega$ -hydroxy telechelic poly(e-caprolactone)-b-polyethylene glycol-b-poly(e-caprolactone) (HO-PCL-PEG-PCL-OH) (triblock copolymer) was realized. Both species HO-PCL-OH and HO-PCL-PEG-PCL-OH showed similarities regarding some spectra (by RMN 1H and 13C) and thermograms (by DSC). Due to the bifunctionality in the homopolymers and diblock copolymers, a series of poly(ester-ether-urethanes) (PEEUs) derived from 1,6-hexamethylenediisocyanate (HDI) were prepared. The analysis of PEEUs also exhibited some similarities between homopolymers and triblock copolymers.

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**BLOCK AND GRADIENT COPOLYESTERS AND THEIR NANOPARTICLES: A THERMAL AND MECHANICAL STUDY**

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DAMIANO BANDELLI, CHRISTINE WEBER, CHRISTIAN HELBING, KLAUS JANDT, ULRICH SIGMAR SCHUBERT

Polyesters represent biodegradable and biocompatible polymers making them useful for medical applications. In particular, applications aiming at release of actives from polyester-based nanoparticles are in focus of our research. The degradation and release behavior is affected by the crystallinity of the polyesters, however, the exact role of this feature is difficult to quantify as additional factors such as the hydrophilicity play a major role as well. Our approach is therefore directed to obtain tailor-made polyesters that vary in their crystallinity but maintain the same hydrophilic / hydrophobic balance (HHB). In this contribution, we show the synthesis of block and gradient-like polyesters from  $\delta$ -valerolactone and  $\delta$ -decalactone with the same HHB as PCL. In this regards we also evaluated the process of copolymerization resulting in gradient polymers. The materials were characterized by means of Size Exclusion Chromatography, Nuclear Magnetic Resonance, Differential Scanning Calorimetry and Thermogravimetric Analysis to assess their structural, thermal and mechanical properties. Stable aqueous nanoparticles suspensions of varying dimensions could be prepared by changing the concentration during the nanoprecipitation. Nanoparticles from all three polymers with a Dh of 170 nm remained stable for four weeks

and were investigated in detail by Atomic Force Microscopy and Scanning Electron Microscopy. All techniques consistently hint towards an altered internal structure of the nanoparticles with constant HHB.

## Poster

### BIO01-POLYACRYLAMID HYDROGELS / CELLULOSE ACETATE AND ITS APPLICATION AS ARTIFICIAL TISSUE IN RATS

JUAN CARLOS SÁNCHEZ-DÍAZ, EMILIO CRUZ-BARBA, AGUSTÍN MARTÍNEZ-RUVALCABA, RUBÉN OCTAVIO MUÑOZ-GARCÍA

Cellulose, methylcellulose (MC), cellulose acetate (AC), and several of its derivatives are used in the food industry as usual. These are additives, with numbers ranging from E460 (cellulose) to E466 (carboxy-methylcellulose, CMC), which offer varying levels of viscosity. The pharmaceutical industry also makes regular use of these compounds. They are, first and foremost, good laxatives but also are used for their thickening qualities, to give consistency to syrups or to produce gels. The mechanical properties of hydrogels are very important to a specific application proposing. In this work is studied the behavior of biomaterials where acrylamide, generally crosslinked, is the crosslinking material in a limited concentration range, obtaining Young's modulus in the order of MPa. The resulting materials are implanted in Wistar rats, which are suitable for testing with artificial tissue. Young's modulus results are presented before and after implantation in a range of 5 to 25% AC concentrations during synthesis. Acrylamide and cellulose acetate form an interpenetrating network through a free radical mechanism, wherein the acrylamide reacts with the molecules of cellulose acetate. Swelling and compression modulus are dependent on the amount of acrylamide, a greater amount of acrylamide is lower swelling and increased compressive modulus, from the composition of 20% this network can have cross-linker or not without a significant difference in swelling.

### BIO02-PREPARATION OF SINGLE AND COAXIAL POLYMERIC MEMBRANES BY ELECTROSPINNING AND THE EVALUATION OF THE EFFECT OF DRUG DISTRIBUTION IN THE FIBER ON RELEASE KINETICS

ARSENIO FÉLIX NÚÑEZ, MARÍA MÓNICA CASTILLO ORTEGA

Electrospinning is a fiber production method in which fibers forming a matrix with interconnected pores are produced using a polymer jet with the use of electrical field. A typical setup consists of a spinneret connected to a high electrical voltage, where the positively charged solution is pulled toward the collector plate by the effect of an electrical field. The major advancement in electrospinning in 2003 was when coaxial electrospinning was introduced, where two concentric layers are formed with necessary features when fiber cross section are analyzed. The unique advantage of coaxial electrospinning is the ability to sequester stimulants in various compartments and modulate the release kinetics by altering the fiber thickness and localization. The controlled drug delivery allows the release of

therapeutic agent loaded electrospun fibers at a controlled rate and timely manner to avoid undesired side effects and high doses of the drug. In electrospinning, successful drug encapsulation is dependent on ensuring the distribution of the drug molecule into the electrospun fiber. Drug characteristics such as instability and solubility, as well as the morphology of the fibers, could significantly affect drug encapsulation efficiency. Multilayered fibers by coaxial electrospinning provide altered release time profiles based on loading location and distribution of the drug in the fibers. In this study, single and coaxial polymeric membranes of polylactic acid will be prepared, both membranes will be loaded with propolis to evaluate the kinetic release of the active agent loaded in the fibers.

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### BIO03-PREPARATION AND CHARACTERIZATION OF PLA, ELASTIN AND GELATIN MEMBRANES OBTAINED BY COAXIAL ELECTROSPINNING

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ITZEL YANIRA LÓPEZ PEÑA, MARÍA MÓNICA CASTILLO ORTEGA

PLA Chronic wounds are those that have failed to restore the anatomical and functional integrity of the skin over a period of three months. Such wounds, unlike acute wounds, remain in a pathological inflammatory stage. Furthermore, these kinds of wounds usually show a high bacterial load which can further complicate wound restoration. The most common etiologies of chronic ulcers include pressure, diabetic foot and vascular ulcers (venous and arterial ulcers). The fundamental goal of tissue engineering is to develop biological substitutes that restore, maintain or improve diseased, injured, or congenitally absent tissues or organs. Strategies for the engineered reconstitution of tissues and organs are typically centered three fundamental approaches: cell based therapy, scaffold based therapy or bioactive molecule based therapy. Among the various approaches, biological achievements regarding cell culture using biodegradable materials are more promising techniques. To achieve these goals, several synthetic and natural polymers have been successfully electrospun into nanofibrous scaffolds or films to act as base matrices. In the recent years, electrospun fibres have been the subject of extensive studies due to their applications in drug delivery, tissue engineering and wound healing. The present work presents the preparation and characterization of membranes based on poly (lactic acid), elastin and gelatin, for their potential use as cell scaffold and release system

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### BIO04-RELEASE PROFILE OF (-) EPICATECHIN FROM ELECTROSPUN/ELECTROSPRAYED AC/PVP/AC POLYMERIC SYSTEMS

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DAMIAN FRANCISCO PLASCENCIA MARTÍNEZ, MARÍA MÓNICA CASTILLO ORTEGA

A drug delivery system consists in a formulation or device, that allows the introduction of a therapeutic agent into the body, which increases its efficacy and safety by controlling the rate, time and site of release of the active agent in the body. The release of the drug from a polymer matrix is determined by several factors such as: morphology, drug-matrix interactions, matrix type, size, drug concentration, among others. When a drug is encapsulated into a matrix, it is expected to carry out tests to determine the mechanism governing the discharge of the drug into the release medium, which help us to extrapolate it to the final application. There are a number of mathematical models that allow us to explain the kinetics, and predict the mechanisms that govern the release of drugs from nano

and micrometric structures, some of them are Korsmeyer-Peppas, Higuchi, zero order, among others. To evaluate the effect of morphology and drug-matrix-medium interactions, fibrous electrospun membranes and coaxial electrospayed spheres with a AC/PVP-Epicatechin/AC configuration were made and characterized by SEM; FTIR and drug release studies were performed by Uv-Vis spectroscopy. It was found that diffusion mechanism was predominant into the spheres whereas fibrous membranes had a more sustained release controlled by the drag and dissolution of PVP into the release medium.

#### **BIO05-PLASMA SYNTHESIS OF THIN FILMS OF POLYALLYLAMINE FOR TISSUE ENGINEERING**

JUAN MORALES-CORONA, ROBERTO OLAYO

In this work, the synthesis by plasma of thin films of polyallylamine under continuous plasma conditions is presented for possible use in surface modification of biomaterials. The thickness of the film depends on both the synthesis time and the power used. The polymers were synthesized with powers between 10W and 100W, and with different times of reaction. They were analyzed by XPS, FTIR, and contact angle and also tested for water resistance and as cell culture surfaces. According to the XPS analysis, 10 min deposit is sufficient for the full coverage of the substrate and remains after immersion in distilled water. At low power (10W), the N/C ratio is 0.28 very close to monomer ratio of 0.33. As the power increases, this ratio decreases up to 0.18. In order to maintain the characteristics of the monomer the best conditions of synthesis are a power of 10 W, time of 10 min and pressure of 18 mTorr. The biological test was done with a culture of fibroblasts on the films. The spectral analysis showed that the films remain chemically unaltered after the water immersion and shows that most of the nitrogen is as amine. This gives a polymer water resistant and with a large number of amines in the surface ideal for biomaterials.

#### **BIO06-SYNTHESIS AND ELECTROSPUN FIBERS OF BIODEGRADABLE POLYURETHANE, CHARACTERIZATION FOR POTENTIAL APPLICATION IN DRUGS RELEASE**

CLAUDIA VASQUEZ, MARIA MONICA CASTILLO, LERMA CHAN

Infection is a frequent complication on exposed fractures that compromise the treatment of bones, it could result in loss of an extremity or life. Now days, the clinical standard of the attention for opened and contaminated fractures is organized on stages, in that the wound is treated first with antibiotics to control the infection, followed by a bone graft. There is applied a graft of biodegradable bone with Hidroxiapatita (HAS) like appatites former in bones, with supported drugs release to prevent the implant from becoming infected, allowing the process of vascularization as much as new bone formation. Current advances in new drugs release systems represent a great opportunity to develop new therapies, or improve the efficiency of available medical treatments. These advances are particularly relevant on the regenerative medicine field, defying to such problems of health as the treatment of wounds in bone and skins repair. At the end, biocompatible materials have been widely studied to improve cellular live integration, and improve medical bioactivity in a located and controlled way. Therefore, in this project membranes of Polyurethane (PU), of biodegradable type (PU, polyester) and nano Hydroxyapatites (nHA) like bone forming,

using Vancomycin (VA) during the drugs release, will be elaborated; since it is an effective antibiotic for the treatment of the osteomyelitis, and it might be a clinical potential therapy for the treatment of infected bones. PU's scaffoldings that contain HA and VA, have the potential of being used in applications of bone tissue engineering and drug release.

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**BIO07-FABRICATION AND CHARACTERIZATION OF FIBROUS CYLINDERS USING ELECTROSPINNING TECHNIQUE WITH POSSIBLE APPLICATION IN BLOOD VESSEL TISSUE ENGINEERING**

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ABRAHAM LEYVA, MÓNICA CASTILLO

The cardiovascular diseases (CVD) are the major cause of death according to the World Health Organization, Vascular tissue engineering is a novel alternative to solve problems when a revascularization surgery is needed, especially when an small-diameter vascular graft is required. In the present work two composite materials with poly lactic acid and gelatin have been fabricated by electrospinning technique. The fabrication process and thermal (TGA, DSC), spectroscopic (FTIR), Mechanical and microscopic (SEM) characterization is presented to compare a blended and a core-shell structures as blood vessel tissue scaffolds, the properties suggest that these materials can be applied if some cellular essays prove them as biocompatible materials

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**BIO08-SYNTHESIS OF PH- AND TEMPERATURE-RESPONSIVE CHITOSAN/POLY(N-ISOPROPYLACRYLAMIDE-CO-ACRYLAMIDE) CORE-SHELL NANOPARTICLES BY SEMI-CONTINUOUS HETEROPHASE POLYMERIZATION**

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ANDRES ORTEGA-GARCIA, ABRAHAM ALVARADO, LOURDES ADRIANA PEREZ CARRILLO, MARTIN ARELLANO, JORGE EMILIO PUIG AREVALO

Thermo-responsive and pH-sensitive core-shell nanoparticles were prepared by semi-continuous heterophase copolymerization of N-isopropylacrylamide (NIPA) and acrylamide (AM) in the presence of chitosan (CS) micelles. After the addition and polymerization of the monomers, the chitosan micelles were crosslinked with glutaric dialdehyde. This polymerization process yielded high conversions and allows increasing the solid content in the system compared to batch emulsion polymerization. Dynamic light scattering (DLS) as a function of reaction time indicates a gradual increase in particle size, which is similar to the CS micelles in the literature. Transmission electron microscopy revealed that the nanoparticles are spherical and polydisperse with an average diameter similar to that obtained by DLS. The nanoparticles were swelled in three different pH buffer solutions (pH of 2, 4 or 7) as a function of temperature and subjected to increasing temperature tests to determine the volume phase transition temperature (TVPT) of the core-shell materials. Our results showed that the TVPT shifted to higher temperature with the increased in AM/NIPA molar ratio. Consecutive heating-and-cooling cycles proved thermo-reversibility. Their performance as drug release carriers with a model drug, doxycycline hyclate, indicates a sustained drug release for more than 50 hours of testing, which makes them suitable to drug release carrier inasmuch as shell (CS) is biocompatible and biodegradable.



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**BIO09-COMPARISON OF CATIONIC AND ANIONIC PEGYLATED NANOGELS FOR LOADING AND RELEASE OF CISPLATIN**

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MARÍA GONZÁLEZ, ÁNGEL LICEA, IVAN ZAPATA

Cis-diamminedichloroplatinum (II) "Cisplatin" is one of most used antineoplastic drugs for various types of cancer. However, several side effects due to its strong toxicity, that cause a decrease in quality of life of the patient, are discouraging for its use. In order to reduce these side effects, its transportation using nanocarriers, such as polymer nanogels, is one alternative to continue its use. It is well known that the tumor tissue shows lower pH values than the physiological one (7.4) and therefore pH-sensitive nanogels are strong candidates for drug delivery into tumor tissue. In this work, two PEGylated nanogels were synthesized with different cross-linked cores: a cationic system with poly(N,N-diethylaminoethyl methacrylate) (PDEAEM) and an anionic system with poly(2-methacryloyloxy benzoic acid) (P2MBA). A surfactant free emulsion polymerization was carried out at different feed compositions and operating conditions. The synthetic conditions were adjusted to yield nanogels in sizes between 100 nm and 200 nm, resulting also in differences in their pH-responsive swelling behaviour. PDEAEM nanogels show swelling at pH values lower than 7, while P2MBA nanogels show shrinkage at pH values lower than 7. A possible interaction between the nanogel and cisplatin through metal coordination with carboxylic acids or with amine groups is expected to yield high loadings of cisplatin in the nanocarrier. The kinetic evaluation of cisplatin release from the synthesized nanogels with anionic and cationic cores is under study and is one of the important factors to determine the best vehicle for cisplatin delivery to tumors.

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**BIO10-DRUG RELEASE SYSTEM BASED ON COLLAGEN-OLIGOURETHANE-SILICA HYDROGELS**

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MAGDALENA RANGEL-ARGOTE, MARÍA LONA-RAMOS, JORGE DELGADO, LAURA CASTELLANO, JOSÉ MATA-MATA, BIRZABITH MENDOZA-NOVELO

New platforms delivering therapeutics to guide soft tissue regeneration or to combat infections are required. The polymerization of collagen molecules along with crosslinking by the urethane chemistry is proposed as an alternative in the development of hybrid gels with controlled structure-property. When incorporated with silica particles, hydrogels support the loading and releasing of dexamethasone and vancomycin at pH 7.4 and 37 °C. The silica content impacts the collagen polymerization process and the collagen network structural parameters, while the oligourethane crosslinking regulates the mechanics and degradation of the material. The efficiency and control of the drug release is dependent on the silica content. After drugs are delivered from the hybrid gels, the effect of dexamethasone on immune cells and vancomycin on bacteria are maintained. Thus, collagen-oligourethane-silica hydrogels combine structure and properties that make them promising templates for loading and delivering drugs in a soft tissue engineering context.

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### BIO11-CHEMICAL INTERACTION BETWEEN POLYANILINE AND DAPSONE MIXTURES IN DRUG DELIVERY ROLES

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MARIBEL GONZÁLEZ TORRES, MARÍA GUADALUPE OLAYO GONZÁLEZ, LIDIA MARÍA GÓMEZ JIMÉNEZ, JUAN MORALES CORONA, ROBERTO OLAYO GONZÁLEZ, ROSARIO RAMÍREZ SEGUNDO, FERNANDO GABRIEL FLORES NAVA, RAFAEL BASURTO SÁNCHEZ, MARÍA DEL ROSARIO MEJÍA CUERO, GUILLERMO JESÚS CRUZ CRUZ

A study of plasma polyaniline to transport dapsone into the human body is presented in this work. This is achieved by absorbing the drug into the polymer in a dapsone solution by cryo-lyophilization with a 10:1 mass polymer:drug ratio. Morphology and chemical structures were studied before and after adding the drug to plasma Polyaniline to analyze if there is chemical interaction between both components. Plasma polyaniline is obtained as a highly cross-linked polymer, which has the potential to be used as an implant in the human body and dapsone is used as an anti-inflammatory drug in the treatment of spinal cord injuries. The results showed that the pores obtained with the cryo-lyophilization were filled and after that, the entire polymeric particles were coated with the drug. However, as the surface was eroded, the chemical analyses suggested that the drug interacted with polyaniline, shifting the energetic distribution of C1s, N1s and S2p orbitals to lower energies which produced the arrival of new chemical states in the mixtures, although some of the initial states of both materials were preserved. These changes were found mainly in dapsone S2p orbitals.

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### BIO12-CHEMICAL COMPARISON OF SOLUBLE AND INSOLUBLE PLASMA POLYPYRROLE STRUCTURES

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GUILLERMO JESÚS CRUZ CRUZ, FERNANDO GABRIEL FLORES NAVA, ROSARIO RAMÍREZ SEGUNDO, LIDIA MARÍA GÓMEZ JIMÉNEZ, MARIBEL GONZÁLEZ TORRES, MARÍA DEL ROSARIO MEJÍA CUERO, JUAN MORALES CORONA, AXAYACATL MORALES GUADARRAMA MARÍA, GUADALUPE OLAYO GONZÁLEZ

A study on the chemical structures of soluble and insoluble plasma polypyrrole (PPy) and polypyrrole doped with iodine (PPy/I) is presented in this work. The polymers were synthesized by glow discharges at 13.56 MHz in the 20 to 100 W interval. Soluble polymers are difficult to synthesize by plasma due to the crosslinking resulted from the constant collisions of accelerated particles with the monomers during the synthesis. However, in resistive glow discharges, the electric potential is higher in the RF than in the grounded electrode, which influences the structure, crosslinking and solubility of the polymers formed in each electrode neighborhood in the same synthesis. As only the soluble fraction can be used to form pure electrospun PPy fibers, this work presents a comparative study of both, soluble and insoluble polypyrrole chemical structures; emphasizing on the evaluation of carbonization and hydrogenation, calculated with the percentages of chemical states obtained from XPS energetic distributions of C1s orbitals.

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### BIO13-ALTERATION OF PLASMA POLYANILINE STRUCTURES IN ELECTROSPINNED FIBERS

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MARÍA GUADALUPE OLAYO GONZÁLEZ, ROSARIO RAMÍREZ SEGUNDO, FERNANDO GABRIEL FLORES NAVA, MARIBEL GONZÁLEZ TORRES, LIDIA MARÍA GÓMEZ JIMÉNEZ, MARÍA DEL ROSARIO MEJÍA CUERO, JUAN MORALES CORONA, AXAYACATL MORALES GADARRAMA, GUILLERMO JESÚS CRUZ CRUZ

A study on the chemical structures of soluble plasma polyaniline (PAn) and polyaniline doped with iodine (PAn/I) during the formation of electrospun fibers is presented in this work. In the electrospinning process, thin flows of polymeric solutions are subjected to high electric potentials (20-30 kV), which forces the fluid to go from the highest to lowest potential electrodes. On the road, the solvent evaporates forming polymeric fibers. This happens rapidly, however, due to the high electric potential applied, the chemical structure of the polymer changes during the process, making fibers with different structure than that of the initial polymeric solution. The analysis was done by XPS comparing C1s and N1s chemical states before and after the fiber formation. In general, the fibers showed higher oxidation than the starting soluble polymers

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### BIO14-SYNTHESIS AND CHARACTERIZATION OF DOUBLE-NETWORK CHITOSAN HYDROGELS FOR SKIN REGENERATION

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YASMANY GARCÍA-RODRÍGUEZ, EUSTOLIA RODRÍGUEZ-VELÁZQUEZ, MANUEL ALATORRE-MEDA

Hydrogels for Tissue Engineering (TE) applications are required to present specific biological and mechanical properties to match the characteristics of the tissue to be regenerated. Among others: (i) they must be biocompatible and biodegradable; (ii) they must have appropriate mechanical properties to replicate as much as possible those of the new tissue; and (iii) they must have pores with appropriate sizes and adequate interconnectivity to allow tissue ingrowth. We herein explore the synthesis and characterization of double network (DN) chitosan hydrogels for their tentative use in skin regeneration. The hydrogels were synthesized by a two-step process entailing the formation of a first covalent network of low molecular weight chitosan cross-linked with glutaraldehyde (CH-HMw:GA), followed by the formation of a second, reinforcing ionic network of high molecular weight chitosan crosslinked with sodium tripolyphosphate (CH-LMw:TPP). The DN hydrogels displayed enhanced mechanical properties relative to their parent covalent and ionic single networks, such as an Elastic Modulus of 71.85 kPa, which is very similar to that of the dorsal forearm (ca. five-fold higher than that of the single networks) and a Strength at break > 250 kPa (at least five-fold higher than that of the single networks). Additionally, the DN hydrogels were found to be degraded by lysozyme, showing a weight loss from 36.59 to 48.77% at 3 and 7 days of incubation, respectively. Finally, the DN showed a cytocompatibility of 85%. Taken together, all these results demonstrate that the chitosan-based DN hydrogels can be considered as candidate scaffolds for skin regeneration.

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### BIO15-RLP-PEG HYDROGELS MICROSTRUCTURED BY LIQUID-LIQUID PHASE SEPARATION

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CRISTOBAL GARCIA GARCIA, HANG KUEN LAU, KRISTI LYNN KIICK

Liquid-liquid phase separation (LLPS) can be used for tuning the microstructure of hybrid hydrogels comprising resilin-like polypeptides (RLPs) and poly(ethylene glycol) (PEG). Entropic and enthalpic contributions from the mixing of the solution components lead to phase separation, and variation in crosslinking times during the kinetics of this phase separation yields microstructures of different sizes based primarily on nucleation and growth mechanisms. Many parameters can be adjusted to achieve desired microstructures, including polymer molecular weight and concentration, ion size and concentration, temperature, and phase separation time. Acrylated versions of the RLPs and PEGs can be used to manufacture the hydrogels by UV photocrosslinking and to manipulate the kinetics of phase separation. Furthermore, the polymer functionality and UV exposure time help to regulate the micromechanical properties by tuning the final crosslink density. The hydrogels exhibit properties that should be useful as resilient materials for regeneration of mechanically active tissues

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### BIO17-RELEASE PROFILE OF CAFFEINE INCORPORATED IN ELECTROSPUN POLY LACTIC-CO-GLYCOLIC ACID FIBERS

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ROBERTO-CARLOS MARTÍNEZ-HERNÁNDEZ, MAYELI ESTRADA-VILLEGAS, JUAN MORALES-CORONA, ROBERTO OLAYO

Electrospinning has been recognized as a simple and versatile method for fabrication of polymer nanofibers. The ultrafine fibers are generated by application of a strong electric field on polymer solution or melt. Various polymers that include synthetic, natural, and hybrid materials have been successfully electrospun into ultrafine fibers. Extensive studies have been conducted to develop biocompatible as electrospun fibrous scaffolds several applications as using biodegradable and biocompatible polymers as a Poly Lactic-co-Glycolic Acid (PGLA). Among the various potential applications, drug delivery is one of the most promising uses. The advantages of using electrospun fibers in drug delivery include: (1) high drug loading (up to 60%) and encapsulation efficiency (up to 100%), (2) polymer diversity to accommodate compatibility with physico-chemically distinct agents, (3) ability to modulate release, and (4) process simplicity and cost-effectiveness. Caffeine is a methylxanthine that stimulates the central nervous system, creating a condition of wakefulness and increased mental activity. Recently, there has been evidence of the role of caffeine as antagonist of adenosine A<sub>2A</sub> receptors in preventing neurodegenerative disorders, such as Parkinson's disease. In this study, 30 and 50 % (w/w) of caffeine was incorporated into PGLA fibers via electrospinning. Scanning electron microscopy (SEM) Fourier transform infrared (FTIR) and Raman spectroscopy, Thermogravimetric analysis (TGA) and Differential scanning calorimetry (DSC) were used to characterize the fibers morphology and physico-chemical properties. The release behavior and kinetics of model drug from PGLA fibers were also studied by in vitro PBS release test. Caffeine was quantified by UV-Vis at 273 nm.

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**BIO18-EFFECT OF THE INTERACTION OF PYRROL POLYMERS WITH IODINE SYNTHESIZED BY PLASMA AND SERUM ALBUMINE PROTEIN IN THE TREATMENT OF TRAUMATIC SPINAL CORD INJURY**

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OMAR FABELA-SÁNCHEZ, AXAYACATL MORALES-GUADARRAMA, STEPHANIE SÁNCHEZ-TORRES, HERMELINDA SALGADO-CEVALLOS, CAMILO RIOS, ARACELI DIAZ-RUIZ, JUAN MORALES-CORONA, MARÍA GUADALUPE OLAYO, GUILLERMO JESUS CRUZ, ROBERTO OLAYO

We have explored the physicochemical changes of the iodine doped pyrrole polymers synthesized by plasma (PPPy/I) and their interaction with the serum albumin protein (SA) as well as the biological repercussions of these changes in the treatment of traumatic spinal cord injury (TSCI). For this, two types of PPPy/I were synthesized, characterized by XPS, FT-IR and contact angle. In vivo microinjection tests were performed in rats with and without TSCI to assess the effect of both biomaterials on post-injury functional recovery, evaluated clinically for 8 weeks according to the BBB scale. Once the functional evaluation period is completed, the treatment site where Microinjection was performed was recovered and analyzed ex vivo by histological techniques and nuclear magnetic resonance (NMR). In this work, the hypothesis was that the interaction with the protein would reduce the mobility of the biomaterial within the spinal cord. As a result, it was observed that both biomaterials interact with SA forming a layer of protein on them, that modifies their superficial physicochemical properties, consequently the biological response in the treatment of TSCI is affected, establishing that under certain conditions PPPy/I can have different effects on the motor functional recovery. This work discusses the physical distribution of the material and the influence of the protein on the global biological response

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**BIO19-CHARACTERIZATION AND CHLORHEXIDINE RELEASE KINETIC OF POLY(LACTIC ACID) NANOCOMPOSITES FILLED WITH EITHER MONTMORILLONITE OR Palygorskite MODIFIED ORGANOCLOYS**

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HÉCTOR ARIEL LOBATO-AGUILAR, JORGE ALONSO URIBE-CALDERÓN, WILBERTH HERRERA-KAO, SANTIAGO DUARTE-ARANDA, JUAN VALERIO CAUICH-RODRÍGUEZ, JOSÉ MANUEL CERVANTES-UC

Nanocomposites made from poly(lactic acid), PLA, and either montmorillonite (MMT) or palygorskite (PLG) modified organoclays at 25% w/w were prepared by solvent-casting method. Antimicrobial agent chlorhexidine acetate (CA) was used as an organic modifier and it was incorporated into nanoclays at 200% of Cation Exchange Capacity (CEC). Nanocomposites were characterized by Fourier Transform Infrared Spectroscopy, X-ray Diffraction and Scanning Electron Microscopy. In vitro release studies of nanocomposites were carried out in phosphate buffered saline (PBS) media. PLA and PLG produced a homogeneous material whereas when PLA and MMT were mixed, a heterogeneous material was generated having clusters of particles. The drug release studies showed an initial burst release within the first 5 hours and then a sustained release of CA up 24 h. CA released from MMT system was higher that observed for PLG ones. The release profiles obtained for nanocomposites were different to those exhibited for the organoclays; in fact, the presence of a polymeric matrix in the system reduces the amount of CA released in the media. The mathematical models for drug release characterization showed that PLG systems exhibit higher drug release rates than those obtained for MMT.

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**BIO20-BIOCOMPATIBLE HOLLOW POLYMERIC PARTICLES PRODUCED BY A BIOMIMETIC APPROACH FOR CELL ENCAPSULATION AND RELEASE**

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EUSTOLIA RODRÍGUEZ-VELÁZQUEZ

Hollow polymeric particles are regarded as exceptional carriers in a wide range of biomedical/technological applications such as drug delivery, food industry, agriculture, etc. However, the synthesis of these particular materials is challenging since it involves conditioning steps that compromise the native structure of the encapsulated cargoes and also the loading efficiency. Filling this gap, we herein describe a simple, yet efficient strategy to produce millimeter-size hollow polymeric particles by a biomimetic approach for cell encapsulation and release. The particles were produced onto biomimetic superhydrophobic surfaces (SHS) upon assembly and double superficial crosslinking of liquid droplets of DNA and methacrylamide chitosan aqueous solutions (CH:MA), leading to liquid-core particles with a hardened hydrogel shell. The hydrogel shell, resulting from the double ionic/covalent crosslinking of CH:MA, endowed the particles with softness to the touch and an outstanding structural stability against manipulation by hand and with forceps. Meanwhile, as demonstrated by cell staining, fluorescence microscopy, and the well-known MTT assay, the liquid DNA core guaranteed a biocompatible encapsulation and subsequent straightforward release of metabolically active cells, which proliferated normally in culture. In the light of the obtained results, the produced soft, resistant, and cytocompatible cell-laden particles hold promise for Tissue Engineering and Regenerative Medicine, where manipulable synthetic carriers are often needed to supply living cells. Also important, to the best of our knowledge, this is the first time hollow polymeric particles have been synthesized in a template-free manner onto biomimetic SHS, proving to be an affordable, cost-effective, and biologically friendly strategy.

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**BIO21-MORPHOLOGY OF CHITOSAN AND POLYETHYLENE GLYCOL BY SAXS: POLYMERIC MATRIX OF TRANSDERMIC ADMINISTRATION**

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RAUL MONTIEL-CAMPOS, IBETH M. GAITÁN-TOLOSA, MIRIAM V. FLORES-MERINO

There are biomaterials that can encapsulate bioactive substances for the treatment of damage or loss of an organ or tissue. Ketoprofen, a nonsteroidal anti-inflammatory drug, is used in medicine to control pain and inflammation. This is absorbed through the gastrointestinal tract, causing alterations such as diarrhea and abdominal pain. With transdermal administration, the risks of oral administration can be avoided. A critical parameter which has a strong effect on drug diffusion and release is the pore structure. In this study, the characterization of the pore sizes and shapes of a polymer matrix of chitosan and polyethylene glycol by SAXS is presented to evaluate the release of ketoprofen as a polymeric matrix of transdermal administration

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### BIO22-ACRYLIC BONE CEMENTS WITH PROPOLIS

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JENNIFER LEWIS, JOSH M.W. HALL, ROSSANA FARIDE VARGAS CORONADO, CARLOS ROLANDO RIOS SOBERANIS, JUAN VALERIO CAUICH RODRIGUEZ

The present study was conducted to assess the effect of propolis addition to an acrylic bone cement. Curing and mechanical properties in tension, compression and bending of propolis containing bone cements were studied and compared with the unmodified bone cement. In addition, the effect of water conditioning during one week was also studied. The results show that the addition of propolis and conditioning does not affect the mechanical properties. However, curing time and maximum temperature were affected by propolis addition.

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### BIO23-THE EFFECT OF DRYING TEMPERATURE ON PROPERTIES PROPERTIES OF CROSSLINKED CHITOSAN

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MARTHA GABRIELA CHUC GAMBOA, ROSSANA FARIDE VARGAS CORONADO, JOSE MANUEL CERVANTES, JUAN VALERIO CAUICH RODRIGUEZ

The present study compares the effects of drying temperature (25°C vs. 150°C) on different chitosan samples including pristine (CHT (Aldrich, Mv=173, 365; DA=70-80%), CHT crosslinked with polyethylene glycol diglycidyl ether (PEGDE) and CHT crosslinked with glutaraldehyde (GA) and their properties studied by FTIR, TGA and XRD. When samples were dried at 25°C, FTIR spectra showed that absorption at 1653 cm<sup>-1</sup> (amide I, C=O stretching) was of higher intensity compared to the band at 1570 cm<sup>-1</sup> (amide II, N-H). However, upon drying at 150°C the opposite occurred on pristine chitosan and GA crosslinked samples were the absorption at 1570 cm<sup>-1</sup> was higher. All samples treated at 150°C exhibited lower mass loss at 200°C indicating that not only free and bound water is lost but also water within crystalline structures. In addition, crosslinking reduced the thermal stability of samples dried at 25°C. Drying at 150°C increased their thermal stability being close to the pristine chitosan. Pristine chitosan films dried at 25°C exhibited crystalline peaks at 2θ=10° and 20° where the first tend to be higher than the second peak. These peaks tend to be reduced with PEGDE crosslinking while they completely disappeared on CHT-GA suggesting it become amorphous. Interestingly, medium crosslinking CHT-PEGDE films showed additional diffraction peaks at 5°, 9°, 11° and 14°. Drying at 150°C resulted in a significant reduction of the 10° peak intensity and in some cases, a shift of the peak to lower angles implying an increase in d-spacing.

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### BIO24-IN VITRO BIOACTIVITY OF POLYMER/HYDROXIAPATITE COMPOSITES FOR BIOMEDICAL APLICATIONS

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GEORGINA CARBAJAL-DE LA TORRE, ANA BEATRIZ MARTÍNEZ-VALENCIA, MARCO ANTONIO ESPINOSA-MEDINA

Bioactive ceramics, such as hydroxyapatite, react with physiological fluids and through cellular activity form tenacious bonds to hard tissue, forming a biologically active apatite surface layer in the presence of body fluids in vitro or in vivo. Thus HA formation on material surfaces upon immersion in acellular simulated body fluid (SBF) is considered a qualitative measure of the material bioactivity. Polylactic/Polycaprolactone/Hydroxyapatite

(PLA/PCL/HA) composites were prepared with different contents (wt%) and the in vitro bioactivity of the composites was conducted for four weeks in SBF solution, and compared with those of hydroxyapatite and Polylactic composites. The results confirmed that the addition of hydroxyapatite improve the formation of bone-like apatite layer on the surface of the composites especially those containing high hydroxyapatite content. The growth of apatite was confirmed by X-Ray Diffraction (DRX), Fourier transformed infrared spectroscopy (FT-IR), and Scanning Electron Microscopy (SEM) characterization. The obtained materials showed different behavior during the bioactivity test, and the study revealed the fact that composite exhibits advantages compared with pure polylactic. Also, the surface reactions of the composites having high hydroxyapatite content were higher than those having low content post-immersion for 14 days. Conclusions prove that the hydroxyapatite matrix could be studied in vivo study in the future for biomedical applications.

#### BIO25-HISTOLOGICAL STUDIES OF A SUPERFICIALLY MODIFIED POLYMERIC SCAFFOLDS IMPLANTED IN VIVO

MARIA FLORES, ATLÁNTIDA RAYA, DIEGO ESQULIANO, ROBERTO OLAYO, JUAN MORALES, PATRICIA ONTIVEROS

This work presents the histological studies of a four different composite scaffolds extracted from the back of rabbit after a 1 month of implantation. The scaffolds were made of Polylactic acid and Hydroxyapatite by Electrospinning and superficially modified by Plasma Polymerization, therefore two kinds of samples were prepared: PLA/HA and PLA/HA/PPy-I, each of them with two different HA concentrations (18.1% and 35.7%). 7 days in vitro test with osteoblasts of autologous mesenchymal stem cells was performed in the biomaterial for the implant and then, in vivo test was done in the back of a rabbit for 30 days. After extraction, tissue was processed for histological studies and dyed with hematoxylin and eosin. Into other sections were used for immunohistochemistry, in this process the osteoblastic cells were identified with broadly reactive anti-rabbit polyclonals (collagen type I and osteocalcin) and finally the preparations were stained with hematoxylin. The images were taken with a light microscope where scaffolds PLA/HA (35.7%)/PPy-I showed higher cell viability which was confirmed by an MTT assay

#### BIO26-HEPATIC REGENERATION WITH SCAFFOLDS MADE WITH 3D BIOPLOTTING

GIBRAN H. RUBIO QUINTANARES, CRISTINA PIÑA BARBA

Hepatic cirrhosis is one of the leading causes of death in Mexico, representing one of the 10 most important public health problems. Cirrhosis is a chronic disease of the liver, consisting of an increase in fibrous tissue and the appearance of nodules, with alteration of the normal structure of the organ. It is the final consequence of various causes that have been injuring the liver for a long time. Currently, there is no cure for this disease, but symptoms can be controlled and relieve complications of the disease. The only cure known until now would be liver transplantation, for which there are very few donors and the procedure for this is very costly, not easily available. This, coupled with the possible rejection of the organ by the patient represents a great challenge for current science and technology. The objective of



this work was to design a scaffold using bioinks and employing 3D bioplotting technique. The bioink was obtained from the collagens type 1 and 3, from Nukbone. The texture of scaffolds was adequated for growing hepatic cells. The XRD showed an amorphous structure for the scaffolds. The IR technique showed that protein structure and the size of pore was measured by SEM. Therefore, the scaffold obtained by this method presents great possibilities to be used in clinical applications

### BIO27-GUIDED BONE REGENERATION USING COLLAGEN-CHITOSAN MEMBRANES CROSSLINKED WITH EDC

MARÍA CRISTINA PIÑA BARBA, JOSÉ LUIS HIDALGO VICELIS, MARCO ANTONIO ÁLVAREZ PÉREZ,  
SUSANA PATRICIA MIRANDA CASTRO

When a dental piece is lost, a reabsorption of alveolar bone occurs, that in some cases, makes it difficult or impossible to place implants. In order to resolve these difficulties, the bone augmentation technique known as Guided Bone Regeneration (GBR) has been developed. In this procedure, the bone graft (decellularized bone) is placed in the cavity left by the tooth loss and a membrane (barrier material) is placed on the graft that separates it from the buccal cavity favoring the regeneration of bone tissue [1-3]. The objective of this work was to develop collagen-chitosan membranes improving their physicochemical and mechanical properties by chemical crosslinking with 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC), to be used in GBR. The membranes were prepared at different proportions of collagen and chitosan by solvent evaporation, crosslinked with EDC and characterized. Differential Scanning Calorimetric exhibited an increase in shrinkage temperature of crosslinked membranes. Mechanical tests presented that crosslinked membranes have the best mechanical properties. Degradation test indicated that crosslinked membranes dissolve slowly. Scanning Electron Microscopy showed an appropriate microstructure for biological applications. Cell attachment and viability tests suggested that crosslinking does not affect the excellent biological characteristics of membranes. In conclusion, crosslinking with EDC improves physicochemical and mechanical properties without affecting the biocompatibility of membranes.

### BIO28-KINETIC STUDY AND DETERMINATION OF THE DEGREE CROSSLINKING OF SEVERAL POLYESTERS –URETHANES OBTAINED FROM POLYESTER-DIOLS WITH DIFFERENT FUNCTIONALITIES

ANA GUADALUPE ALPIZAR-NEGRETE, KARLA A BARRERA-RIVERA, RICARDO VERA-GRAZIANO,  
ANGEL MARCOS-FERNANDEZ, ANTONIO MARTINEZ-RICHA

There is a current interest on increasing the performance of polymeric materials by different techniques. Based on the knowledge of their chemical nature, the control of molecular weight and the crosslinking nature of the final product, better materials can be created. Crosslinking of polymeric materials results in the modification of different polymer properties. Diols such as  $\alpha$ ,  $\omega$ -telechelic PCL diols (HOPCLOH) (obtained by ring –opening polymerization (ROP) of  $\epsilon$ -caprolactone (CL)) have been used as precursors of biodgradable polyurethanes PUs. In this work, PUs with certain degree of crosslinking have been obtained from PCL-polyols

having functionalities higher than 3. Mixtures of  $\alpha$ ,  $\omega$ -telechelic PCL diols (HOPCLOH) with commercial multifunctional PCLs (CAPA3091 and CAPA4101, with functionalities  $f=3$  and  $f=4$  respectively), were reacted with hexamethylene diisocyanate (HDI) in a stoichiometric ratio NCO: OH, to obtain biodegradable crosslinked PUs. Gel fraction content, swelling properties, weight loss and mechanical properties were evaluated. Polymers obtained using PCL with a functionality of four ( $f=4$ ) demonstrated to be more resistant to weight loss and show a higher percentage of gel fraction and swelling; on the other hand, the PUs derived from PCL with functionality of three ( $f=3$ ) showed a higher percentage of weight loss and lower percentage of gel fraction and swelling. Obtained polymers were also characterized by solid state NMR, FT-IR, DSC, TGA and WAXD.

### BIO29-REPLACEMENT OF TRACHEA USING DECELLULARIZATION TECHNIQUES

CRISTINA PIÑA, DAVID M GIRALDO, DAVID GARCIA DIEGO

Although it is known that all decellularization methods result in an alteration of the architecture, a potential loss of the surface structure and composition of the tissue, efforts were made to develop a method that would allow us to preserve the best possible extracellular matrix. For obtain a tracheal organ decellularized scaffold, porcine tracheas were used, physical methods and chemical and biologic agents were used in combination to lyse cells. This treatment was qualitatively evaluated by SEM and histological techniques: DAPI, Sfranine-O and H&E; collagen type II was following by immuno fluorescence by anti-MHC-I and anti-MHC-II in frozen section. The scaffolding capacity of decellularized matrices was following during two weeks by MSCs seeding on the scaffold obtained from human adipose tissue for in vitro behavior of the matrices through immunofluorescence by, anti-SOX9, anti-Col II and anti-RUNX2. The microscopic evaluation and immunofluorescence technique showed that the decellularization process was effective, providing a cell-free scaffold formed by the EMC of the trachea in which the structure and composition of the ECM is maintained, is fully biocompatible to be colonized by human cells that were able to adhere into this scaffold.

### BIO30-HEPATIC REGENERATION WITH SCAFFOLDS MADE WITH 3D BIOPLOTTING

CRISTINA PIÑA, JUAN M. PÉREZ-OSORIO, GIBRAN H. RUBIO QUINTANARES

Hepatic cirrhosis is one of the leading causes of death in Mexico, representing one of the 10 most important public health problems. Cirrhosis is a chronic disease of the liver, consisting of an increase in fibrous tissue and the appearance of nodules, with alteration of the normal structure of the organ. It is the final consequence of various causes that have been injuring the liver for a long time. Currently, there is no cure for this disease, but symptoms can be controlled and relieve complications of the disease. The only cure known until now would be liver transplantation, for which there are very few donors and the procedure for this is very costly, not easily available. This, coupled with the possible rejection of the organ by the patient represents a great challenge for current science and technology. The objective of this work was to design a scaffold using bioinks and employing 3D bioplotting technique. The bioink was obtained from the collagens type 1 and 3, from Nukbone. The texture of scaffolds

was adequated for growing hepatic cells. The XRD showed an amorphous structure for the scaffolds. The IR technique showed that protein structure and the size of pore was measured by SEM. Therefore, the scaffold obtained by this method presents great possibilities to be used in clinical applications. Acknowledges: To DGAPA – PAPIIT for financial support through project number IG-100117

### **BIO31-ELECTROMAGNETIC ACTIVATION OF AMINED POLYMERIC COATINGS ON TITANIUM MEMBRANES WITH POTENTIAL APPLICATION TO MODIFY TUMOR CELLS**

LIDIA MARÍA GÓMEZ JIMÉNEZ, GUILLERMO JESÚS CRUZ CRUZ, MARIBEL GONZÁLEZ TORRES, FRANCISCO GONZÁLEZ SALGADO, JUAN MORALES CORONA, ROBERTO OLAYO GONZÁLEZ, ROSARIO RAMÍREZ SEGUNDO, FERNANDO GABRIEL FLORES NAVA, MARÍA DEL ROSARIO MEJÍA CUERO, MARÍA GUADALUPE OLAYO GONZÁLEZ

Polypyrrole doped with iodine (PPy/I) and Polyallylamine (PAI) synthesized by plasma were used to cover titanium membranes in order to evaluate their electromagnetic absorption. That could be applied in cancer treatments with biocompatible moldable implants, able to absorb electromagnetic energy, which increase their chemical reactivity with external electromagnetic pulses to modify tumor cells. Polymeric conjugated chemical structures might absorb electromagnetic radiation from an external source to do this function in specific wavelength intervals. Plasma PPy/I has its highest absorption between 200 and 325 nm, with another less intense absorption from 325 to 450 nm due to its heteroaromatic nature. PAI has its highest absorption in the 200-300 interval, due to its aliphatic nature. In isolated conditions, PPy/I and PAI activation energies with superficial electromagnetic beams were calculated in the 0.1-4.0 eV and 1.0-12.5 eV intervals, respectively. The stability of polymeric coatings on the metallic surface was tested by immersion for 1 month in PBS solution at 37°C. After that, the coatings remained adhered to the surface without peeling or fractures. The contact angles of the coatings were around 90°, in the middle between hydrophilicity and hydrophobicity, which contributes to a major adhesion stability.

### **BIO32-EVALUATION OF BIOACTIVITY OF PLLA FLEXIBLE MEMBRANES, MODIFIED BY THE ADDITION OF PLLA-3-ARM**

IVAN ANTONIO NEUMANN, ROSA MARÍA JIMÉNEZ-AMEZCUA, JUAN MANUEL VIVEROS PAREDES, ALEJANDRO AARON PEREGRINA LUCANO, EDUARDO MENDIZABAL MIJARES, ANDREZA MARIA RIBEIRO, THAIS HELENA SYDENSTRICKER FLORES-SAHAGUN

The use of biodegradable polymers in regenerative tissue engineering and in bone implants is increasingly practiced in the biomedical area due to its good mechanical properties, good biocompatibility, and complete degradation in living organisms, without adverse side effect. The main objectives of the present study were to the synthesis of PLLA and PLLA-3-Arm (copolymer of PLLA and glycerol) through bulk polymerization for the subsequent production of blends of both polymers at different ratios for bone engineering applications. PLLA/PLLA-3-Arm polymer blends were obtained in the concentrations of 50/50, 60/40, 70/30, 80/20, and 90/10 (weight:weight), followed by their characterization through differential scanning calorimetry, FTIR, thermogravimetric analysis, tensile tests, contact angle

measurements, SEM, TGA and TF- XRD. The biomimetic process was carried out by 7, 14, 21 and 28 day using Kokubo solution as Body fluid simulator solution. The presence of calcium phosphates on the surface of samples was confirmed through analysis of scanning electron microscopy, the microphotographs revealed that the membranes were porous and pore size was about 20 $\mu$ m. In vitro bioactivity evaluation showed that the composite membranes were able to induce the formation of hydroxyapatite layer on their surfaces, demonstrating their potential application in bone engineering.

### BIO33-SYNTHESIS AND CHARACTERIZATION OF METHYL METACRYLATE-CO-ETHYL GLYCOL DIMETHACRYLATE COPOLYMERS MADE BY EMULSION POLYMERIZATION

ROMÁN ALEJANDRO VALLE LÓPEZ, ROSAURA HERNÁNDEZ MONTELONGO, LOURDES ADRIANA PÉREZ CARRILLO, JUAN HUMBERTO PÉREZ LÓPEZ, ABRAHAM GABRIEL ALVARADO MENDOZA, MARTIN RABELERO VELASCO

The synthesis by emulsion polymerization and characterization of copolymers made of ethylene glycol dimethacrylate and methyl methacrylate is presented here. Different monomer weight ratios were used in the synthesis and the effect on reaction kinetics, final conversion and glass transition temperature ( $T_g$ ) were studied. The characterization of latex and copolymers was carried out by quasi-elastic light scattering, infrared spectroscopy and differential scanning calorimetry. Stable latexes, mono-dispersed with particle diameters less than 50 nm were obtained. Infrared spectra and the presence of a single  $T_g$  value are evidence of the successful copolymerization of these monomers. It was found that the particle size, reaction kinetics and glass transition temperature depend on the composition of the system

### BIO34-INVESTIGATING NANOCOMPOSITES OF POLYLACTIDE (PLA) AND TUNGSTEN DISULFIDE (WS<sub>2</sub>) FOR THINNER, RADIO-OPAQUE BIORESORBABLE VASCULAR SCAFFOLDS (BVS)

EDGAR ERNESTO RUIZ BELLO, KARTHIK RAMACHANDRAN, TIZIANA DI LUCCIO, JULIA KORNFIELD

Coronary Heart Disease (CHD) is the leading cause of death in the world. The current standard of care for CHD is the deployment of a permanent metal stent to restore blood flow through occluded arteries. However, permanent metal stents induce fatal complications such as Late Stent Thrombosis (LST). A promising alternative to metal stents are BVSs, transient implants made from poly L-lactide (PLLA) that supports the occluded artery for 3-6 months, but is completely resorbed in 2-3 years, leaving behind a healthy artery with no risk of LST. However, the thicker profile of current BVSs (~150 $\mu$ m vs 80 $\mu$ m for metal stents) cannot access smaller arteries and the poor radio-opacity of PLLA makes it challenging for surgeons to implant BVSs under X-ray guidance. We hypothesize that a nanocomposite of poly-lactide (PLA) and tungsten disulfide (WS<sub>2</sub>) nanotubes offers a viable solution for a thinner, radio-opaque BVS. We select WS<sub>2</sub> as it is well tolerated in vitro and offers radio-opacity similar to platinum, the current standard for radio-opaque markers. We probe the impact of a flow-field on the crystallization behavior of PLA and PLA-WS<sub>2</sub> and use an in situ optical technique to characterize the concomitant change in their microstructure. We

discovered that even a relatively low concentration of WS2 (0.05wt%) strongly favors the formation of oriented precursors in PLA, which grow to form lamellar superstructures called "shish-kebabs". This favorable morphology induced by WS2 has the potential to enhance strength in a thinner profile, which can enable a new generation of BVs.

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#### BIO35-DETERMINATION OF BIOACTIVE MATERIALS OBTAINED FROM SIMULATED BODY FLUID (SBF)

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ROBERTO MENDOZA SERNA, ATENEA JOSEFINA CHONG SANTIAGO, MARINA CABALLERO DIAZ, GLORIA ALICIA DEL ANGEL MONTES

In this research the bioactivity of mixed systems obtained through the Sol-Gel process was determined using appropriate amounts of silicon tetraoxide (TEOS), which were incorporated into a simulated body fluid (SBF). For this, the following FeO, NiO and Va2O5 systems were synthesized, which were then placed in 35 ml of simulated body fluid (SBF) at a temperature of 37 ° C contained in sterile polyethylene packages, with an ionic concentration close to the human blood plasma; which was obtained from the method of T. Kokubo to be able to determine the presence of the bonds that make up the bioactivity in the samples using the Fourier Transformed Infrared Spectroscopy (FTIR). In the systems obtained, the Ca / P ratio was determined by an elemental analysis (EDS), which must be 1.5 to 2, to be considered as bioactive material.

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#### BIO36-STUDY OF MODIFIED COLLAGEN SCAFFOLDS FOR THE HEALING OF CUTANEOUS WOUNDS IN RATS WITH EXPERIMENTAL DIABETES

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GUADALUPE ESTEFANÍA VILLANUEVA-ORNELAS, LAURA E. CASTELLANO, BIRZABITH MENDOZA-NOVELO

Collagen-based biomaterials have undergone numerous innovations in the field of tissue engineering and biomedical applications. Three dimensional collagen scaffolds are invaluable for soft tissue engineering applications, especially for treating chronic wounds, such as burns, leg ulcers, and decubitus ulcers. Properties of scaffolds based on type I collagen (main component of the extracellular matrix) are limited due to their poor mechanical properties, fast degradation. However, chemical crosslinking is a process intended to slow down or prevent degradation of collagen scaffolds, to inhibit the recognition of surface epitopes by the host, and to provide improved mechanical properties. Male Wistar Rats (8-week-old) were used for the study, animals were divided into healthy rats and DM(diabetes mellitus) rats, that were generated by an intraperitoneal injection of streptozotocin (65 mg/kg body weight). The dorsal hair of the rats were removed and six 8-mm-diameter, full-thickness wounds were created with a biopsy punch at either side of the dorsal central line. All wounds in each rat were randomly treated by control and Scaffolds like CH:(Collagen/hexamethylene diisocyanate(HDI)), CL: (Collagen/Lysine-Diisocyanate (LDI)), CHD: (Collagen/HDI/Dexamethasone), CLD:(Collagen/LDI/Dexamethasone). The percentage of wound closure was evaluated after 28 h, 4 and 12 days. In healthy rats, it was observed that by the 10th and 11th days, the CHD and CLD scaffolds showed a 100% wound closure percentage, while CH and CL groups

maintained percentages of 80 and 90% on day 12. In general, the wounds of DM rats closed slower compared to healthy rats.

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### BIO37-POLY(ESTER-URETHANES): SYNTHESIS, KINETIC STUDY, CHARACTERIZATION AND DRUG-DELIVERY BEHAVIOR

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MARLA GONZALEZ-CORNEJO, KARLA A BARRERA-RIVERA, ANTONIO MARTÍNEZ-RICHA

Polyurethanes (PU) are produced by the condensation reaction of a diisocyanate and a bifunctional reagent, for example the polyols. Biodegradable polyurethanes are generally prepared by using easily hydrolyzable polyols, such as polycaprolactone diol (PCL), polyacrylic acid (PAA), polylactic acid (PLA), and polyglycolic acid (PGA), as soft segments. Biodegradable polymers also are commonly biocompatible, water soluble, low crystalline or having low melting point. These polymers need to possess the desired biocompatibility, suitable mechanical properties and predictable biodegradability. In recent decades it has been synthesized in a large number of polymers and has evaluated its behavior in contact with biomolecules, viruses, bacteria, body fluids, cells and organisms. These studies are part of the growing trend of designing smart polymers and employing them in the field of biomedicine. The primary objective of controlled delivery is to provide the appropriate amount of the active agent at the right time and in the right place. This release method is commonly used to prolong the time that the therapeutic dose is effectively present using a single dose. In this work, synthesis and characterization of polyurethanes containing alpha-amino acid moieties using a chemoenzymatic process is presented. The release profiles of different drugs at three different pHs will be discussed. In most of the cases studied, drug release was a two-stage process: an initial rapid release stage followed by a second slower release stage. Mechanical tests were also performed on the synthesized polyurethanes to obtain tensile-elongation diagrams.

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### BIO38-SYNTHESIS AND ADSORPTION OF SEMISYNTHETIC MUCIN-LIKE BRUSH POLYMERS ONTO COLLAGEN

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LUIS NAVARRO, DANIEL FRENCH DREW WANG, ASHUTOSH CHILKOTI, FARSHID GUILAK, STEFAN ZAUSCHER

Mechanical and biological deterioration of articular cartilage is an irreversible process retarded by lubricin (PRG4) —a mucinous glycoprotein that naturally forms a protective coating on the surface of cartilage. Drawing inspiration from lubricin's structure, we designed a new set of bioconjugates with protein-based binding domains and antifouling brush polymers. We synthesized these bioconjugates by combining ATRP and copper-catalyzed click chemistry, and characterized them by NMR, IR, GPC, SLS, and SDS-PAGE. We studied their adsorption behavior by quartz crystal microbalance (QCM) and found that they strongly bind to collagen model surfaces. Our results will contribute to the rational design of innovative, bio-inspired polymers for the treatment of osteoarthritis.

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### BIO39-CYTOTOXICITY OF COPPER CONTAINING POLYURETHANES

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JORGE FROYLÁN XOOL TAMAYO, ROSSANA FARIDE VARGAS CORONADO, FABIOLA ELIZABETH VILLA DE LA TORRE, VÍCTOR ERMILO ARANA ARGAEZ, IVAN HUMBERTO CHAN ZAPATA, JUAN VALERIO CAUICH RODRÍGUEZ

Copper is a trace metal involved in endothelial cell proliferation and acts as proangiogenic factor. Besides, this metal has cofactor properties and oxygen transport has been reported. However, copper excess have implications in human health. Therefore, in this study copper complexes were prepared with D-penicillamine, L-penicillamine, L-cysteine and glutathione and then used as filler of polyurethanes prepared with PCL, HMDI and L-cysteine as chain extender. First, cytotoxicity of D-penicillamine, L-penicillamine, L-cysteine and glutathione was first assessed by MMT assay using polymorphonuclear cells obtained from peripheral blood. Then, cytotoxicity of D-penicillamine-Cu, L-penicillamine-Cu, L-cysteine-Cu and glutathione-Cu complexes was studied. Finally, cytotoxicity of copper containing polyurethanes was studied. Cell viability was over 70% with D-penicillamine, L-penicillamine, L-cysteine and glutathione in the concentration range between 10 and 400  $\mu$ M. For D-penicillamine-Cu, L-penicillamine-Cu, L-cysteine-Cu and glutathione-Cu complexes, cell survival was above of 83 % in the concentrations of 200 and 400  $\mu$ M. In conclusion, the data showed that all the components of copper containing polyurethanes were not toxic to PMN cells

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## Invited Presentations

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### METALLOCENES ENCAPSULATION IN MICELLAR SOLUTIONS OF FUNCTIONALIZED ACRYLIC HOMOPOLYMERS

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ODILIA PEREZ, CAROLINA VENTURA, ALBA NIDIA ESTRADA, CARLOS A. GUERRERO,  
MARICELA GARCÍA

Amphiphilic polymers (PA's) have been widely studied for special applications in controlled release of drugs, or as nanocontainers for organic and photochemical reactions, as well as for supporting of catalysts in polymerization processes. In the present work libraries of PA's based on poly(n-stearylmethacrylates) (PSMA's) and poly(n-hexylmethacrylates) (PHMA's) were synthesized by RAFT technique, using a high-throughput approach. The effect of controlled molar masses of several PSMA's and PHMA's was studied on the formation of micelle-like structures in non-polar solvents. The use of a highly electrophilic compound like methylaluminoxane (MAO) in hexane solutions of these PA's, led to self-assembled particles (inverse micelle-like structures) with encapsulated MAO, which were characterized by dynamic light scattering (DLS) and TEM. The encapsulated MAO within PA's particles, were useful to activate a zirconocene complex (BuCp<sub>2</sub>ZrCl<sub>2</sub>) for ethylene polymerizations, where the nascent polymer (HDPE) showed spherical morphology.

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### METAMORPHOSIS FOR NEW MATERIALS

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BRENT SUMERLIN

Advances over the last two decades in the area of macromolecular engineering have allowed access to polymers with complex architectures, compositions, and functionality. While the composition and functionality of many polymers can be altered post-synthesis, for example by postpolymerization modification, the architecture of a polymer is typically considered a static inalterable feature that is predetermined by the functionality of the monomers or initiator used during polymerization. Our recent work has focused on macromolecules with dynamic architecture that undergo dramatic topological transformations via a process we term macromolecular metamorphosis. Examples include metamorphosis from a linear amphiphilic block copolymer or hyperbranched polymer into comb, star, and hydrophobic block copolymer architectures. This approach was also employed to obtain gels that undergo programmed crosslink exchange such that the molecular weight between crosslinks increases on heating. Topological transformations of this type represent an entirely new approach to stimuli-responsive materials.

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### APPLICATIONS OF HYPERVALENT IODINE COMPOUNDS IN THE SYNTHESIS OF FUNCTIONAL POLYMERS

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NICOLAY V. TSAREVSKY, HONGZHANG HAN, RAJESH KUMAR, AVICHAL VAISH, YAKUN CAO

Hypervalent (HV) iodine(III) compounds of the type ArI<sub>2</sub> (Ar = aryl, L = carboxylate, halide, or azide), can participate in thermal and/or photochemical homolytic cleavage reactions affecting the weak (three-center-four-electron) HV bonds I-L. These reactions yield the monovalent iodine compound ArI in addition to radicals derived from the "ligands" L. The latter can be used to initiate polymerization or to functionalize pre-made, e.g., polymeric,



materials. In addition, the ability of HV iodine(III) compounds to participate in ligand exchange reactions with nucleophiles (e.g., carboxylates, (pseudo)halides, etc.), make them very useful precursors of functional materials. For example, various synthetic strategies involving ligand exchange and subsequent homolysis reactions of HV iodine(III) compounds, which lead to the formation of branched functional macromolecules will be presented, including i) copolymerizations of vinyl monomers and multivinyl crosslinkers in the presence of HV iodine(III) compounds, in which the latter serve as radical sources and/or transfer agents, and ii) HV iodine(III)-mediated in-situ formation of inimers from carboxylate-containing monomers for self-condensing vinyl polymerization. Last, the preparation of branched and crosslinked dynamic and self-healing polymers containing HV iodine(III) groups as "building blocks" will be described.

### NEW METHODOLOGY IN CONDENSATION METATHESIS CHEMISTRY

KEN WAGENER

Recently we have created a new methodology regarding condensation metathesis reactions, both those producing polymers (ADMET) as well as cross metathesis and ring closing metathesis conversions. This aspect of our work will form the basis for the presentation. It will focus mainly on the polymer side of condensation metathesis. We will describe what is new to offer in this regard, with a focus on simple synthesis of pure polyethylene as well as on precision aliphatic polysulfones, which melt at 175 C, approximately 40 C higher than high density polyethylene. Our earlier work on polysulfones is already in the literature.<sup>1</sup> The new methodology mentioned herein is not yet published. Polycondensation chemistry is quite old of course, yet in the world of metathesis the parameters involving condensation have been limited in a number of ways. What we have done is to expand upon our recent review of metathesis polycondensation<sup>2</sup> and an article specifying how to conduct a proper ADMET reaction.<sup>3</sup> Simple metathesis condensation can be extended beyond conventional wisdom and methods. The polysulfone work is of interest in that large quantities of precision aliphatic polysulfones are easily produced. Our work in this chemistry is now turning towards potential applications to examine whether or not precision offers benefit or not. Details of the new methodology will be provided along with a description of what could be possible by applying these thoughts to other systems.

### Oral Presentations

#### MOLECULAR MIXOLOGY FOR RAFT POLYMERIZATION

JEFFREY M. TING, DEBORAH K. SCHNEIDERMAN, ANATOLII A. PURCHEL, THERESA M. REINEKE, STUART J. ROWAN, MATTHEW V. TIRRELL

Over the past decade, reversible addition-fragmentation chain transfer (RAFT) polymerization has greatly expanded the creative capabilities of polymer scientists and engineers to create well-defined, sophisticated materials across countless areas of research. Much like molecular gastronomists in the culinary world, RAFT chemists balance measured amounts of monomer, initiator, and chain transfer agent under oxygen-free settings to form concoctions that benefit from the technique's high functional group tolerance and mild

reaction conditions. Recently, new developments in light-initiated and enzymatic techniques have enabled functional polymers to be synthesized in open vessels without restrictive heating and external degassing prerequisites. To further advance the ease and versatility of RAFT polymerization, we investigated the polymerization of hydroxyethyl acrylate (HEA) in ill-defined aqueous solvents, including assortments of beer, wine, liquor, and fermentation broth. We show that, by combining traditional RAFT ingredients together with glucose-based enzymatic deoxygenation, poly(HEA) can be attained with precise control over molecular weight and narrow dispersity. This was achieved with sugared rail drinks and top-shelf cocktails alike. Other water-soluble monomer families were also examined following this approach, establishing its broad applicability and utility to the RAFT polymerization repertoire. This robust design strategy enables polymer microstructures with tunable properties to be more easily and reliably prepared under imperfect environments, simplifying general protocols in the high-throughput screening and materials discovery landscapes, with opportunities to lower separation costs of precursor monomer mixtures that are often associated with manufacturing bio-based polymers.

#### PREPARATION OF POLY(METHYL METHACRYLATE-CO-METHACRYLIC ACID) NANOPARTICLES BY SEMICONTINUOUS HETEROPHASE POLYMERIZATION IN ORDER TO BE USED AS ANTICANCER DRUG CARRIERS/DELIVERIES

JOSÉ ROBERTO LÓPEZ MUÑOZ, HENED SAADE CABALLERO, GRACIELA MORALES, FRANCISCO JAVIER ENRÍQUEZ-MEDRANO, RAUL GUILLERMO LÓPEZ

Scientific reports related to nanotechnology applications in antitumoral prevention, detection and treatments have considerably increased in the last few years. Efficiency in drug delivery and decrease/elimination of negative side effects are the seminal challenges in order to get more effective cancer therapies where the development of novel techniques or materials have been the focus of these reports. Different kind of nanostructures such as liposomes, micelles and metallic nanoparticles have been tested for loading and release of anticancer drugs, however, the use of polymeric nanoparticles (PNP) have gained importance for these purposes because they offer features related to greater stability and loading capacity, less toxicity, etc. On the other hand, low particle sizes (between 10 and 50 nm) are required in these systems for increasing the probability to overpass the physiological barriers to act directly on cancer cells. In these sense, the Semicontinuous Heterophase Polymerization (SHP) offers the possibility to obtain PNP in the desired size range. In this work polymerization aspects for obtaining PNP of poly(methyl methacrylate-co-methacrylic acid) by SHP stabilized in a latex containing around 11% solids, with a composition MMA/MAA molar ratio equal to 2/1, a number average molecular weight around  $3.9 \times 10^5$  g mol<sup>-1</sup> and an average particle size around 10 nm are presented and discussed. Specifically, compositions, molecular weights and particle sizes evolutions along the polymerization reaction are reported, as well as studies related with the predominantly chains termination mechanism. PNP have been obtained in order to be later loaded by different mechanisms with several anticancer drugs such as daunorubicin, doxorubicin and paclitaxel.

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### STUDIES IN SOLUTION OF STAR-SHAPED POLY(N-VINYLCAPROLACTAM) WITH SIX ARMS VARYING END-GROUPS

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NORMA AIDE CORTEZ-LEMUS, ANGEL LICEA-CLAVERIE, ANA A. CASTRO-HERNANDEZ, ARTURO ZIZUMBO LOPEZ

Poly(N-vinylcaprolactam) (PNVCL) star-shaped polymers with six arms were prepared by reversible addition-fragmentation chain transfer (RAFT) polymerization using trithiocarbonate or xanthates. The PNVCL star polymers prepared using trithiocarbonate contain carboxyl or an aliphatic alkyl chain end (propyl or undecyl). The thermosensitive behavior of the star polymers was studied in aqueous by measuring the lower critical solution temperature (LCST) by dynamic light scattering (DLS). For a same molecular weight star polymer, the  $D_h$  measured in water of the star polymer with propyl end group is greater than the  $D_h$  of the star prepared with xanthates. Nevertheless, the stars prepared with undecyl end group shown a bimodal distribution. Possibly, this behavior could be a result of interconnected aggregates in aqueous solution. Furthermore, the viscosity of dilute solutions of PNVCL star polymers in ethanol was measured at 35 °C by using an Ubbelohde viscometer. It was found that the intrinsic viscosity of stars containing the undecyl segment is greater than those containing propyl. For its part, the intrinsic viscosity of the stars prepared with xanthates was much lower.

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### TOWARDS THE ATRP OF BUTADIENE

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ALEX ASANDEI

While the controlled radical polymerization (CRP) of conventional monomers such as styrene and acrylates has seen significant progress over the last two decades, the metal mediated CRP of reactive, gaseous/low boiling monomers conjugated dienes such as butadiene and isoprene, is still in its infancy. To this end, we have carried out a comprehensive investigation of the reaction variables in the ATRP of butadiene including the type of ATRP (normal vs ICAR), the nature of the halide (Cl vs Br), initiator fragment (allyl, benzyl, ester etc), ligand (aromatic/aliphatic amines, phosphines, etc), as well as solvent and temperature effects. The rational selection of these parameters towards the minimization of side reactions in the synthesis of well-defined polybutadiene with high chain end functionality, suitable for the ATRP synthesis of block copolymers will be presented.

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### EFFECT OF TRIMETHYLSILYLDIAZOMETHANE -METHYLATING AGENT- ON THE DEGRATION OR REMOVAL OF RAFT FUNCTIONALITY OF POLY ACRYLIC ACID

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LILIANA LOPEZ-PEREZ, HORTENSIA MALDONADO-TEXTLE, ENRIQUE JAVIER JIMENEZ-REGALADO, CLAUDE ST THOMAS

In this investigation, we describe the effect of thimethylsilyldiazomethane -a methylating agent of acrylic monomers- on the degradation or removal of Reversible Addition-Fragmentation chain Transfer (RAFT) functionality of polyacrylic acid. It worth mentioning that due to the Size Exclusion Chromatography (SEC-THF) suitability, well-defined polyacrylic acid and its chain extended hydrophobe (co)polymers were usually methylated before analysis. Notwithstanding, scared reports are revealed the effect of methylating agent on functionality of acrylic (co)polymers. A series of hydrosoluble PAAs have been synthesized in dioxane at 70 °C employing three different RAFT chain transfer agents (a dithiobenzoate, a symmetric trithiocarbonate and an asymmetric trithiocarbonate). Functionalized

homopolymers were prepared and narrow molecular weight distribution were obtained. Polymers were characterized and successful removal or degradation of RAFT functionalization was confirmed by FT-IR, NMR, UV-vis, MALDI-TOF and SEC. Furthermore, the homopolymers (PAAs) were chain extended by styrene and acrylic acid. The SEC traces of PAAs obtained using a symmetric CTA show bimodal distribution which explain the degradation of distribution is acquired. Whilst the FT-IR and UV-vis analysis polymers before and after methylation demonstrated the removal of RAFT functionality at the polymeric chains. The results from this study are clearly exhibited the effect of trimethylsilyldiazomethane on the degradation of RAFT functionality of PAAs especially when the functionality is located into the middle of the polymeric chains.

#### USING 2D MATERIALS AT FLUID-FLUID INTERFACES TO ACCESS HYBRID STRUCTURES

BRAD RODER, PEIRAN WEI, QINMO LUO, CHRISTINA HEMMINGSEN, AL DE LEON, EMILY PENTZER

Fluid-fluid interfaces are a rich landscape for chemical reactions and transformations and by tuning the properties of these interfaces, the long-term stability of the system can be controlled and the interface can be made active and responsive. We will report the assembly of 2D materials at different fluid-fluid interfaces, including oil-water, oil-oil, and ionic liquid-water, and demonstrate the applications of these systems. 2D nanomaterials (i.e., nanosheets) have properties distinct and complimentary to their spherical and rod-like counterparts which are more commonly studied. Using graphene oxide (GO) nanosheets and their functionalized analogues, materials and assemblies that are multifunctional (e.g., antimicrobial, thermally conductive, good gas barriers, etc.) are accessed. Thus, by combining fundamental organic chemistry reactions and the assembly of 2D materials, structure-property relationships are understood, and the next generation of functional materials are prepared.

#### A NOVEL SYNTHESIS OF LADDER POLYMERS THROUGH POLYMERIZATION BY SUPERACID CATALYSIS

JOSÉ MANUEL RODRÍGUEZ MOLINA, LILIAN IRAÍS OLVERA GARZA, MIKHAIL ZOLOTUKHIN

A novel series of ladder-type polymers (3a-3d) was synthesized in one step using superacid catalysis in the reaction of macrocyclic monomers (1a-1d) and trifluoromethyl ketones (2a-2b). Polymerizations were performed at room temperature and the superacid trifluoromethanesulphonic acid (TFSA) with different solvents: dichloromethane, nitrobenzene and tetrachloroethane. The polymers obtained are soluble in most polar solvents and their ladder type chemical structure was revealed through <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR. The molecular weight obtained (MW) based on the macrocycles and trifluoromethyl ketones is about 10,000 to 30,000. These polymers also have high thermal stability, as well as gas permeation in membranes and gas absorption. The mechanism of polymerization will be discussed.

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## STABLE RADICAL POLYMERS FOR CHARGE TRANSPORT STUDIES

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ALICIA CINTORA, CHRIS OBER

Nitroxide radicals such as TEMPO have been thoroughly studied in the context of electrochemistry and magnetic labeling. More recently, polymers bearing TEMPO side groups, such as poly(2,2,6,6-tetramethylpiperidinyloxy methacrylate), further denoted poly-TEMPO-methacrylate (PTMA), have been used as alternative materials in energy storage systems, such as rechargeable organic radical batteries. Although devices have been created using stable radical polymers, the charge transport mechanism has not been thoroughly studied, and many of these devices fail after a few cycles. In order to improve current advancements in the field, the charge transport in nitroxides must be further studied. This work focuses on creating platforms in which to study charge transport along oriented pathways via various phase morphologies in block copolymers containing PTMA. These directed pathways are used to confine the conducting species in an insulating matrix in order to study the charge transport mechanism. Various morphologies are developed in thin polymer films via thermal or solvent vapor annealing. The block copolymers have been synthesized via anionic polymerization, and their phase morphologies have been observed using Atomic Force Microscopy (AFM) and Grazing-Incidence Small Angle X-Ray Scattering (GISAXS). Investigating phase behavior in these block copolymers allows charge transport to be studied, and organic energy storage systems containing stable radical polymers can be further improved.

## Posters

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### SYNTH01-A NOVEL METHODOLOGY FOR THE SYNTHESIS OF THREE COMPONENT FORCED GRADIENT POLYMERIC MATERIALS

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FRANCISCO JAVIER RIVERA-GÁLVEZ, LUIS JAVIER GONZALEZ-ORTÍZ, MIGUEL ÁNGEL LÓPEZ-MANCHADO, CARLOS FEDERICO JASSO-GASTINEL

A methodology for the synthesis of 3 component polymeric materials was developed, trying to optimize mechanical properties. Using butyl acrylate (BA), styrene (S), and 4 - vinylbenzyl chloride (VBC), as monomers, the method consisted of a seeded (with polystyrene as the starting seed) semicontinuous free radical emulsion reaction where the 3 components were sequentially feeded by pairs, with S as the common monomer. The sequential comonomer feeding profiles (S - BA and S - VBC) were chosen looking for a forced gradient composition within the chains to be formed along the reaction to obtain chains rich in S, then rich in BA and later rich in VBC. 25/60/15 and 15/60/25 for BA/S/VBC overall compositions were obtained on a weight percentage basis, where the final conversions were generally ca 95 % in approximately 135 minutes for both compositions. As a reference, a core shell type polymeric material was also prepared with the comonomer pairs in two stages. For DMA testing certain differences in T<sub>g</sub> were obtained inverting the comonomer feeding order. For stress - strain tests some of the forced gradient polymeric materials (FGPM) presented similar modulus but higher deformation capacity than the reference material. The micrographs using atomic force microscopy showed smaller phase domains than the reference materials. By the results, the synergic mechanical performance of the FGPM compared to the reference material can be explained by the better component interaction which is reached

by the better phase compatibility that can be inferred by the trajectories in loss modulus plots and AFM micrographs.

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### SYNTH02-SOLID-SUPPORTED RAFT POLYMERIZATION OF METHYL METHACRYLATE ON A MERRIFIELD RESIN IMMOBILIZED CHAIN TRANSFER AGENT BY THE Z-GROUP

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CARLOS CASAS-SOTO, ALEJANDRO VEGA-RIOS, VELIA OSUNA

Raft polymerization of methyl methacrylate mediated by Merrifield Resin-supported 4-Cyano-4-(phenylcarbonothioylthio)pentanoic acid via the stabilizing Z-group was investigated. The tethering of the RAFT agent to a solid substrate using this route allowed the effective separation of the living polymer chains from dead chains and other side products from the reaction by simple filtration. After polymerization the tethered polymer was removed from the support by a radical addition fragmentation cleavage process in order to recover the RAFT agent. The microspheres were characterized by elemental analysis and FTIR spectroscopy. Molecular weight and molecular weight distribution of the cleaved polymer were determined by gel-permeation chromatography.

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### SYNTH03-PREPARATION AND CHARACTERIZATION OF BIOBASED EPOXY-RESINS FROM COTTONSEED OIL

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ERIKA FLORES-LOYOLA, KARINA CRUZ-ALDACO, NURIA BURGOS, ALFONSO JIMENEZ

Most of polymers are prepared from nonrenewable petroleum derivatives, thus renewable raw materials have being an important issue of study, to obtain polymers with similar properties to those petroleum based ones. Vegetable oils are becoming important in this field due to their functional groups can be reacted to produce different polymers such as polyurethanes, polyamides, polyesters and epoxy resins among others. Vegetable oils as castor, soy, and palm are being used as alternatives for polymer preparation. In this work films of epoxy resins were prepared using cottonseed oil, a highly unsaturated oil, by photoinitiated cationic polymerization using different amounts of triarylsulphonium hexafluoroantimonate (TSHA) and triarylsulfonium hexafluorophosphate (TSHP). The films were characterized by Infrared spectroscopy (FT-IR), thermogravymetric analysis (TGA), differential scanning calorimetry (DSC), and scanning electronic microscopy (SEM). Results shown that the procedure used for epoxidize cottonseed oil allows yielding up to 70%. The reactions following was carried out by FTIR from which it was observed the correspondent signals for epoxy resins in all films. In the process of cationic photoinitiated polymerization with TSHA and TSHP there was not difference in the morphological behavior of the films, in both cases non-porous and compact films were obtained. All materials shown glass transition temperatures below room temperature, no matter the photoinitiator used nor their concentration. Degradation temperatures were founded around 350°C, the initiator content affected this value although not in an important manner. This results shows to cottonseed oil as a potential renewable raw material to obtain epoxy resins with good thermal properties.

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**SYNTH04-BREATHING ATRP REACTIONS: FULLY OXYGEN-TOLERANT POLYMERIZATIONS ASSISTED BY ENZYMES**

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ALAN ENCISO, LIYE FU, ALAN RUSSELL, KRZYSZTOF MATYJASZEWSKI

In this presentation, we address the first ATRP reaction that can be fully conducted in open air without the need of degassing with inert gases. The experiments were conducted with assistance of glucose oxidase (GOx) and pyruvate, which through a cascade of reactions inspired in the aerobic respiration of cells, consumes O<sub>2</sub> and releases CO<sub>2</sub>. This system allowed the controlled polymerization via aqueous ICAR-ATRP of OEOMA500, where low dispersities ( $1.09 \leq \bar{D} \leq 1.2$ ) were obtained, even when high DPs were targeted. Successful chain extension with OEOMA300 also demonstrated livingness of the polymerization ( $\bar{D} = 1.3$ ). The discovered conditions showed that larger scale polymerizations can be pursued in high volumes. In addition, the self-promoted polymerization of polymer brushes from glucose oxidase was achieved, probing that the conditions employed are mild and suitable for modification of biological systems, due to the low amounts of catalyst required (ppm) and short time of the reaction (1 to 2 hours). Also, through a cascade of enzymatic reactions (based on GOx-catalase system), oxygen was employed as the fuel to grow polymers via ATRP from proteins and synthesize protein-polymers bioconjugates. These experiments are pioneering steps in the synthesis of bioconjugates by an enzymatic machinery using ATRP.

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**SYNTH05-SYNTHESIS AND COMPARATIVE BEHAVIOR OF RUTHENA(II)CYCLES BEARING BENZENE LIGAND IN THE RADICAL POLYMERIZATION OF STYRENE AND VINYL ACETATE**

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VANESSA MARTÍNEZ CORNEJO, LARISSA ALEXANDROVA, RONAN LE LAGADEC, JESSICA OLVERA MANCILLA, JOSÉ ALBERTO OVIEDO FORTINO

The synthesis of polymers with well-defined compositions, architectures and functionalities has been of great interest in polymer chemistry. The "living" radical free polymerization is a novel method that allows us to obtain new materials and to improve their properties in traditional monomers. The atom transfer radical polymerization (ATRP) method is one of the most promising, which can apply to a great number of monomers. The most important component in ATRP is the catalyst; therefore several complexes of metals have been applied in this process, including different transition metals, such as ruthenium, copper, iron, rhenium and nickel. In this work a series of half-sandwich ruthenium(II) complexes of the type  $[\text{Ru}(6\text{-C}_6\text{H}_6)(\text{N}(\text{N})\text{C})\text{L}]\text{PF}_6$  (L = PPh<sub>3</sub>, P(nBu)<sub>3</sub>, SbPh<sub>3</sub>, MeCN), bearing cyclometalated N,N-dimethylbenzylamine (1a-d) and 2-phenylpyridine (2a-d) moieties, has been efficiently prepared by ligand substitution. The catalytic activity of the complexes in the radical polymerizations of vinyl monomers was evaluated, and a comparative structure-activity analysis was performed.

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**SYNTH06-ANIONIC COPOLYMERS THICKENERS CONTAINING HYDROPHOBIC MONOMERS PREPARED BY INVERSE EMULSION POLYMERIZATION**

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JOSE HERNANDEZ-BARAJAS, ROCIO DEL CARMEN RAYA-ELIZARRARAZ

In this investigation, we report the synthesis of copolymers of acrylamide/acrylic acid partly neutralized with ammonium hydroxide using small amounts of hydrophobic monomers and obtained by inverse emulsion polymerization. These copolymers show a 38,000 to 60,000 cps RVT Brookfield viscosity range (2% by weight of inverse polymeric emulsion with spindle 6 at 25°C). This behavior is checked by rheological measurements (viscosity versus shear

rate). Using behenyl methacrylate with 30 units of ethoxilation as hydrophobic monomer, it is observed that the viscosity with this monomer is much higher than the same monomer with 25 units of ethoxilation. This means that the length of hydrophilic moiety (measured by the ethoxylation units) is important, if we want to obtain higher viscosities. We conclude that the big viscosities obtained in these copolymers are due to the associations of the hydrophobic monomers that form tridimensional networks and aggregates and not only by chemical reticulation (methylen-bis-acrylamide is also used in the formulation of the copolymers).

The viscosities of the thickeners obtained with the anionic copolymers developed in this study ( $\approx 26\%$  solid weight percent) are comparable to the viscosities of commercial concentrated thickeners of the same copolymers ( $\approx 64\%$  solid weight percent). Then, the proposed synthesis procedure allows us a reduction of time and costs due to the fact that it is not longer necessary the use of vacuum distillation techniques to concentrate the non-concentrated anionic polymeric inverse emulsion.



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## Invited Presentation

### GAS TRANSPORT PROPERTIES OF PURE AND MIXED GASES ON MODIFIED COPOLYMERS FROM ISATINE AND ACEANTHRENEQUINONE

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MA. ISABEL LORÍA-BASTARRACHEA, ANGEL MONTES-LUNA, OLIVIA HERNÁNDEZ, MIKHAIL ZOLOTUKHIN, ALBERTO RUIZ-TREVIÑO, MANUEL AGUILAR-VEGA

A copolymer bearing equal amounts of isatine and aceanthrenequinone moieties (POH186) was synthesized by polycondensation. The original copolymer was modified with the introduction of tert-butyl and pyrene side groups. The copolymer and its modified structures were characterized showing that they have limited solubility in chloroform and N-methyl-2-pyrrolidone, NMP. They also show high thermal stability given its highly aromatic nature with onset decomposition temperatures above 430°C. The copolymers may show intrinsic microporosity, PIM, and they may find application as gas separation membranes. Permeability coefficients, P, for five gases He, O<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub> and CO<sub>2</sub> show that the introduction of the lateral bulky groups tert-butyl and pyrene decrease P for all gases tested depending on the bulkiness of the side group. The decrease in P gives place to an increase in gas separation factors. This decrease in P is due to a lowering on the diffusion coefficients for all gases tested. Mixed gas permeation measurements, a mixture CH<sub>4</sub>/CO<sub>2</sub> (90/10), indicate that the gas separation tendency is maintained but there is a small increase in CO<sub>2</sub> P coefficient and separation factor as compared to the pure gas measurements. It was also noticed that the initial copolymer behaves as a PIM while the modified copolymers behave as glassy polymers.

### POLY (OXINDOLARYLENE)S AS GAS SEPARATION MEMBRANES

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F. ALBERTO RUIZ TREVIÑO, MIKHAIL ZOLOTUKHIN, MANUEL AGUILAR VEGA

Poly (oxindolarylene)s is a high-molecular weight average polymer family that possesses high chemical resistance, no detected high glass transition temperature and excellent mechanical properties. In addition, it can be synthesized at low reaction temperatures with a great variety of rigid aromatic repeating units that can bear specific functionalities to improve their ability to be processed as polymer membranes with conventional techniques, and moreover to be thermally-treated to tune their gas separation selectivity-permeability combination of properties and at the same time to cross-link their repeating units to avoid the common densification problem associated to annealing time. It will be shown that poly (oxindolarylene) membranes holding a repeating unit made up of basic isatine and 9H-fluorene or fused biphenyl, possess attractive selectivity-permeability combination, for the gas pairs O<sub>2</sub>/N<sub>2</sub> and CO<sub>2</sub>/CH<sub>4</sub>, which falls close to or in between the two Robeson's upper bound limits. Even though its strong chemical resistance -cannot be dissolved in common solvents- represent a major advantage for its application, it also represents a major drawback in terms of its ability to be processed as a film or eventually as hollow fiber. To sort this problem, the repeating unit is modified through the incorporation of bulky thermally-labile functionalities to produce polymers which can be dissolved by common solvents, and then through several thermal-treatments protocols modify the repeating unit to recuperate the original selectivity-permeability combination of the highly chemical stable membrane. It will be also shown that carefully and simultaneously incorporating bulky and unsaturated thermally-labile groups to cross-link polymer chains, another typical problem -polymer densification rate- can be suppressed.

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## SYNTHESIS AND CHARACTERIZATION OF SULFONATED BLOCK COPOLYMERS BASED ON PMMA-PS FOR PROTON EXCHANGE MEMBRANE FUEL CELLS

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CLAUDIA PIÑÓN-BALDERRAMA, ULRICH S. SCHUBERT, CARLOS GUERRERO-SÁNCHEZ,  
ROBERTO OLAYO-VALLÉS, JOSÉ BONILLA-CRUZ

Charged block copolymers possessing ionic conductivity properties has rapidly increase scientific interest in the last years due their potential applications as proton exchange membranes in fuel cells (PEMFC). In this sense, diblock copolymers were synthesized by a reversible addition fragmentation charge transfer (RAFT) polymerization technique based on PMMA and PSt. Block copolymers were synthesized in the range of 14-75 KDa., with narrow polydispersity 1.08-1.17. The highest sulfonation level was ~90% of the total available styrene units and it was quantified by elemental analysis. Thin films (~30 nm) of block copolymers were directly deposited on silicon wafer by spin coating techniques and then was undergoes to solvent vapors (SVA) and thermal annealing (TA) treatments in order to reach the equilibrium morphology. Morphologies of Block copolymers obtained were evaluated by atomic force microscopy (AFM) before and after sulfonation. It was found that highly sulfonated blocks exhibited partially ordered nanostructures even without any SVA or TA treatment typically required to reach the thermodynamic equilibrium. This effect was triggered by the introduction of sulfonic acid groups (SO<sub>3</sub>H), which modified the interaction parameter that governs the self-assembly process of the system. Proton conductivity measures were evaluated by electrochemical impedance spectroscopy (EIS) in bulk membranes and it was found that conductivity increase in two orders of magnitude after SVA (from 10<sup>-6</sup> to 10<sup>-4</sup> S/cm) which give us indication that well-defined ionic paths were induced after treatment where the proton conduction could be carried out in an efficiently way. Morphology of the bulk membranes would be studied in order to establish a relationship between structure and ionic conductivity.

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## TOUGHENING ANION EXCHANGE MEMBRANES

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MICHAEL HICKNER

Anion exchange membranes (AEMs) provide a pathway to platinum-free fuel cells, large-scale batteries, and novel water treatment technologies. However, several challenges must be overcome before anion exchange membranes become competitive with their proton exchange membrane (PEM) counterparts. The conductivity and stability of AEMs must be improved for deployment in long-lived applications such as fuel cells and advanced batteries. Additionally, the mechanical properties of AEMs must be addressed in order to extend their lifetimes in applications where there is a large transmembrane pressure. We have demonstrated a number of strategies for toughening poly(phenylene oxide) (PPO)-based anion exchange membranes. In one example, we employed thiol-ene crosslinking of PEG-PAGE networks that interpenetrated quaternary ammonium functionalized PPO. These semi-interpenetrating networks of hydrophilic, crosslinked polymers and cationic PPO showed high elongation at break, a critical metric for toughness. In another example, we used Jeffamine crosslinking of cationic PPOs to toughen membranes. The high molecular weight between crosslinks lent the membranes high elasticity that could be controlled by the crosslink density. This talk will demonstrate how blending elastic components with ionic materials can improve the properties of ion-conducting membranes.

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**HYDROCARBON, SOLID POLYMER ELECTROLYTES FOR ACIDIC AND ALKALINE  
ELECTROCHEMICAL DEVICES**

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STEVEN HOLDCROFT

Full scale commercialization of Proton Exchange Membrane Fuel Cells (PEMFCs) is imminent yet fundamental knowledge in specialized areas is still required in order to resolve persistent technical barriers associated with high materials costs and limited reliability, versatility, and performance. Perfluorinated proton-exchange polymers form the basis of standard high-performance PEMFCs but difficult synthetic chemistry hampers further materials development. Hydrocarbon proton-exchange materials, on the other hand, are founded on well-established and versatile synthetic chemistry that allows for rapid materials development, and offer a less expensive alternative to perfluorinated polymers. In the corollary case of Anion Exchange Membrane Fuel Cells, the search continues for an alkaline-stable, polymeric hydroxide-conducting medium. Solutions to these challenges require the undertaking of rigorous systematic studies on model polymers and representative materials of known and controllable molecular structure and preferred nano-morphology. In this presentation the evolution and properties of unique proton- and hydroxide-conducting polymers being developed at Simon Fraser University will be described.

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**BLOCK COPOLYMERS FOR MORPHOLOGY CONTROL AND MECHANICAL STABILITY IN BULK  
HETEROJUNCTION ORGANIC PHOTOVOLTAICS**

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JORGE MOK, ZHIQI HU, RAFAEL VERDUZCO

State-of-the-art organic photovoltaics (OPVs) are comprised of donor and acceptor organic semiconductors blended to form a co-continuous, bulk heterojunction phases. While systematic variation of processing conditions can dictate various morphological characteristics, control over the properties and composition of the donor-acceptor interface is limited. Block copolymers with donor and acceptor conjugated polymer blocks provide an innovative approach to dictating the donor-accepter interfacial structure and understanding its relationship to charge separation and photovoltaic performance. In this work, we report the development of all-conjugated block copolymer additives for tailoring the electronic properties and morphology of bulk heterojunction photovoltaics. We demonstrate that small quantities of all-conjugated block copolymers can significantly enhance the open-circuit voltage, and that incorporation of a flexible linker is detrimental to charge separation. We also demonstrate an improved route to flexible and mechanically robust organic photovoltaics using block copolymer additives. These materials offer improved performance and insight into the properties and function of bulk heterojunction OPVs.

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Oral

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**EVALUATION OF DIFFERENT MACROPOROUS RESINS IN AN ELECTRODEIONIZATION PROCESS FOR ARSENIC REMOVAL**

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ADRIANA NAHÚM GUTIÉRREZ LÓPEZ, JUDITH CARDOSO MARTÍNEZ JORGE GABRIEL VAZQUEZ ARENAS

Arsenic generates adverse effects on human health, whence it is necessary to develop efficient and low-cost technologies to remove it. In this direction, just a few techniques are competent for its treatment, as a result of its structure which hampers its chemical or biological transformation. Electrodeionization (EDI) is a promising hybrid technology that synergistically combines ion exchange membranes and resins in an electrolytic cell, thus, promoting the migration of ionic species throughout the application of an electric potential difference. However, it has been scarcely explored for the removal of arsenic species. In the present work, we tested a commercial anionic exchange resin (Amberlite IRA-900) and compared its performance with two synthesized resins (4-vinylpyridine/divinylbenzene matrix, functionalized with methyl iodide and 1,3-propanesultone). The resins were characterized by electrochemical impedance spectroscopy to select those with the highest ionic conductivity. Additionally, adsorption isotherms, maximum capacity of adsorption and kinetics and adsorption rates were obtained to evaluate the adsorption kinetics. We fitted the experimental data to Langmuir and Freundlich adsorption models. Subsequently, the resins are assembled into an EDI cell containing a dimensionally stable anode (Ti/RuO<sub>2</sub>-IrO<sub>2</sub>) and a stainless steel cathode. The effective area of the EDI cell is 24cm<sup>2</sup>, and the flow rate was 12ml min<sup>-1</sup>. The synthetic solution was prepared using a 1000 µg mL<sup>-1</sup> of an Arsenic (V) standard and deionized water and tested at different applied current densities and flow rates.

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**COLORIMETRIC SENSOR FOR TILAPIA FRESHNESS CONTROL**

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ANGÉLICA DOMÍNGUEZ-ARAGÓN, ALEJANDRO VEGA-RIOS, SERGIO G. FLORES-GALLARDO, E. ARMANDO ZARAGOZA-CONTRERAS

Fish is a worldwide consumed food; thus, there is a great interest to develop methodologies for evaluating fish freshness in real time. In the fish industry, attributes such as appearance, color, smell, and texture have been evaluated as quality control parameters; however, these procedures are labor intensive and require specialized equipment. As the fish deteriorates, due to microorganism growth propagation, a variety of basic volatile amines (trimethylamine, dimethylamine, and ammonia) are produced. These products are collectively known as TVB-N (total volatile basic nitrogen). Therefore, the TVB-N level is an indicator of fish freshness, because its presence produces an alkaline atmosphere, which indicates the degradation activity beginning. This research reports the synthesis of a poly(ortho-phenylenediamine-co-aniline) copolymer and its application as a colorimetric sensor for tilapia (Cichlidae family) freshness control. The sensor operation is based on the changes that the polyanilines and its copolymers undergo because of the pH change, which generates color changes. The sensor detects the TBV-N presence, produced during fish spoilage, indicating the freshness degree. First, the sensor sensitivity to the pure amines' vapor was evaluated, showing that the sensor responds by producing a color change from red to yellow, which was dependent on the amine solution pH and exposure time. Assays on tilapia have verified that the copolymer response enabled the fish spoilage real-time monitoring

during refrigeration storage at 10°C. The characterization by cyclic voltammetry and UV-vis spectroscopy indicated the suitability for obtaining functional materials to develop a TBV-N chemical sensor.

### STUDY AND DESIGN OF CONJUGATED POLYMERS TYPE "D AND A" IN A BULK HETEROJUNCTION ARCHITECTURE

LORENA CARRASCO VALENZUELA, ALEJANDRO VEGA RIOS

Photovoltaic cells based on organic semiconductors have attracted considerable interest as a possible alternative to conventional inorganic photovoltaic technologies. Solar cells with Bulk Heterojunction (BHJ) polymer architecture have been investigated because of their low cost, and their high potential as renewable energy conversion devices. In addition, properties, including support, mobility and solubility adaptation between donor and acceptor polymers, are also crucial for achieving high efficiency of polymer solar cells. Among the conductive polymers, PEDOT has been the most used and has several advantages, such as its high functionality and its transparency. In addition, it behaves as a barrier to oxygen that can diffuse from the anode to the device. PANI has emerged as a very attractive candidate due to its transparency, chemical stability, relatively easy synthesis and conductivity. PEDOT and PANI can act as an oxygen barrier and as a planar layer to inhibit electrical shorts and improve the life of the device, resulting in improved brightness and efficiency. Although poly(3,4-ethylenedioxythiophene): polystyrenesulfonate (PEDOT: PSS) is insoluble in organic solvents, it is often used as a transparent material that transports holes, simple processing and appropriate work function. Doping the PEDOT with PSS allows it to become soluble in aqueous media, facilitating its deposition on ITO surfaces through spin coating the most common method used in the manufacture of organic devices. Therefore, several highly conductive materials, PEDOT and PANI, have been studied as possible replacements for PEDOT: PSS as the hole injection or transport layer.

### OPTIMIZATION OF DIRECT ARYLATION POLYMERIZATION CONDITIONS FOR THE REALIZATION OF HIGH EFFICIENCY ORGANIC PHOTOVOLTAICS

BARRY THOMPSON

In recent years direct arylation (DArP) polymerization has emerged as a simplifying alternative to prevalent cross coupling polycondensation reactions for the synthesis of conjugated polymers. DArP attractively bypasses the need to metallate a monomer prior to installing a reactive group, avoids extra synthetic steps, waste, and purification challenges. While DArP has proven successful for realizing a broad range of conjugated polymers, careful analysis of structure reveals that defects are often present when compared to those polymers synthesized by traditional methods such as the Stille polycondensation. These defects have been a significant detriment to polymer properties and electronic device performance, notably in organic solar cells. Here our recent efforts toward optimizing reaction conditions are discussed from a structure-property and structure-device standpoint within the context of polymer solar cells. We have synthesized a wide variety of conjugated polymers ranging from poly(alkylthiophenes) to alternating donor-acceptor copolymers, as well as random and semi-random polymers. Synthetic conditions cover a range of ambient and high temperature approaches in which solvent, catalyst, ligand, and additive are correlated with presence of structural defects in the polymer such as homo-coupling and branching. The emerging conditions of oxidative direct arylation polymerization are also discussed. The influence of defects on optical and electronic properties are evaluated and

correlated with performance in polymer solar cells. Optimal conditions are ultimately identified for each polymer class. Efforts toward expanding the scope of DArP are discussed along with strategies for effectively scaling this promising polymerization.

#### CONTRIBUTION OF ENTROPIC AND ENERGETIC SELECTIVITIES ON GAS SEPARATION PERFORMANCE OF CMS MEMBRANES DERIVED FROM BLENDS OF RIGID POLYMERS

JOSÉ MANUEL PÉREZ-FRANCISCO, JOSÉ LUIS SANTIAGO-GARCÍA, MARIA ISABEL LORIA-BASTARRACHEA, MANUEL AGUILAR-VEGA

In the present work, we report the study of entropic selectivity on gas separation performance of carbon molecular sieve membranes (CMS membranes) derived from blends of the rigid polyimide PI DPPD-IMM and a commercial polybenzimidazole. CMS membranes show an enhancement of gas permeability coefficients for smaller gases (He, O<sub>2</sub> and CO<sub>2</sub>), up to five times, with respect to membrane precursors. CMS membranes derived from precursors with polyimide concentration  $\geq 75\text{wt}\%$  have an excellent relationship between gas permeability coefficients and ideal selectivity and they were located above the upper bound for CO<sub>2</sub>/CH<sub>4</sub> and O<sub>2</sub>/N<sub>2</sub> gas pairs as the result of the formation of micropores and ultramicropores as was elucidated by the WAXD analysis. Gas separation performance was correlated with entropic and energetic selectivities. The results show that entropic selectivity, which is related to the pore size and the size and shape of penetrant, is an important factor in gas separation properties of carbon membranes, founding that CMS membranes, which overpass the upper bound, have entropic selectivity higher than unity. Energetic selectivity showed a negative contribution to gas separation performance of CMS membranes.

#### EFFECT OF ION CONCENTRATION ON CONDUCTIVITY OF POLY(3,4-ETHYLENEDIOXYTHIOPHENE) PREPARED BY EMULSION POLYMERIZATION

PILAR SANTOS-PERCINO, ENRIQUE PÉREZ-GUTIÉRREZ, JUDITH PERCINO-ZACARÍAS

Poly(3,4-ethylenedioxythiophene) (PEDOT) is one of the most used polymer in organic and hybrid electronic devices such as organic light emitting diodes and organic solar cells. Its properties as hole transport material depends mainly on its ionic character as well as polymer properties. In this work PEDOT was prepared by oxidative polymerization of 3,4-ethylenedioxythiophene under high-concentration emulsion conditions in the presence of 2-naphthalenesulfonic acid sodium salt acting as an emulsifier and a doping agent and Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> as an oxidant. It was found that the electrical conductivity of the synthesized polymer was related with the concentration of sodium in the naphthalenesulfonic salt. Pellets of PEDOT were prepared and used for measure the resistivity of the material polymer with resistivity in the range of MΩ/□ to some Ω/□ was obtained.

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Poster

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**FPOLO1-SYNTHESIS OF MEMBRANES FROM TITANIUM PRECURSORS FOR THE SEPARATION OF GAS MIXTURES**

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ATENEA JOSEFINA CHONG SANTIAGO, ROBERTO MENDOZA SERNA, LUCILA VALDEZ CASTRO, JOSE OCOTLAN FLORES FLORES

The objective of this research was to perform the synthesis of five mixed systems composed of SiO<sub>2</sub>-TiO<sub>2</sub> applying the Sol-Gel method, for the use of these as membranes in the separation of gaseous mixtures, for which in the synthesis the precursor was changed of titanium from each of them (methoxide, ethoxide, propoxide, isopropoxide, butoxide). In the synthesis methodology the reaction was carried out between the precursor of Titanium which was previously chelated with acacH (acetylacetonate 2, 4 pentanedione) in a 2: 1 molar ratio, and the previously hydrolyzed silicon sol. Once the homogeneous soles were obtained, the characterization was carried out by UV-Vis and FTIR spectroscopies up to the moment of gelation of the soles. At this point the excess ethanol was removed from each of the gels, dried, calcined and were ground for a TG study to determine the heat resistance of the materials obtained, as well as an analysis of Textural Properties to obtain data on the influence of the precursor on each of the materials, separation factor of the membranes synthesized and applied in gas mixtures.

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**FPOLO2-SYNTHESIS AND CHARACTERIZATION OF NEW SULFONATED POLYAMIDES DERIVED FROM OLEIC ACID**

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CARLOS CORONA-GARCÍA, ARLETTE A. SANTIAGO, JOEL VARGAS

The present work reports on the self-metathesis reaction of oleic acid using the Grubbs 2nd generation catalyst to produce the difunctionalized monomer 1,18-octadec-9-enedioic acid (DIC) which was subsequently used in polycondensation reactions at high temperature with the diamines 4,4'-(hexafluoroisopropylidene)bis(p-phenyleneoxy) dianiline (HFDA) and 2,5-diaminobenzenesulfonic acid (DABS), respectively. Triphenylphosphite (TFF) was used as catalyst, 1-methyl-2-pyrrolidone (NMP) in addition to pyridine were used as solvents. The degree of sulfonation of the polyamides was adjusted by controlling the molar ratio of the sulfonated diamine DABS to the fluorinated diamine HFDA. From the synthesized polyamides dense films membranes were prepared by the solution-evaporation method using dimethylformamide (DMF) as solvent. The chemical structures of the new materials were confirmed by the FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and <sup>19</sup>F-NMR which showed the presence of amide groups and sulfonic groups in the proposed concentrations. The water absorption values (W<sub>u</sub>) at room temperature for the synthesized polymers ranged from 1.9 % to 17.0 %. The ion exchange capacity (IEC), determined by chemical titration, for the sulfonated membranes were between 1.86 mmol/g and 0.67 mmol/g. The new polymers were fully characterized by thermomechanical analysis (TMA), thermogravimetric analysis (TGA) and X-ray diffraction measurements (XRD), among others. Acknowledgements We thank CONACyT for generous support with contract 239947. Financial support from DGAPA-UNAM PAPIIT through the projects IA101317 and IA101817 is gratefully acknowledged.

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### FPOL03-POLYANILINE COPOLYMERS FOR SUPERCAPACITOR ELECTRODES

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ANGÉLICA DOMINGUEZ-ARAGÓN, CLAUDIA A. HERNÁNDEZ-ESCOBAR, E. ARMANDO ZARAGOZA-CONTRERAS

Energy consumption/production that relies on fossil fuel combustion is having a severe worldwide impact on economics and ecology. The electrochemical energy production is under consideration as an alternative energy/power source, as long as this energy consumption is designed to be more sustainable and environmentally friendly. Electrically conducting polymers are among the most promising materials for high-performance supercapacitor fabrication, due to the good intrinsic conductivity, low band gap, suitable morphology, fast charge/discharge kinetic processes, and low cost. In this research, polyaniline, polydiphenylamine (PDPA), and two copolymers with molar ratios 1 to 1 and 3 to 1 of precursor monomers (anilinium dodecyl sulfate and diphenylamine) were synthesized via an oxidative polymerization in a water/ethanol interfacial system. The copolymers' structure and morphology exhibited PAni or PDPA characteristics, depending on the monomer molar ratio. More importantly, electrochemical characterization indicated that PDPA properties can be modified and improved by the copolymerization with an aniline monomer. Particularly, the copolymer with PAni precursor highest content showed a specific capacitance of 634.89 F g<sup>-1</sup> at 1 A/g, the charge-discharge test indicated that the capacitance loss during the charge/discharge cycles was lower than 25% of the initial capacitance. Diphenylamine-co-aniline copolymers cycling stability was improved with DPA content, which suggests its potentiality for the design of supercapacitor electrodes.

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### FPOL04-VARIATION OF ELECTRICAL AND THERMAL PROPERTIES OF PSSNA-CO-PEGA GRADIENT COPOLYMER DEPENDING OF ITS COMPOSITION

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CLAUDE ST.THOMAS, ALEXIS VÉLEZ DE LA FUENTE, JUDITH CARDOSO MARTINEZ RICARDO, IVÁN RODRÍGUEZ RAMÍREZ

The monomer proportions and synthesis method of copolymers can determine the bulk material properties such as decomposition temperature, electrical conductivity and the mechanical resistance, being its study of great interest for industrial and technological purposes. In this work, it was decided to study the influence of the monomer proportions in the properties of PSSNa-co-PEGA gradient copolymer. These copolymers were synthesized via a RAFT controlled polymerization in water using ACPA as initiator, varying the proportion between the both monomers in the aim to study their physicochemical behaviors. The thermal analysis was carried out by DSC, TGA and DEA respectively. The results exhibited a variation of the T<sub>g</sub> ca. to 10°C (from -50 to -40°C) which decreases when the proportion of PEGA was increased and the samples presented semi-crystallinity. The thermal decomposition showed the same behavior for any proportion of material. The nanocomposites showed a decrease of around 20°C for the PEG predominant monomer and 5°C for the PSSNa predominant monomer. The electrical properties were measured by a Bio-logic potentiostat/galvanostat varying between the both nanocomposites and unspoiled polymer by 2 magnitude degrees (x10<sup>-7</sup> – x10<sup>-5</sup> S cm<sup>-1</sup>) Data demonstrated that the positive charges in the MMT helps to canalize the charge in the whole system and that the nanocomposites were efficiently formed even when the polymer was fully synthesized before its incorporation.



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#### FPOL05-CROSS-LINKED CONDUCTIVE BINDER FOR LI-ION BATTERY SI ANODES

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ANDREA MIRANDA, TRACY LI, HYOSUNG AN, KASTURI SARANG, JODIE LUTKENHAUS, RAFAEL VERDUZCO

Numerous of advances in wearable technology have inspired a growing demand for light-weight, flexible batteries with long lifetimes. To answer this call, many attempts have been made to stabilize the Si-alloy Li-ion storage mechanism in Li-ion battery anodes, which faces issues of low electronic conductivity and volume expansion often leading to battery death. A multi-functional binder may hold the key to unlocking the high theoretical capacity of Si in Li-ion batteries. Previous work in the literature has shown the benefits of functional binders. Non-conductive cross-linked binders have alleviated the stresses of Si particles reacting with lithium and, separately, conductive binders have increased local electronic conductivity of the anodes. By combining these functionalities, we have shown stable cycling performance, especially considering the improved flexibility and mechanical integrity of the anodes. A systematic approach to cross-linking conductive PEDOT:PSS demonstrates that a cross-linked, conductive binder stabilizes the capacity retention of Si anodes. Electrode surface and cross-section morphology is observed before and after cycling to compare SEI formation on the anodes using various methods of crosslinking PEDOT:PSS. Electrical conductivity, peel tests, nanoindentation show marked improvement of the binder properties upon crosslinking. Tensile failure tests of the crosslinked binders quantify mechanical improvements in the conductive binder that we propose help alleviate strain from the volume expansion caused by Si-Li alloy.

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#### FPOL06-MESOMORPHISM AND PHOTOLUMINESCENCE OF METHACRYLIC POLYMERS BEARING CYANO TERPHENYL GROUPS

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ISAURA FELIX-SERRANO, ROSA JULIA RODRÍGUEZ-GONZÁLEZ, LETICIA LARIOS-LÓPEZ, IVANA MOGGIO, EDUARDO ARIAS DÁMASO NAVARRO-RODRÍGUEZ

Methacrylic polymers, carrying a didodecyloxy-p-terphenyl laterally substituted with one or two cyano groups, were synthesized and studied from the liquid crystal and optical points of view. The chemical structure was confirmed by <sup>1</sup>H-NMR spectroscopy. These new polymers are fairly soluble and thermally stable up to 300°C. Their mesomorphic behavior was studied by differential scanning calorimetry (DSC), polarizing optical microscopy (POM) and X-ray diffraction (XRD). The polymer bearing one cyano group melts at lower temperature, and displays a mesomorphic behavior over larger temperature interval as compared to that bearing two cyano groups. Polymers showed only non-ordered smectic phases with molecules arranged in single layers. Optical properties were studied by UV-Vis absorption and fluorescence spectroscopies. Molecules absorb and emit in the blue spectral range, a region of high energy. The fluorescence quantum yield is high ( $\geq 54\%$ ) suggesting that these new fluorescent liquid crystal polymers have potential use in modern optical systems.

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## Invited Presentations

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### CARBON DIOXIDE SWITCHABLE TECHNOLOGY IN POLYMER CHEMISTRY

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MICHAEL CUNNINGHAM

Carbon dioxide has emerged as a new, innovative "trigger" for stimuli-responsive materials. It is abundant, inexpensive, nontoxic and environmentally benign. Carbon dioxide switchable polymers are a class of stimuli-responsive polymers for which CO<sub>2</sub> is a trigger used to change the polymer properties. However, in addition to making stimuli-responsive polymers, carbon dioxide switchable technology can be used as a valuable process alternative in polymer chemistry. In this lecture, the use of CO<sub>2</sub>-switchable technology for polymerization processes will be presented, including the use of switchable solvents to conduct copper-catalyzed ATRP polymerizations and subsequently remove the metal catalyst. We have designed three approaches to remove copper catalyst and recycle the ligands after atom transfer radical polymerizations, all based on using materials whose properties can be switched using only CO<sub>2</sub> and any nonacidic gas as triggers. The first approach involves the use of a CO<sub>2</sub>-switchable solvent as the medium for the ATRP reaction. The second approach involves using a conventional ATRP solvent such as toluene to conduct the polymerization. Finally, we demonstrate the effectiveness of the CO<sub>2</sub> switching approach in organocatalyzed atom transfer radical polymerization (O-ATRP) using a new CO<sub>2</sub> switchable photo-initiated catalyst, which can be extracted from the polymer and reused. In all methods, residual copper in the polymer was <5 ppm, while residual ligand was <3 ppm. The feasibility of recovering and re-using the ligand or photo-initiated catalyst for subsequent polymerizations is also established.

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### INTERFACIAL POLYMER ENGINEERING: APPLICATIONS TO POLYMER FLOCCULANTS AND POLYMERIC SOLIDIFIERS

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JOAO SOARES

In this presentation, I will give an overview of the research activities being carried out in my group in the area of polymer reaction engineering, focusing on three main areas: 1) polymer flocculants for oil sands tailings remediation, 2) polymer flocculants for the removal of fines from effluents of non-aqueous extraction processes, and 3) polymeric solidifiers for the containment of oil spills. Polymer flocculants have long been used to treat oil sands tailings, but they are generally based on acrylamide monomers. Polyacrylamide (PAM) is a hydrophilic polymer that can lead to fast settling rates, but traps water inside its flocs, creating difficulties for the long-term dewatering of the flocculated sediments. I will explain in my talk how modifying the basic structure of PAM with hydrophobic components, or using polymers based on completely different monomers, can lead to the development of more effective flocculants for oil sands tailings that could be designed for a particular application. The other two research areas that I plan to discuss in this presentation have only started recently in my group. I will discuss the concept of using hyperbranched functional polyolefins as a flocculant for fines in non-aqueous bitumen extraction processes, and also give an overview of our research approach in developing polymeric solidifiers to contain oil spills.

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## DEGRADATION OF PET WITH ETHYLENE CARBONATE TO OBTAIN DIFUNCTIONAL MACROGLYCOLS

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KARINA ESPINOZA GARCÍA, RODRIGO NAVARRO CRESPO, AURELIO RAMÍREZ HERNÁNDEZ, ANGEL MARCOS FERNÁNDEZ

Commercial PET was chemically degraded using ethylene carbonate as reactant and KOH as catalyst. Using model reactions, the chemical species produced during the degradation of PET were identified by NMR. Hydrolysis was the main degradation mechanism during the first 8 h of reaction with a strong decrease in the molecular weight and the attachment of some short polyether chains, mainly diethylene glycol. From 8 to 12 h reaction time carbonate groups were incorporated into the oligomer chains and some short polyether chains substituted ethylene glycol molecules in between the terephthalate rings without a significant change in the molecular weight. From 12 to 24 h reaction time only minor changes in the molecular weight and the chemical structure of the oligomers took place. Quantification of the signals allowed for the full determination of the final degradation product. After 24 h reaction a paste was obtained, composed of difunctional oligomers of approximately  $2000 \text{ g} \cdot \text{mol}^{-1}$  molecular weight with short polyether chains, mainly diethylene glycol, connecting the terephthalate rings and a significant content of carbonate groups. Degradation for a longer time, 48 h, produced a viscous liquid composed of difunctional polyester oligomers with the same chemical species than the PET material degraded for 24 h but with lower molecular weight, approximately  $1100 \text{ g} \cdot \text{mol}^{-1}$  and much lower content of carbonate groups. The chemical structure of the resulting oligomers make them attractive candidates as macroglycols for the preparation of thermoplastic polyurethanes.

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## FLUORESCENCE EMISSION COLOR CHANGES OF ACRYLONITRILE DERIVATIVES. SYNTHESIS, STRUCTURE, AND OPTICAL PROPERTIES

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PAULINA CEBALLOS, MARGARITA CERÓN, VENKATESAN PERUMAL, ENRIQUE PÉREZ-GUTIÉRREZ, JOSE BONILLA, M. JUDITH PERCINO

Solid state lighting (SSL) of model organic compounds has attracted much attention due to their potential applications in devices such as light-emitting diodes, photovoltaic devices, and sensors. Tuning and controlling the wavelength of emission of an organic material is crucial to identify the appropriate application, and the optical properties of different dyes in the solid state strongly depend on the molecular structure and intermolecular interactions. Recently, organic chromophores that exhibit quenching of fluorescence in the solid state have been reported, and this phenomenon is termed aggregation-caused quenching (ACQ). In contrast, when the emission of fluorescence depended on the presence of the solid state, the process was termed aggregation-induced emission (AIE) or aggregation-induced emission enhancement (AIEE). Herein, we report results from optical characterization (absorption and emission) of  $\alpha, \beta$ -unsaturated acrylonitrile with structures of electron donor D-p-A acrylonitrile derivatives. The investigation reveals differences in the characteristic emission such as an enhancement in fluorescence in solvent, as well as in the solid state. Their photophysical properties have been investigated to evaluate the effect of the substituents, which afforded a dye that exhibited emission depending of the morphology.

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**DIACETYLENE-CONTAINING POLYMERS: THEIR CROSS-LINKING, HYDROGENATION OF DIACETYLENE GROUPS AND APPLICATIONS**

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MIRIAM F. BERISTAIN, TAKESHI OGAWA

The oxidative coupling polymerization of terminal bisacetylenic compounds is a useful method to obtain unique functional polymers. The polymerization takes place in solution under mild conditions at room temperature without concern of presence of water, provided that the monomer and polymer are soluble in the solvents employed and extremely high molecular weights can be achieved. The functionality and morphology of polymers depend on the spacer group. For example, the polymers with high second order nonlinear optical susceptibility can be obtained using polar chromophores. Some of the crystalline polymers undergo topochemical cross-polymerization developing 1,4-polydiacetylenes, and some are amorphous; but amorphous polymers also undergo cross-linking by light or heat, depending on size of spacer groups, and those with bulky groups are less vulnerable to cross-linking. Such cross-linking can be used to fix the poled chromophores for nonlinear optical polymer films and to increase their mechanical properties. However, sometimes premature crosslinking can be a serious problem for storage of polymers. The characteristics of crosslinking of different polymer films will be presented. The hydrogenation is thought to be a solution to avoid premature crosslinking, as well as obtaining novel polymers, which are not easy to obtain for conventional methods. Catalytic hydrogenation of some diacetylene-containing polymers was carried out using different palladium catalysts and was found that the catalyst activity depended on the support.

**Oral**

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**SYNTHESIS AND CHARACTERIZATION OF NEW PHOTO-CURABLE POLYURETHANES BEARING COUMARIN DERIVATES**

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RODRIGO NAVARRO, RUBÉN SEOANE-RIVERO, JOSÉ MARÍA CUEVAS, ÁNGEL MARCOS-FERNÁNDEZ

Nowadays polymeric materials able to recover from a damage through the action of external stimuli is arousing great interest in the scientific community. The use of light as a trigger has the advantage that the light-triggered processes can be halted and resumed "on demand" by turning off and on the excitation light. Coumarins are capable of absorbing radiation and undergo a reversible photo-dimerization reaction. Through these photoactive reactions, the final properties of the polymeric material can be easily modulated. The combination of the photo-activity of these molecules and the versatility of the polyurethanes allows the preparation of new tailor-made polymeric materials. Linear segmented polyurethanes bearing photoactive coumarin moieties within the soft segment, the hard segment or distributed between both segments were successfully synthesized. These polyurethanes contain flexible chains of polycaprolactone as soft segments and, isophorone diisocyanate and butanediol as hard segments. The synthesized coumarin derivate presented in this work overcome the problems previously encountered in other coumarin derivative. The photoreversibility of the coumarin moiety was studied by different techniques (UV and Raman) and the physical properties of the photo-irradiated polyurethanes were evaluated and compared with non-irradiated polymers and with previously described similar materials prepared in our group.

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## THEORETICAL-EXPERIMENTAL EVALUATION OF THE ION EXCHANGE PROCESS OF THE ARSENIC OXYANIONS IN MACROPOROUS HYPER-CROSS-LINKED RESINS USING A HYDROGEOCHEMICAL MODEL

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DANIEL VILLEGAS MARTINEZ, ANGEL ALBERTO MÉNDEZ HERNÁNDEZ, JUDITH MARÍA DE LOURDES CARDOSO MARTÍNEZ, NADIA VALENTINA MARTINEZ VILLEGAS, ELOÍSA ANLEU ÁVILA, JOSÉ ANTONIO ARCOS CASARRUBIAS

A novel macroporous hyper-crosslinked resins for the removal of toxic As(III) and As(V) oxyanions from aqueous solutions were synthesized by post cross-linking precursor resins prepared by suspension polymerization of vinylbenzyl chloride (VBC) and divinylbenzene (DVB). These polymers were functionalized with pyridine and 1,3-propanesultone to increase their capacity to remove the oxyanions. Adsorption studies were conducted and the kinetic and adsorption capacity were studied. The equilibrium adsorption data were fitted with Langmuir, Freundlich and Redlich–Peterson adsorption models and the model parameters were evaluated. The kinetic experimental data were fitted to the models, such as the pseudo-first order and pseudo-second order models. The polymer was characterized by mercury intrusion porosimetry to determine the specific surface area, the pore volume and pore size; a spectrophotometric method based on the determination of the number of moles of nitrates ions exchanged for chlorides was used to determine the ion-exchange capacity; the protonation–deprotonation behaviour was determined by potentiometric titration technique, a thermogravimetric analysis determined the decomposition temperature of the resin; the charge, charge density and isoelectric point was determined using zeta potential and finally the scanning electron microscopy (SEM) was used to analyse their morphology properties. The data obtained were used and analysed by protoFit GUI V2.1 program and PHREEQC 3.1.2 in order to know the surface species distribution into the resin. The initial research results showed that the anion exchange capacity for the resin functionalized both with pyridine and propanesultone is 2.27 meq/g and 4.18 meq/g respectively.

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## HYDROXYLATION OF LIGNIN IN DEEP EUTECTIC SOLVENTS FOR SUSTAINABLE REPLACEMENT OF PHENOL IN RESINS

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JOSUE D. MOTA-MORALES, SHU HONG, HAILAN LIAN

ZnCl<sub>2</sub> mixed with several hydrogen bond donors (HBD) forms deep-eutectic solvents (DESs) that are capable to dissolve and improve the chemical reactivity of wheat straw alkali lignin under different temperatures and times of pretreatment. The chemical structure of the resulting modified lignin was studied by several techniques including UV, FT-IR, <sup>1</sup>H, <sup>13</sup>C and <sup>31</sup>P-NMR spectroscopies, TGA, NALDI-TOF MS and ICP. The chemical treatment resulting from dissolution of lignin in the DESs produced an increase of total phenolic hydroxyl of the fraction precipitated upon addition of water. Depending on the HBD used, different mechanism of hydroxylation and even selective demethoxylation occurred in the lignin, mainly through β-O-4' linkages. Finally modified lignin was used as a phenol replacement in the synthesis of phenol-formaldehyde (PF) resins with similar adhesive, thermal and mechanical properties of conventional ones.

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### AFFORDABLE MICROFLUIDICS APPROACH TO COLLAGEN MICROVESSELS FORMATION

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EDGAR ERNESTO RUIZ BELLO, DANIEL PAREDES, BIRZABITH MENDOZA NOVELO, JORGE DELGADO

Targeted delivery and release of drugs is one of several applications of biopolymer based matrices. Collagen in particular is widely known for its properties, such as excellent biocompatibility and well-established structure. With the emergence of microfluidics technology, the capacity to generate drug delivery vehicles has increased the applicability of these biomaterials. Within this study, an affordable method for creating collagen microvessels is being developed. Type I fibrillar collagen was extracted from rat tails by separating the tendons and hydrolyzing the protein with an acidic solution. An easy-to-use microfluidics chip was created using Teflon tubing. T-shaped junction and co-flowing streams methods were tested, controlling flow streams of collagen and mineral oil independently by two syringe pumps. After droplet formation at the junction, a section of tubing was submerged in a heat bath at 37°C. Different flow rates, temperatures and pH levels were tested to ensure gelation inside the tubing. In a first step to this study, collagen microspheres were obtained with relative success using the two methods previously mentioned. After establishing the basis for droplet formation, we will proceed to generate microvessels with the co-flowing streams method, which showed better results in our chip configuration.

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### SYNTHESIS OF CO<sub>2</sub> RESPONSIVE CELLULOSE NANOCRYSTALS VIA RAFT-MEDIATED GRAFT MODIFICATION

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JOAQUIN ARREDONDO, MICHAEL CUNNINGHAM, PHILIP JESSOP, PASCALE CHAMPAGNE

Cellulose is the most abundant natural polymer on Earth. From cellulose, cellulose nanocrystals (CNC) can be obtained through various hydrolysis processes. This material has become the subject of much attention from the scientific community due to its outstanding mechanical, optical and physical-chemical properties, in addition to its high natural abundance, and low toxicity. There is interest in grafting different types of polymers onto CNC as their applications are limited due to their poor dispersibility in low polarity and non-polar systems. The potential versatility and value of modified CNC can be enhanced even further if the polymers used in the grafting process are CO<sub>2</sub> responsive, including for example poly(dimethylaminoethyl methacrylate) (PDMAEMA), poly(diethylaminoethyl methacrylate) (PDEAEMA) and poly(diisopropylaminoethyl methacrylate) (PDPAEMA), since stimuli responsive composites have shown promise in applications such as Pickering emulsifiers, water treatment and as polymer reinforcing agents. In this work, we report the grafting of CNC surfaces via grafting-from and grafting-to using reversible addition fragmentation chain transfer (RAFT). The CNC surfaces were first chemically modified with a RAFT agent capable of mediating polymerization of these monomers. A grafting-from polymerization was then performed using the CO<sub>2</sub> switchable monomers DEAEMA, DMAEMA and DPAEMA. The grafting-to approach was also undertaken as a comparative assessment where the respective CO<sub>2</sub> responsive polymers were synthesized and fully characterized prior to grafting.

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**THERMOPLASTICS VULCANIZATES: EFFECT OF THE CROSSLINKING SYSTEM AND TYPE OF DIENE TERMONOMER**

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NUNO MARQUES, ANA VERA MACHADO, MARTIN VAN DUIN

Thermoplastics vulcanizates (TPVs) are a particular class of TPEs, which are obtained via dynamic vulcanization, i.e. the selectively crosslinking of the rubber while it is melt mixing with the thermoplastic phase. The crosslinking enhances the viscosity and elasticity of the rubber phase and, as a result, the final TPVs morphology comprises crosslinked rubber particles dispersed in a thermoplastic matrix, even if large amount of rubber is used. Therefore, TPVs combine the melt processability of thermoplastics with the elastic and mechanical properties of thermoset crosslinked rubbers. Although, Even though TPVs are commercially available from the 1970's and a large number of studies have been published, many fundamental questions, related to the effect of dynamic crosslinking and crosslinking system on the morphology, its mechanism and final properties, are still not understood. Since resol it yields TPVs with better colour characteristics a peroxide is a good alternative as crosslinking system. However, it some drawbacks have been identified: peroxide results in degradation of PP and also reacts with oil, thus decreasing crosslinking efficiency. Thus, the main objective of this work is to get new insights on the effects of both crosslinking systems, resol and peroxide, and the type of diene termonomer on rubber crosslinking efficiency and PP degradation. TPVs with two different type of diene termonomer rubbers (ENB-EPDM and VNB-EPDM) were mixed with PP and two dissimilar crosslinking systems (resol and peroxide) and were dynamic vulcanised in a batch mixer. Samples were collected along the time in order to correlate the evolution of morphology with the crosslinking reaction. The EPDM gel content and the degree of swelling were used as a crosslinking measurement. PP degradation was evaluated by SEC and rheology. The results obtained show that the higher gel content values were obtained with the resol. For the peroxide systems, the values were higher for VNB than for ENB rubber, indicating that VNB enhances crosslinking by peroxide.

**Poster**

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**REACT01-GRAFTING OF N-VINYLCAPROLACTAM AND 2-HYDROXYETHYL METHACRYLATE ONTO POLYPROPYLENE FILMS FOR BIOMEDICAL APLICATIONS**

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GEOVANNI GONZÁLEZ-HERNÁNDEZ, EMILIO BUCIO, LUISA ISLAS

The aim of this work was to graft 2-hydroxyethyl methacrylate (HEMA) and N-vinylcaprolactam (NVCL) onto polypropylene films (PP) using  $\gamma$ -radiation to endow the films with swelling capabilities and better surface properties. Different grafting conditions were tested including varying the dose (10–70 kGy), reaction temperature (45–70 °C), and monomer concentration (10–50 vol. %); and two different grafting methods were compared. First, weighed PP films were placed in glass ampoules for their exposure to a  $^{60}\text{Co}$   $\gamma$ -source in the presence of air, at room temperature. This was done to promote the formation of peroxides and hydroperoxides, which are thermally unstable and lead to the formation of free radicals, on the films. Then, 8 mL of a HEMA solution in water or NVCL solution in heptane were added to the preirradiated ampoules. To remove any oxygen in the system, the ampoules that contained HEMA were bubbled with argon, while the ampoules that contained NVCL were degassed by a freeze-thaw process. The ampoules were then sealed and heated at different temperatures (45–70 °C) for 6 or 24 h depending on which

compound, HEMA or NVCL, respectively, was being grafted. To remove any unreacted monomer or homopolymer, the films were soaked in acetone for 6 h, and then ethanol for 18 h, before being dried under vacuum overnight. The binary graft was achieved using two different methods. The first method involved two-steps, where one compound was grafted first (PP-g-HEMA or PP-g-NVCL), and the other compound was grafted thereafter. For this binary graft, each compound was grafted using the same procedure outlined for the single graft. In addition, for this two-step method the grafting order was changed to analyze its effect on the chemical properties of the copolymer, that is to say, we obtained (PP-g-HEMA)-g-NVCL and (PP-g-NVCL)-g-HEMA samples. The second method involved the use of the direct irradiation method, where PP was irradiated alongside a solution of HEMA/NVCL (50:50 vol. %) in toluene. For this method, the irradiation dose was varied between 50–90 kGy to obtain different grafting yields. The chemical structure of PP before and after grafting was studied using infrared spectroscopy (FTIR-ATR) and thermal analysis (DSC and TGA). In addition, the water contact angle, swelling properties, and LCST of the different films were compared.

### **REACT02-DESING OF HYPER-CROSSLINKED RESINS FOR REMOVE CR (VI) IN SYNTHETIC WATER**

ANGEL MÉNDEZ, DANIEL VILLEGAS, ELOISA ANLEU, JUDITH CARDOSO, JOSÉ ARCOS

Chrome is one of the elements that can be found in the wastewater from a variety of industrial processes. The toxicity depends on the state of oxidation and concentration, being of particular importance the elimination of hexavalent chromium present in aqueous systems, for its recognized carcinogen. According to IARC (International Agency for Research on Cancer) classified at the Cr (VI) in Group I (carcinogenic confirmed in humans) that is related to the exposure of Cr (VI) with the development of lung cancer. In this work it was designed a hyper-crosslinked resin capable of adsorbing oxyanions with Cr (VI). Hyper-crosslinked resin was synthesized by polymerization in solution of vinylbenzyl chloride and divinylbenzene in the presence of a mixture of toluene and n-heptane as inert porogens in amounts (50-50) % by volume, based on the monomers used during the reaction, at a temperature of 80° C for a period of 8 hours at 86 rpm. It was subsequently functionalized by reaction of Friedel-Crafts type with pyridine and after with 1,3-propanosultone for quaternized the N of pyridine. Resin precursor was characterized by infrared (FTIR), thermogravimetry (TGA), scanning electron microscopy (SEM) and elemental analysis. It was assessed the performance of resin as adsorbent of Cr (VI) in experiments in batch and column packed at pH=2 obtaining a maximum of adsorption of Cr (VI) of 54 mg/g of resin used.

### **REACT03-BIOBASED EPOXY THERMOSETS FROM WHEAT GERM OIL**

ALFONSO BARAJAS CERVANTES, PEDRO ORTEGA GUDIÑO, INÉS JIMÉNEZ PALOMAR, KERRY KIRWAN, JORGE RAMÓN ROBLEDO ORTÍZ, MARTÍN RIGOBERTO ARELLANO MARTÍNEZ

The substitution of thermosets polymers derived from petroleum by those obtained from renewable resources has taken interest in the most demanding specialized industries mainly because it can be a strategy to eliminate the effect of the fluctuating price and of course, to assure the increasing demand. Due to its biodiversity and its growing technological development, Mexico plays a vital role in the synthesis of these polymers based on renewable resources, as it is among the top 10 oil and vegetable grease producing countries worldwide. The objective of the present work was to analyze the viability of wheat germ oil as a precursor of epoxy resins synthesized from the Prileschajew epoxidation method to



obtain thermosets polymers based only on renewable resources, characterize their mechanical properties and identify if for themselves it comply the specifications for use in the industry. Preliminary results show low mechanical properties in flexural and tensile tests compared to the commercial epoxy resin based on Diglycidyl ether of bisphenol A, suggesting that for application in specialized industries such as automotive it is necessary to reinforce the materials with Fiberglass frameworks or as reported in the literature, by mixing the resin based on renewable resources with the commercial one.

#### REACT04-FUNCTIONALIZATION OF POLYPROPYLENE IN MELT BY N-PHENYLMALIMIDE GRAFTING

NOEMI JARDON MAXIMINO, GREGORIO CADENAS PLIEGO, CARLOS ALBERTO ÁVILA ORTA,  
LUIS EDMUNDO LUGO URIBE

The N-phenylmaleimide monomer was synthesized from maleic anhydride and aniline in equimolar proportions, requiring two steps for its preparation. The first step consisted in the formation of maleamic acid and the second step consisted in the cyclization of the monomer in acid medium to a refluxing temperature of xylene. The characterization of N-phenylmaleimide consisted of an analysis of FTIR, <sup>1</sup>H NMR and <sup>13</sup>C NMR. In order to optimize the functionalization process of the N-Phenylmaleimide monomer in melt, polypropylene functionalization reactions were first carried out with maleic anhydride to study the effect of the monomer concentration and the initiator concentration (PDC) on the degree of grafting. Subsequently, grafting reactions of the N-phenylmaleimide monomer were carried out with polypropylene. The degree of grafting was estimated by FTIR spectroscopy analysis.

#### REACT05-PREPARATION AND CHARACTERIZATION OF CROSSLINKED MUCILAGE OF NOPAL (OPUNTIA FICUS INDICA) WITH EPICHLOROHYDRIN, POTENTIALLY ADSORBENT MATERIAL OF POLLUTANTS IN WASTEWATER

BARBARA BERENICE AVILA MORALES, MIGUEL CHAVEZ GUTIERREZ, DELIA SOTO CASTRO

Dyes in wastewater are very difficult to treat contaminants because of their synthetic origin and the stability provided by their aromatic structures. For its degradation, it is necessary to consider its molecular structure, and the type, number and position of the molecular substituents to determine the possible interactions with some adsorbent. Biological materials can be effective in the decontamination of wastewater through biosorption such as alginates, agricultural residues, cellulosic materials, chitosan, bacteria, algae, cactus plants, xanthan and guar gum. The mucilage obtained from nopal (*Opuntia ficus indica*) is a biopolymer widely studied and has been used in Chile and Mexico as a water purifier and is known to reduce turbidity and hardness in the spring waters. On the other hand, the starch and its modified forms represent a promising class of adsorbent materials. In this work, nopal mucilage microcapsules were spray-dried on a Yamato model 311S equipment under inlet and outlet temperature conditions of 140 °C and 70 °C, respectively, at a pressure of 0.28 MPa and a flow rate of 7 mL/min. Cross-linking of the biopolymers with epichlorohydrin (0.1, 0.4 and 0.7 %P/P) was performed stirring the mixture at a set temperature and time in a salt bath. The temperature conditions (50, 60 and 70 °C), reaction time (8, 12 and 24 h) and pH of the NaOH (5.0 M) were varied to determine optimum cross-linking conditions. The morphological, mechanical and thermal characterization of the crosslinked materials was performed by the FTIR, SEM, TGA, DSC, TEM and TMA techniques.

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REACT06-COMPARISON OF CARBONIZATION, HYDROGENATION AND OXIDATION IN  
THERMAL AND PHOTO DEGRADATION OF EXPANDED POLYSTYRENE

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INDIRA SACHENKA MEJÍA TORRES, ELENA COLÍN OROZCO, MARÍA GUADALUPE OLAYO GONZÁLEZ, ROSA MARÍA VALDOVINOS, ROSAS, IVÁN GALILEO MARTÍNEZ CIENFUEGOS, MIRIAM SÁNCHEZ POZOS, GUILLERMO JESÚS CRUZ CRUZ

Expanded polystyrene (EPS) is one of the most used polymers in disposable containers for food, which is causing a great accumulation in the environment due to its slow biodegradability. Thermal (120°C) and photo-irradiated (295-365 nm wavelength) treatments of this material were studied in this work to evaluate its degradation at different depth levels from the surface: 0, 30, 60 and 90 nm, as a function of the exposure time. The main chemical changes in the structure were followed by IR and XPS spectroscopies. The study focused on quantify and compare carbonization, oxidation and hydrogenation in the EPS structure between thermal and photo conditions which can be similar to some solar collectors studied to degrade EPS and other non-easily degradable polymers to avoid their environmental accumulation. The results showed that carbonization has the main influence in the thermal treatment, which increased up to 6.6% extending far beyond the surface, while oxidation occurs mainly on the EPS surface in the photo-irradiated treatment, increasing up to 9.7%. In general terms, the results showed stratification in the degradation treatments with different pattern in both processes.

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## Invited Presentation

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### NANOSTRUCTURAL DESIGN, SYNTHESIS AND CHARACTERIZATION OF FUNCTIONAL POLYMER SURFACES

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KENNETH J. WYNNE

Soft surface science and engineering in the context of this work emphasizes coatings (~50  $\mu\text{m}$ , bulk) rather than nanofilms, but nanosurface (1-2 nm) functionality is obtained by tailored surface modifiers. Targets for this work are antimicrobial effectiveness with cytocompatibility, stability, and economy. These criteria are considered essential for transformation of conventional polymers into "soft" biomaterials for urological applications. Polyurethanes with brush-like soft blocks having PEG and quaternary side chains are used to modify conventional polyurethanes. One physical criterion is stability of nanosurface quaternary charge density monitored by zeta potentials. Figure 1 shows zeta potentials for a biomedical grade polyurethane (Tecoflex SG80A) and a new PEG/quat soft block modifier. Interestingly, the zeta potential for the modified coating is about 100 mV higher than the control polyurethane. Charge density that was determined by zeta potential measurements encouraged carrying out "sandwich" tests that mimic antimicrobial effectiveness in a confined environment. Taken together, a body of evidence is being acquired to support our model for developing Antimicrobial-But- Cytocompatible (ABC) nanosurfaces on conventional polymers used in biomedical applications. The significance of this work lies in the development of antibiotic and biocide resistant bacteria or "super bugs". Thus one of the challenges in this work is to show that bacteria cannot develop resistance to modified surfaces.

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### NANOCOMPOSITES FOR BIOMEDICAL & ENVIRONMENTAL APPLICATIONS

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GABRIEL LUNA-BARCENAS

In this talk I will discuss some applications in which the proper combination of synthesis and characterization methods help fine-tune the performance of a nanocomposite. In this regard, the extensive use of the polysaccharide chitosan (CS) has triggered many interested applications due to the presence of primary amine and hydroxyl groups. In acidic aqueous media, the primary amine protonates giving rise to hydrogen abstraction, chelation, and other bonding forces when in the presence of an "appropriate" substrate. For this, I will present two examples that our group has developed: 1. Antibacterial Skin Patch. Chitosan-silver (CS/Ag) nanocomposite either in the form of nanoparticles (AgNP) or as ionic dendritic structures (Ag<sup>+</sup>). The antibacterial activity of the resulting nanocomposites in the form of films is studied against two bacteria, Gram-positive *Staphylococcus aureus* and Gram-negative *Escherichia coli*. The collective action of AgNP and Ag<sup>+</sup> ions facilitate the enhancement and synergetic antibacterial activity below certain critical concentration. The nanocomposites containing 1 wt.% of silver nanoparticles and about of 2 wt.% of silver ions exhibit a maximum antibacterial activity, which is close to their electrical percolation threshold. 2. Cu<sup>++</sup> Detection Electrode. We developed electrodes with chitosan-gold nanoparticle (CS-AuNPs) based membranes. Adsorption of the positively charged Cu<sup>++</sup> is related to its interaction with the complex formed by the protonated amino groups of CS with the carboxylate groups that adsorbs onto AuNPs and with the C=O group of amide I groups of CS. For the first time, the relation between percolation threshold and detection

limit of copper ions has been established. Impedimetric method shows superior properties; detection limit ca.  $10^{-7}$  M, linear response range  $10^{-7}$ - $10^{-3}$  M of  $\text{Cu}^{++}$ .

## Oral

### PREPARATION AND CHARACTERIZATION OF MECHANICAL AND BIOLOGICAL PROPERTIES OF GELATIN-GALLIC ACID/ZNO NANOCOMPOSITE BIO-ADHESIVE FOR MEDICAL APPLICATIONS

SONIA NOEMÍ RAMÍREZ BARRÓN, SAÚL SÁNCHEZ VALDÉS, REBECA BETANCOURT GALINDO, MARIA DAS GRAÇAS CARNEIRO DA CUNHA, MARIA TEREZA DOS SANTOS CORREIA, BERTHA ALICIA PUENTE URIBINA

There are in nature some unusual adhesives such as the mussel feet, commonly called mussel foot proteins (fps). The singularity of these bioadhesives resides in their adhering performance to all kinds of surfaces and, more astonishing, under a wet environment. It has been shown that its adhesiveness is due to L-DOPA-containing proteins. Nevertheless, the high cost of extraction of these proteins has limited its application. Researches have opted to add L-DOPA analogues to the backbone chain of diverse synthetic or natural polymers. The Gallic acid (GA) is an antioxidant polyphenolic, which possess a catechol group and differ from each other by an additional hydroxyl group. Such as L-DOPA, GA has the capacity to interact strongly with Ti- (IV), Fe +3, and other surfaces. To improve bio-adhesive characteristics, it has been opted to add antimicrobial properties into the bio-adhesive to prevent infection in patients for medical applications. The ZnO nanoparticles (NZnO) have received noticeable attention in the medical area due to their excellent antibacterial properties. The proposal of this work is the development of a bio-adhesive from GA modified gelatin, with the incorporation of NZnO as antimicrobial agent. In this investigation, the bio-adhesive nanocomposites were characterized by FT-IR, NRM, TEM and XPS. The adhesive strength, swelling performance and degradation time were investigated. In addition, the biological properties such as antimicrobial and cytotoxicity were evaluated. The results confirmed that these bio-adhesives meet the required bio-adhesive, mechanical and antimicrobial characteristics to be used for medical applications.

### POLYMER GRAFT-MODIFIED CO<sub>2</sub>-SWITCHABLE CELLULOSE NANOCRYSTALS PREPARED BY NITROXIDE-MEDIATED POLYMERIZATION AND THEIR USE AS PICKERING EMULSIFIERS

JOE GLASING, JUSTINE YOUNES, JEAN BOUCHARD, PHILIP G. JESSOP, PASCALE CHAMPAGNE, MICHAEL F. CUNNINGHAM

We have studied solid-stabilized (Pickering), stimuli-responsive oil-in-water emulsions using polymer graft-modified CO<sub>2</sub>-switchable cellulose nanocrystals (CNC). Following functionalization of the CNC surface with glycidyl methacrylate, CO<sub>2</sub>-switchable poly(N,N-(diethylamino)ethyl methacrylate) (PDEAEMA) and poly(N-3-(dimethylamino) propyl methacrylamide) (PDMAPMam) macroalkoxyamines with low dispersities, high livingness and chain end functionalities were grown through nitroxide-mediated polymerization (NMP) and grafted to the nanocrystals. The success of the grafting reactions was demonstrated by <sup>13</sup>C CP-MAS and FT-IR spectroscopy, as well as elemental and thermogravimetric analysis.

The CO<sub>2</sub>-responsiveness of the graft-modified CNC was demonstrated by zeta-potential measurements and reversible phase shuttling experiments in oil and water. The surface and interfacial properties of the graft-modified CNC were characterized by surface and interfacial tensiometer measurements. The stability of the solid-stabilized emulsions at different pH was investigated, and the resulting droplet size measured using optical microscopy. Depending on the pK<sub>a</sub>H of the polymer grafted to the CNC and the polarity of the oil phase, the stability of the emulsions could be controlled by bubbling CO<sub>2</sub> and N<sub>2</sub>, which led to protonation/deprotonation of the tertiary amino groups on the CNC surface. Various factors, including chain length of the grafted polymer, graft densities, total amount of CO<sub>2</sub>-switchable groups on the CNC surface, and concentration of Pickering stabilizer and their effect on the properties of the emulsions were investigated.

#### DEVELOPMENT OF GRAPHENE OXIDE EPOXY/THIOL-ENE NANOCOMPOSITES AND THE STUDY OF THEIR ELECTRICAL CONDUCTIVITY

RICARDO ACOSTA ORTIZ, AIDA ESMERALDA GARCIA VALDEZ

In this work is reported a study where it was obtained photocurable reduced graphene oxide (rGO) epoxy/thiol-ene composites. A difunctional tertiary amine functionalized with allyl groups as the curing agent along with the pentaerythritol tetrakis mercaptopropionate were used as the components of the thiol-ene system. After dispersing the graphene oxide in the epoxy resin diglycidyl ether of bisphenol A (DGEBA), the photocurable formulations were subjected to a dual photo-thermal treatment, achieving full conversion of epoxy groups in 10 minutes. Additionally, a study using monofunctional models compounds analogs to the epoxy resin, curing agent and multifunctional thiol, was carried out in order to confirm the reduction of the graphene oxide under the conditions of photocuring. It was demonstrated by FT-IR spectroscopy, Raman spectroscopy, and XPS, the reduction of graphene oxide during the curing of the epoxy resin. The mechanical properties of the cured test specimens were determined using dynamic mechanical analysis (DMA). The electrical conductivity of the nanocomposites is also reported.

#### SELF-ASSEMBLED THREE-DIMENSIONAL STRUCTURE BASED ON GRAPHENE OXIDE AND CALCIUM CARBONATE PARTICLES USING POLYETHYLENIMINE

ALMA DANIELA SALAZAR-AGUILAR, GLADIS JUDITH LABRADA-DELGADO, FERDINANDO TRISTÁN-LÓPEZ, SOFÍA MAGDALENA VEGA-DÍAZ

Carbon nanomaterials, like graphene oxide (GO) and reduced graphene oxide (rGO), have attracted great interest during last few years because of their potential applications in electrochemical devices, energy storage, catalysis, enzyme adsorption, drug delivery, biosensors, etc. Recently, it has been observed that the performance of some devices is increased when using three-dimensional structures made of nanomaterials due to an increase of active material per projected area. The current challenge is to obtain self-sustained three dimensional materials made with nanostructures, like GO or rGO, preserving their nanometric properties in macroscopic structures to maximize their performance and ease their manipulation to elaborate devices. Then, the control of the structure in these macroscopic structures is the key step to achieve better performance. In this study, a self-sustained three-dimensional structure was obtained using calcium carbonate microparticles, polyethyleneimine (PEI) and graphene oxide by combining sacrificial

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template and layer-by-layer (LbL) techniques. Polyethylenimine, a well-known polyelectrolyte, allows to control self-assembly of graphene oxide on the surface of calcium carbonate particles, while these, by using different particle diameter, are strongly related to the size and distribution of the porous structure in the final self-sustained structure after their elimination using an acidic solution.

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#### INVERTED OPAL LIKE STRUCTURE OBTAINED USING POLYETHYLENIMINE MODIFIED SILICON OXIDE PARTICLES AND GRAFENE OXIDE

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JOSÉ IVÁN RODRÍGUEZ-RODRÍGUEZ, SOFÍA MAGDALENA VEGA-DÍAZ, FERDINANDO TRISTÁN-LÓPEZ, GLADIS JUDITH LABRADA-DELGADO

One of the main goals in material science is the synthesis of new nanostructured materials, particularly those where micro and nanostructure is well tuned. One of the main methods of synthesis is based on molding. The quality of the replicates depends on the degree of order in the colloidal crystal and the conditions of mineralization and removal of the mold. Throughout this procedure, some problems arise. The most important is the affinity of the template with the coating, due to this it is important to use some agents with the appropriate characteristics to improve the coatings. An alternative is the use of polyelectrolytes like polyethyleneimine (PEI). PEI is a branched polyamine well known for its physisorption properties. It is also known to mediate the binding of nanostructured metal oxides with various compounds due to the amino group present in their chain. The present work will study the formation of three-dimensional structures analogous to inverted opals using PEI to favor the interactions between the template and the graphene oxide (GO), where the PEI has the dual function of acting as a bridge between the particles and GO, and improving the dispersion of the silicon oxide particles in the suspension. In this way, the PEI facilitates the coating of the silica particles with several sheets of GO, obtaining a more uniform and orderly coating. Later the silicon oxide particles are removed leaving their imprinting on GO.

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#### OBTAINING A BIOPLASTIC BY EXTRUSION – INJECTION MOLDING METHOD FROM RESIDUES OF THE FISHERY INDUSTRY

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IRAIIS ARAGON LUCERO, MIGUEL CHAVEZ GUTIERREZ, GUSTAVO HINOJOSA ARANGO, MARIA ISABEL FELISBERTI

In recent decades, the use and study of biopolymers have increased compared to conventional polymers. Gelatin is a biopolymer derived from the hydrolysis of collagen that has been extensively studied for the production of plastic films and composite materials. However, there are few studies regarding its processing by the extrusion-injection molding method. The objective of this work was to obtain a bioplastic material from fishery residues by means of the extrusion-injection molding method. Gelatin was extracted from the bones of Indo-Pacific blue marlin (*Makaira nigricans*) and cartilage from the silky shark (*Carcharhinus falciformis*). The residues were washed and cleaned to remove any remaining meat. The extraction was carried out with an acid-base treatment. The clean material was treated with a sequence of 2% NaOH, 2% H<sub>2</sub>SO<sub>4</sub> and 1% citric acid. Each treatment took 45 min respectively and was performed in duplicate and followed by a wash to pH = 7. The final extraction was carried out with distilled water at 45°C for 24 hrs. The extract was filtered to remove impurities and dried in petri dishes in an oven at 60°C for 16 hrs. After drying, the material was manually sprayed and stored in an airtight container at 25°C. The average yield of gelatin extraction was 3 g for every 100 g of residue. After extraction, gelatin was wetted

with 10% by weight glycerol, used as plasticizer, and used to obtain specimens. The formulation was manually mixed for 10 min prior to extrusion and, later, extruded at 120°C in the three heating zones, 100 rpm for 2 min, in a co-rotating extruder DSM Xplore, model MC-5. The material obtained in the extruder was injected with the following processing conditions: temperature of 120°C in the feed and 45°C in the mold, a pressure of 0.80 Bar for 24 seconds in a molding injector DSM Xplore IM-5. Our methodology for the transformation of fisheries residues into bioplastic is an innovative approach for the integral use of targeted fish species.

### **THERMAL AND VIBRATIONAL CHARACTERIZATION OF NANOCOMPOSITES OF POLY( $\epsilon$ -CAPROLACTONE)-CO-POLY(ETHYLENE GLYCOL) AND FUNCTIONALIZED CARBON NANOTUBES**

LEONARDO CAJERO-ZUL, SERGIO NUÑO-DONLUCAS, FERNANDO LOPEZ-DELLAMARY

In this work, nanocomposites synthesized with a polymer matrix of poly( $\epsilon$ -caprolactone)-co-poly(ethylene glycol) (PCL-co-PEG) with star structure, and functionalized carbon nanotubes (CNTs) were characterized thermally and by infrared spectroscopy.

### **SYNTHESIS OF FLEXIBLE POLY (ETHYL METHACRYLATE-CO-BUTYL ACRYLATE) FILMS BY SEMICONTINUOUS HETEROPHASE POLYMERIZATION**

ERNESTO GONZÁLEZ, ABRAHAM GABRIEL ALVARADO MENDOZA, ROSAURA HERNÁNDEZ MONTELONGO, LOURDES ADRIANA PÉREZ CARRILLO, SUSANA LÓPEZ CUENCA, MARTIN RABELERO VELASCO

The copolymerization in semicontinuous heterophases under monomer-starved conditions of ethyl methacrylate-butyl acrylate is presented here. Stable latexes with particle diameters smaller than 50 nm and narrow size distributions were obtained using a low surfactant concentration and producing a ratio of polymer formed to a surfactant employed of 30/1. The effect of the monomers ratio on reaction kinetics, polymerization rate, particle diameter and glass transition temperature ( $T_g$ ) was studied. The copolymerization was verified by differential scanning calorimetry and infrared spectroscopy, the morphology of the nanoparticles obtained was analyzed by transmission electron microscopy. Flexible and translucent films were obtained and analyzed for their mechanical tensile properties. In all cases stable latexes were obtained with conversions greater than 90% and particle sizes less than 100 nm. The synthesis of the copolymers was confirmed by FTIR and the  $T_g$ 's obtained were displaced as a function of the monomers composition. The mechanical properties obtained show that as the content of the butyl acrylate is increased, the films become softer and more flexible.

### **SYNTHESIS OF NANOCELLULOSE FROM POLYMERIC BIOMASS: AGAVE TEQUILANA WEBER**

TANIA LARA-CENICEROS, JOSÉ BONILLA-CRUZ, A. GARCÍA-GARCÍA A., ARIZPE-ZAPATA, U. MÁRQUEZ-LAMAS, E. HERNÁNDEZ-FRANCISCO, ARA CARBALLO, Z. ALI, CHUN-YANG YIN

In nature, a large number of plants synthesize extra-cellular skeletal structures consisting of a matrix reinforced by fibrous biopolymers. Cellulose is the most abundant and renewable natural biopolymer on Earth, and is the most important example of reinforcing element in plants. In this work lignocellulosic materials were obtained from polymeric biomasses of Agave Tequilana Weber: pineapple and penca. Cellulose nanofibrils (CNFs) were synthesized by a combination of chemical and physical treatments. The influence of

these diverse methods over the final crystallinity, morphology and size of the CNFs is discussed. The materials resulted after each treatment step were followed by different characterization techniques: SEM, XRD, XRF, Fluorescence, FTIR, TGA and DSC in order to elucidate what happen after each treatment step. SEM reveals the surface modification of the nanofibrils with the different chemical and physical treatments. XRD showed the appearance of crystalline structures related with the nanocellulose structure. Finally, we obtained semi-crystalline Cellulose nanofibrils (CNFs) by facile synthetic approaches.

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#### SOLVOTHERMAL SYNTHESIS METHOD FOR THE PREPARATION OF POLYMERIC CARBON NITRIDE OXIDES

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MANUEL EDUARDO MARTINEZ CARTAGENA, SALVADOR FERNANDEZ TAVIZON, JOSE ROMAN TORRES LUBIAN, JORGE ROMERO GARCIA

We have developed a simple one step solvothermal method to synthesize g-C<sub>3</sub>N<sub>4</sub> oxides from urea; varying the preparative method it is possible to obtain oxygen containing materials as well as phosphorous-doped graphitic carbon nitrides. The products are prepared by heating urea-toluene suspensions in Teflon-clad pressure vessels; when mixtures of urea-phosphorous pentoxide are similarly treated, phosphorous containing materials can be isolated. All products contain a large amount of oxygen, the highest reported thus far for oxidized nitrides and, depending on the conditions employed, can also incorporate varying amounts of P. The reported gC<sub>3</sub>N<sub>4</sub> oxides syntheses rely on the nitride's thermal preparation followed by oxidation by methods used in the synthesis of GO, the yields of both steps are low; by comparison the yields of the solvothermal method are in the order of 70%, based on urea. We present the materials' characterization by commonly used analytical means. Thus the materials' DRX reflections show  $2\theta=10.76$  y  $28.27^\circ$  signals, in agreement with those reported for oxidized gCNs; SEM and TEM observations corroborate the presence of stacked layers of 2D materials that in some instances show a porous structure. NMR analysis is consistent with the presence of a OH contained in a triazine moiety and XPS analysis permits discerning the presence of the expected bonds and to determine the contents of oxygen and phosphorous within the samples. High yield and preparation ease of the synthetic approach will facilitate the use of the gC<sub>3</sub>N<sub>4</sub> oxides in several applications under study.

#### Poster

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#### NANO01-BIOSYNTHESIS OF SILVER NANOPARTICLES USING AGAVE TEQUILANA WEBER VAR. AZUL FIBERS AS TEMPLATE

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EDGAR JOSÉ LÓPEZ-NARANJO, AIDA ALEJANDRA PÉREZ-FONSECA, JORGE RAMÓN ROBLEDO-ORTIZ, RUBÉN GONZÁLEZ-NÚÑEZ, LUIS JAVIER GONZÁLEZ-ORTIZ, MARÍA JUDITH SÁNCHEZ-PEÑA, PRISCILLA MÚÑIZ-MENDOZA

The use of natural fibers over synthetic fibers is attractive due to several reasons including their low environmental impact, renewability, biodegradability, relative low cost, lightness, acoustic and thermal insulation properties. Although the insertion of natural fibers on the industrial, building and commercial markets has experienced a growth rate of 13% over the last 10 years, the mechanical properties of natural fiber composites are lesser than those of synthetic composites. This problem can be overcome through surface modification of the fibers, to improve the interfacial bonding between the fibers and the polymer matrix. The use of nanoparticles to modify fibers' surface offers remarkable advantages, due to their



interfacial interactions on polymer branches. Although it has been demonstrated that natural cellulose fibers can be used as support for nanoparticle synthesis, most of the literature reports on the modification as been applied to cotton fibers. Therefore, the use of unconventional natural fibers as solid supports is attractive as they exhibit heterogeneous and oxygen-rich structures, which can result in different nanoparticle morphologies and distributions that could confer varied macroscopic properties to the fibers. Thus, the main aim of this work is to synthesize silver nanoparticles (AgNPs) using Agave tequilana Weber var. azul extract as reducing agent and Agave tequilana Weber var. azul fibers as template.

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#### NANO02-EFFECT OF MOLECULAR WEIGHT AND REACTION PARAMETERS IN THE SYNTHESIS OF METALLIC NANOPARTICLES USING PVA AS REDUCING-STABILIZING AGENT

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RAÚL ENRIQUE DE JESÚS PÉREZ-PARRA, EDGAR JOSÉ LÓPEZ-NARANJO, AIDA ALEJANDRA PÉREZ-FONSECA, RUBÉN GONZÁLEZ-NÚÑEZ, MILTON OSWALDO VÁZQUEZ-LEPE, LUIS JAVIER GONZÁLEZ-ORTIZ, ARAHÍ ALVARADO-ARÁMBURO

Recently, the interest in the synthesis of metallic nanoparticles (MNPs) using green chemistry routes has increased. The synthesis of MNPs via green chemistry routes must take into consideration three main specific aspects: the choice of non-toxic solvents, an environmental friendly reducing agent and, a biodegradable stabilizing agent. Poly vinyl alcohol (PVA) is a biodegradable, synthetic, innocuous and highly water-soluble polymer commonly used in food packaging, desalination membranes, and membranes by evaporation. Due to its high solubility in water and stabilizing properties, it constitutes a good candidate to be used in the synthesis of MNPs in aqueous solution as both, reducing and stabilizing agent. It is also known that the molecular weight of the reducing-stabilizing agent directly influences the shape, size and morphology of the synthesized MNPs. Therefore, in this work the effect of PVA molecular weight and reaction parameters on the shape, size and morphology of MNPs synthesized through a low-cost and safe green chemistry route is reported.

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#### NANO03-INFLUENCE OF REACTION PARAMETERS ON THE MORPHOLOGY OF BIOSYNTHESIZED SILVER NANOPARTICLES

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MARCO ANTONIO PONCE-VILLALOBOS, EDGAR JOSÉ LÓPEZ-NARANJO, AIDA ALEJANDRA PÉREZ-FONSECA, JORGE RAMÓN ROBLEDO-ORTIZ, LUIS JAVIER GONZÁLEZ-ORTIZ, ALEJANDRO MANZANO-RAMÍREZ, ARAHÍ ALVARADO-ARÁMBURO

Up to now, different methods for the synthesis of silver nanoparticles have been developed. These methods include chemical synthesis, electrochemical techniques, ultraviolet irradiation and photodetection technique. Of these methods, chemical reduction is the most common route used to synthesize silver nanoparticles (AgNPs). Nevertheless, chemical synthesis involves the use of toxic compounds. As a consequence, green techniques, which employ microorganisms, plant extracts or plant biomass for the synthesis of AgNPs have recently received vast attention, since they are considered cost-effective and environmentally friendly alternatives to traditional methods for the synthesis of different shaped and sized AgNPs. It is known that intrinsic properties of metal nanostructures can be tailored by controlling their size, shape, composition, crystallinity and, structure. Particular emphasis has recently been placed on the control of the morphology during the synthesis of AgNPs, since mastery over the shape of a nanostructure enables control over its properties and usefulness for a given application. Therefore, in this work we report an extensive study of the effect of different experimental parameters on the morphology of AgNPs synthesized

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through a green chemistry method, using a natural extract obtained from Agave tequilana Weber var. azul as reducing agent.

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#### NANO04-GOLD NANOPARTICLES SYNTHESIZED VIA MICROWAVE AND THEIR USE IN THE DEGRADATION OF NITRO COMPOUNDS

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DIANA GARCÍA-TERÁN, JOSÉ BONILLA-CRUZ, RUBÉN MENDOZA-CRUZ, LOURDES BAZÁN-DÍAZ, MIGUEL JOSÉ-YACAMÁN, TANIA LARA-CENICEROS

Nanoparticles morphology (size and shape) is very important to obtain materials with unique properties with potential applications in photonics, information storage, electronic and optical detection systems, therapeutics, diagnostics, photovoltaics, and catalysis. Typically, gold nanoparticles (AuNPs) are synthesized under aqueous process during long reaction times and using toxic reducing agents. In this work we present a simple, green and facile methodology assisted by microwave (MW) in short times, to obtain different morphologies and highly crystalline AuNPs, using PVP as reducing and stabilizer agent. The effect of PVP molecular weight is discussed in the syntheses of AuNPs. We report a highly reproducible method to obtain anisotropic crystalline nanostructures (nanotadpoles) using a fast and simple method assisted by MW in short time without the use of a "seed method" which is usually used for the synthesis of anisotropic nanoparticles. The functional nanocomposites (PVP-AuNPs) with different sizes and morphologies were used as catalytic materials for the p-nitroaniline (p-NA) degradation in aqueous media. The ratio p-NA:NaBH<sub>4</sub> was studied in order to optimize the p-NA degradation times.

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#### NANO05-SYNTHESIS OF CELLULOSE NANOWHISKERS FROM NOPAL CLADODES

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TANIA LARA-CENICEROS, JOSE BONILLA-CRUZ, A. GARCÍA-GARCÍA, A. ARIZPE-ZAPATA, G. SOSA-LOYDE, A. CARBALLO, Z. ALI, CHUN-YANG YIN

Nopal (*Opuntia ficus-indica*) is an indigeneous and endemic cactacea of the desertic and semidesertic áreas from América. In México, there are 104 species of *Opuntia*, and have different uses: consumed as feedstock, consume of their fruit (tuna) and as a vegetable, furthermore to its use in ranches as fences. Cellulose, the most abundant biopolymer, is a polysaccharide consisting of a long chain of D-glucose repeat units, which form part of the nopal cladodes. In this work is presented a facile and tunable approach to obtain Cellulose nanowhiskers (CNWs) from nopal cladodes, using basically a combination of chemical and physical treatments. In order to extract the lignin and hemicellulose (who helps to maintain together the cellulose microfibrils) a variety of chemical treatments were carried out (sosa treatment for soaking the cladodes, soxhlet extraction, etc). The successful elimination of lignin was verified by FTIR and Fluorescence. After the chemical extraction, different mechanical treatments using high shear rates (ultraturax), lyophilization and ultrasonic dismembrator were used. The influence of these diverse methods over the final crystallinity, morphology and size of the CNWs is discussed. SEM analysis showed our evidences.

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### NANO06-OBTAINING OF CELLULOSE NANOCRYSTALS BY HYDROLYSIS FROM AGAVE BAGASSE

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MANUEL GALLARDO SÁNCHEZ, JOSÉ ANZALDO HERNÁNDEZ, ROSA MARÍA JIMÉNEZ AMÉZCUA, ROGELIO RAMÍREZ CASILLAS, EMMA REBECA MACÍAS BALLEZA, SALVADOR GARCÍA ENRÍQUEZ

The process of obtaining cellulose nanocrystals from agave bagasse Tequilana Weber var. Azul has acquired great importance because it is a very abundant agroindustrial residue. Furthermore, in the literature it is found that these nanomaterials are very relevant due to their abundance, strength, stiffness, low weight and biodegradability. In the present work, we report a study of two hydrolysis routes for the production of cellulose nanocrystals from these wastes; The first involves a hydrolysis with sulfuric acid and the second with hydrochloric acid, varying parameters such as temperature, reaction time and concentration, in both cases a cellulosic pulp was obtained from an alkaline cooking and a series of bleaching stages. Obtaining a Kappa number of 26, a percentage of alpha cellulose of 93%, a viscosity of 11.53 cp, a degree of polymerization of 830 and a degree of brightness of 76%. The agave bagasse, bleached pulp and nanocrystals were characterized by FTIR, XRD and NMR, which were compared with Whatman paper, which has a high degree of alpha cellulose.

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### NANO07-REOLOGIC CHARACTERIZATION OF POLY (LACTIC ACID)/CELLULOSE NANOCRYSTALS

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SOLEDAD CECILIA PECH COHUO, JORGE ALONSO URIBE CALDERÓN, DENIS RODRIGUE, GONZALO CANCHÉ ESCAMILLA, ALEX VALADEZ GONZÁLEZ, VÍCTOR VLADIMIR ALMÍCAR FERNÁNDEZ ESCAMILLA

Poly (lactic acid) (PLA) is a linear biopolymer with good chances to replace other polymers based on petroleum in packing application for food; but, it presents low barrier properties and low melt strength. The latter reduces the processability of PLA in order to produce thin films by blow-extrusion[1]. The melt strength of PLA can be increase by adding pristine and modified cellulose nanocrystals (NCC) from bagasse fiber of Agave Tequilana Weber as rheological modifiers. In this work, the effect of adding pristine NCC (A) and NCC-g-poly (2 ethyl hexyl acrylate) (B) at different proportions (0.5, 1 and 2 wt.%) was evaluated as modifier on shear and extensional rheological properties of PLA/NCC. The thermal properties of unprocessed PLA (PLAV), extruded PLA (PLAP), and PLA/NCC nanocomposites were evaluated by TGA and DSC. It was found that the processing increase slightly the crystallinity of PLA (crystallinity of PLAV was 11% and 18% for PLAP); PLA/(grafted NCC) exhibited higher degrees of crystallinity than PLA/(pristine NCC) nanocomposites or PLAV and PLAP. On the other hand, the TGA results showed B nanocomposites are more thermal stable than A nanocomposites. PLAV showed a Newtonian behaviour in the shear rheological tests, PLAP and NCC nanocomposites exhibited a pseudoplastic behaviour. The B nanocomposites showed higher values of complex viscosity, loss and storage modulus than A nanocomposites, PLAP and PLAV; the above suggested that grafted NCC and PLA matrix present a certain interaction between them. In addition, the extensional rheological results showed a similar behaviour to shear rheology ones.

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#### **NANO08-RHEOLOGICAL BEHAVIOR OF AQUEOUS SOLUTIONS OF CELLULOSE NANOCRYSTALS**

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MANUEL ALBERTO GALLARDO SÁNCHEZ, ROSA MARÍA JIMÉNEZ AMÉZCUA, ROGELIO RAMÍREZ CASILLAS, J. FELIX ARMANDO SOLTERO MARTÍNEZ, SALVADOR GARCÍA ENRÍQUEZ, EMMA REBECA MACÍAS BALLEZA

The agave blue tequilana Weber bagasse is an agroindustrial waste obtained from production of Tequila in denomination origin region. It has been reported that the agave bagasse can be used as raw material for animal feeding, in the production of ethanol, in the elaboration of cyto and biocompatible hydrogel films, as reinforcement materials for composites, among others uses. It is also possible to obtain a colloidal suspension of cellulose, which have nanometric size and improve the mechanical properties of composites because of the abundance of hydroxyl groups. In this work, it has been isolated cellulose nanocrystals (CNs) from bagasse of blue agave by acid hydrolysis with sulfuric and chloric acids. When an acid hydrolysis is realized, the surface of CNs is negatively charged and a self-aggregation process occurs. The rheological behavior of aqueous solutions of cellulose nanocrystals is studied as a function of time and temperature of acid hydrolysis, hydrolysis route (HCl or H<sub>2</sub>SO<sub>4</sub>), concentration of CNs and temperature. The results show a non-Newtonian behavior. The shear stress and the viscosity increase with CNs concentration and diminish with temperature.

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#### **NANO09-ANTIOXIDANT AND ANTIFUNGAL ACTIVITIES OF PHB-TPS/CLAY/EUGENOL BIONANOCOMPOSITES FILMS**

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KARLA GARRIDO-MIRANDA, BERNABÉ L. RIVAS, MÓNICA PÉREZ

Bionanocomposites based on polyhydroxybutyrate (PHB) and thermoplastic starch (TPS) containing of 3 wt.% of organo-modified montmorillonite clay and eugenol were prepared by melt mixing and characterized. The properties thermal, mechanical, morphology, antimicrobial and antioxidant of the bionanocomposites films with eugenol have been investigated. The PHB-TPS/Clay/Eugenol bionanocomposites films showed microbial inhibition zones against the botrytis cinerea. Antioxidant activity assays showed that the bionanocomposites films with eugenol had scavenging activity on DPPH radical. Finally, the mechanical and thermal properties did not present changes significant with respect to the PHB. These results revealed that bionanocomposites show great potential as a biodegradable packaging especially for applications in food.

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#### **NANO10-PREPARATION AND CHARACTERIZATION OF POLY(UREA)URETHANE NANOPARTICLES**

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MÓNICA MAYTÉ VASQUEZ-ALFARO, MARÍA ELISA MARTÍNEZ-BARBOSA, AMIR DARÍO MALDONADO-ARCE, JUAN VALERIO CAUICH-RODRIGUEZ, JOSÉ MANUEL CERVANTES-UC, LERMA HANAIY CHAN-CHAN

Polymeric nanoparticles (PNPs) are structures with a diameter ranging 10-100nm (Wilczewska, 2012). PNPs can be conveniently prepared either from preformed polymers or by direct polymerization of monomers. There are several methods for the preparation of PNPs from preformed polymers such as nanoprecipitation, solvent evaporation, salting-out, dialysis and supercritical fluid technology. The choice of preparation method is made on the basis of a number of factors such as the type of polymeric system, area of application, size requirement, etc. (Rao, 2011) In this work, PNPs were prepared from preformed poly(urea)urethane (PUU) by nanoprecipitation method and Taguchi experimental design

methodology. Four factor and three levels were chosen for Taguchi L9 array: Precipitation temperature (5, 25, 45 °C), PUU concentration (0.75, 3, 9mg/mL), surfactant concentration (0.025, 0.125, 0.25 % w/v) and speed rate (400, 800, 1200 RPM). Morphology and size of PNPs were characterized mean Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS). MINITAB 17 software was used for analyzing results and for obtaining mean and signal-noisy plots. ANOVA analysis was used for determining significant results. Optimum conditions for smaller PNPs (around 60nm) were 0.75mg/mL of PUU, 25°C of temperature, 0.125% w/v of surfactant concentration and 1200 RPM.

#### **NANO11-POLYURETHANE NANOCOMPOSITE MEMBRANE USING BIODEGRADABLE DIOL AND FUNCTIONALIZED CARBON NANOTUBES PREPARED BY PHASE INVERSION METHOD**

VICTOR HUGO ANTOLIN CERON, SERGIO MANUEL NUÑO DONLUCAS, ANTONIO MARTINEZ RICHIA

Fabrication conditions of microporous thermoplastic polyurethane to produce small diameter porous materials are studied. Porosity variations due to various factors such as concentration of PU solution (20, 25, 30 % wt/wt), effect of coagulant temperature (40, 50 and 60 °C) and carbon nanotube concentration (0.5, 1, 2 % wt/wt) are discussed. The membrane's morphology and microphase organization were investigated by scanning electronic microscopy (SEM), differential scanning calorimetry (DSC), infrared spectroscopy (FTIR) and tensile strength test. The soft segment of PU was made of poly( $\epsilon$ -caprolactone-co-ethylene glycol) (PCL-EG) using a chemico-enzymatic route to obtain a biodegradable diol to increase the biocompatibility and biodegradability of resulted material, and isophorone diisocyanate (IPDI) as hard segment to prepare a material approved by medical purpose. Membranes are prepared by a wet phase inversion process using N,N dimethylformamide (DMF) as solvent and water as no solvent. Increasing the polymer concentration to 30 % and coagulant temperature 60 °C decreases the macrovoid formation. This enhances the tensile modulus of PU films. By using this process adjustment may be made on the morphology as they are important factors in design and fabrication of small-diameter membranes. This work is a brief presentation of our results concerning the synthesis and application of biodegradable polyurethane which is thermoplastic elastomer precursor for membrane preparation, we investigated the optimization of membrane morphology, in order to improve their applicability in vascular grafts, soft tissue replacement or drug delivery systems.

#### **NANO12- EFFECT OF AMMONIUM AND AMINOSILANE MONTMORILLONITES ORGANO-CLAYSON THE CURING KINETICS OF UNSATURATED POLYESTER (UP) RESIN NANOCOMPOSITES**

MARIA VARGAS

The curing kinetics of UP nanocomposites prepared by incorporating different amounts of two kinds of organo-montmorillonite (organo-MMT): trimethyloctadecacylammonium chloride (TMOA) and aminopropyl-triethoxysilane (APTES) were studied by non-isothermal differential scanning calorimetry (DSC) experiments. Small angle X-ray scattering (SAXS) was used for measuring the d-spacings in the modified organo-clays, and no intercalation of UP into these clays was observed for the nanocomposites. HRTEM images showed dispersed and agglomerated platelets in UP/APTES 2 and 10 wt%. DSC analysis showed two peaks in UP resins and UP/organo-MMT, and a decrease in the exothermal peak temperature (Tp1 and Tp2) for nanocomposites with the heating rate as compared with those of neat UP system; thus, the higher the heating rate, the higher the curing reaction rate. This effect was

more clearly on the UP/MMT-APTES nanocomposites. The effective activation energies ( $E_a$ ) were determined with the mode-free isoconversional Starik's method. Sesták-Berggren model was chosen to simulate the reaction rate with a good match achieved. Thermal gravimetric analysis showed that the cured UP/APTES at high concentration were slightly more stable than UP and TMOA.

#### NANO13-STRUCTURAL & SPECTROSCOPIC STUDY OF ZINC SELENIDE QUANTUM DOTS DISPERSED IN PLASTISOL

RAQUEL LEDEZMA RODRÍGUEZ, LAYZA A. ARIZMENDI GALAVIZ, RAMIRO ANGUIANO JARAMILLO, ISaura G. YAÑEZ FLORES, RONALD F. ZIOLO

Research in semiconductor quantum dots (QDs) continues to be a hot bed of activity as their applications span broad areas of interest including optoelectronics, lasers, solar cells, biomedicine, computing, communications and solid state lighting. Equally important are hybrid QD polymer nanocomposites (NCs) because they combine the properties of these 0D nanostructures with the technological feasibility of polymers. As part of a larger effort to advance the fundamental understanding of the formation and behavior of QD polymer NCs and their interface, we chose to work with the wide-bandgap semiconductor ZnSe particularly because of its prominent and unique applications in nonlinear optical devices. Here, we report the results of a study to optimize the dispersion of ZnSe QDs in plastisol films to improve the dispersibility and overall optical quality of the QD hybrid films. The NCs were synthesized by mixing oleic acid as stabilized ZnSe QDs at 0.5 to 5 wt % with plastisol formulation. Films were prepared on glass substrates by casting at room temperature and curing at 170°C. Film characterizations were performed using XRD, TEM, HRTEM, EDXA, TGA, UV-Vis and photoluminescence spectroscopies.

#### NANO14-KINETICS OF IBUPROFEN RELEASE FROM NANOPARTICLES OF POLY (ETHYL CYANOACRYLATE)

JESÚS AUGUSTO BALLEÑO, EDUARDO MENDIZÁBAL, RAÚL GUILLERMO LÓPEZ, MAITE RENTERÍA, ADRIANA PATRICIA MENDIZÁBAL, HELEN SAADE

Ibuprofen-loaded poly(ethyl cyanoacrylate) nanoparticles were prepared by semicontinuous heterophase polymerization in the presence of ibuprofen. Nanoparticles with diameters between 10 and 58 nm, loaded with up to 7 % of ibuprofen were obtained. To determine the amount of drug released UV spectroscopy was used. The wavelength that usually has been used to determine the presence of ibuprofen is 264 nm, however, the absorption bands of the PECA and the IB overlap at that wavelength; then the measurements were done at pH 7.5 and a wavelength of 220 nm, using the second derivative of the spectra to obtain more accurate measurements. Four models were used to fit the experimental release data. The analysis of the Ibuprofen release data indicated that the Weibull model is the one that best fit the experimental data. Also, it was found that IB release starts at a slow rate in contrast with the burst of the drug concentration in the plasma when IB is administrated in oral dosing. The ibuprofen is released within the first 80-120 min.

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**NANO15-NANOSTRUCTURED MAGNETIC POLY( $\epsilon$ -CAPROLACTONE)/HEMATITE-ALUMINA  
COMPOSITE SYNTHETIZED BY SOL-GEL METHOD**

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NANCY NELLY ZURITA-MÉNDEZ, MARCO ANTONIO ESPINOSA-MEDINA, AMADEO SANCHEZ-CASTILLO, GEORGINA CARBAJAL-DE LA TORRE

Magnetic nanoparticles have been studied for the last years due to their properties which are employed in biomedical areas as hyperthermia, magnetic resonance imaging (MRI) agents, biosensors, magnetic carriers and targeted drug delivery. In this context, the aim of this study is to elaborate a nanostructured magnetic poly( $\epsilon$ -caprolactone)/hematite-alumina composite by sol-gel synthesis in order to take advantage of the biocompatibility and biodegradable properties of the poly( $\epsilon$ -caprolactone) (PCL) matrix and simultaneously to take advantage of the alumina (Al<sub>2</sub>O<sub>3</sub>) porosity as a possible repository for a drug delivery system. The precursor used at first, was a mixture of stoichiometric aluminum isopropoxide Al(OC<sub>3</sub>H<sub>7</sub>)<sub>3</sub> and ferric chloride (FeCl<sub>3</sub>) at 85°C during 72 hours of reaction in propanol as solvent and 6M nitric acid as catalyst under continuous stirring. The resulting sol was then dried to 60°C during 48 hours and taken for a DSC/TGA analysis for the establishment between the temperature and physical properties of the product obtained. The thermal treatment was realized at 1100°C and posteriorly the gel was added in situ with poly( $\epsilon$ -caprolactone). Characterizations using Fourier Transform Infrared spectroscopy (FTIR), X-Ray Diffraction analysis (XRD) and Scanning Electron Microscopy (SEM) and hysteresis parameters showed the formation of magnetic hematite and porous alumina coated by a poly( $\epsilon$ -caprolactone) matrix.

**NANO16-NANOCOMPOSITES BASED ON HIGH IMPACT POLYSTYRENE, SiO<sub>2</sub> NANOPARTICLES  
AND Mg(OH)<sub>2</sub>: INFLUENCE OF THE SiO<sub>2</sub> AND Mg(OH)<sub>2</sub> RATIO ON THE REACTON KINETICS,  
MORPHOLOGY, IMPACT STRENGHT AND FLAMABILITY**

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A. UBALDO ALARCÓN, F. SORIANO-CORRAL, R. E. DIAZ DE LEON, E. DÍAZ BARRIGA-CASTRO

SiO<sub>2</sub> nanoparticles (SiNP's) were modified using radiofrequency plasma in the presence of styrene monomer (St). Unmodified and modified SiNP's were characterized by infrared spectroscopy (FTIR), thermogravimetric analysis (TGA) and transmission electron microscopy (TEM), to know the degree of modification. Unmodified and modified SiNP's were mixed with Mg(OH)<sub>2</sub> (MAGNIFIN H5MV) and incorporated in the reaction system, where St is polymerized in the presence of polybutadiene, using 0.1 wt-% of benzoyl peroxide as initiator. During the St polymerization the reaction conversion as a function of time was evaluated. Molecular weight distribution (MWD), gel content (GC) and grafting degree (GD) were determined. The morphology of all composites was observed using transmission electron microscopy (TEM). While, the impact strength is measured in accordance to ASTM D256 and the flammability tests (FR) were carried out. The presence of SiNP's and the Mg(OH)<sub>2</sub> increased the reaction time due to the chemical interactions with the organic modification of nano and microparticles. It was corroborated with the increment of the molecular weight in the PS matrix of all compounds. The stage where the morphology is fixed was shifted to higher time and the final morphology was core-shell for all compounds. The SiNP's was encapsulated in the elastomeric phase and the modification of SiNP's increased the impact strength.

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## Invited Presentation

### ROTATIONAL MOLDING OF HYBRID COMPOSITES BASED ON LINEAR LOW DENSITY POLYETHYLENE WITH DIFFERENT CONCENTRATIONS OF GROUND TIRE RUBBER AND MAPLE FIBRE

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YAO DOU, DENIS RODRIGUE

In this work, ground tire rubber (GTR) and maple wood fibre (MF) were dry-blended with linear low density polyethylene (LLDPE) to produce hybrid composites via rotational molding. The idea is to control the final properties of these composites by a balance between rigidity and strength (MF) combined with toughness and elasticity (GTR). To further improve on the overall properties, particle surface treatment was also studied to get better dispersion and interfacial adhesion. From the samples produced, a complete set of characterization was done in terms of morphological (SEM), thermal (DMA, DSC, TGA) and mechanical properties (tensile, flexural and impact). The results show that for the range of parameters studied, optimum compositions can be determined depending on the final applications. Regression models are used to predict these conditions.

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### NEW APPROACHES TO IMPROVED POLYMER PERFORMANCE

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MICHAEL JAFFE

Ordered copolymer backbones and the blending of high performance polymers, aromatic heterocyclics and LCPs can provide attractive routes to improved performance (mechanical properties, chemical, thermal and dimensional stability) at lower cost. Blending of polyimides with higher temperature polymers such as m-PBI provides improved temperature capability in complex systems but test the limits of polymer blend theory and often lead to compositions on the edge of metastability. Blending of all aromatic LCPs results in behavior highly dependent on processing conditions and demonstrate a competition between miscibility and trans-esterification, depending on the blend process details. Controlling the sequence distribution in copolymers allows a broad range of performance from polymers with identical backbone chemistry. While systems have not yet been identified with improved cost-performance, the potential for unusual behavior, coupled with interesting and unexpected chemical and physical behavior renders these systems of recurring academic and commercial interest.



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Oral

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**INFLUENCE OF AMINE-ALCOHOL MODIFIED POLYPROPYLENE (PP) AS COMPATIBILIZER ON PHYSICAL PROPERTIES OF CARBON NANOFIBER REINFORCED PP NANOCOMPOSITES**

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SAUL SANCHEZ, JOSE MANUEL MUÑOZ, ISAURA YAÑEZ, OLIVERIO RODRIGUEZ, EDUARDO RAMIREZ, ROGELIO RAMIREZ

The effect of plasma functionalized carbon nanofibers (CNF) with acrylic acid (AA) and amine alcohol (DMAE) on physical and mechanical properties of polypropylene-CNF nanocomposites prepared by melt mixing was studied. The behaviour of these functionalized CNF via plasma was compared with a CNF functionalized by oxidation with a mixture of sulphuric acid (H<sub>2</sub>SO<sub>4</sub>) and Nitric acid (HNO<sub>3</sub>). Two different types of compatibilizers were used: an amine alcohol modified PP (PPgDMAE) and a maleic anhydride grafted PP (PPgMA). The CNF functionalization was evidenced by Raman spectroscopy, comparing the ratio of peaks at 1371 and at 1590 cm<sup>-1</sup>. Dispersion of the CNF was assessed using scanning microscopy, and the effect of the type of CNF functionalization on the dispersion was evidenced. A notorious increase in thermal stability, mechanical and electrical properties and crystallization rate were observed. A great effect on the storage modulus was obtained when using PPgDMAE and AA functionalized CNF. The mechanical properties of flexural and impact strength showed an effective load transfer when using this CNF and compatibilizer system, which was attributed to the better functionalized CNF dispersion and the strong interactions between this CNF and the polymer matrix. Keywords: Functionalized carbon nanofibers; polypropylene; compatibilization.

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**EFFECT OF COPPER-DOPED GNPS ON THE THERMAL CONDUCTIVITY OF EPOXY COMPOSITES**

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FABIOLA LÓPEZ-BARAJAS, LUIS FRANCISCO RAMOS-DE VALLE, SAUL SÁNCHEZ-VALDÉS, RICARDO ACOSTA-ORTIZ, ROSARIO RANGEL-RAMÍREZ, BLANCA M. HUERTA-MARTÍNEZ

The thermal conductivity was evaluated on epoxy composites with different content of graphene nanoplatelets doped with copper (Cu-GNPs). The composites were prepared using the epoxy resin diglycidyl ether of Bisphenol-A (DGEBA) as polymeric matrix and diamino diphenyl sulphone (DDS) as curing agent. The Cu insertion in GNPs was performed by high energy ball-milling process during 1, 2 and 4 hours. The interaction Cu-GNPs was evaluated by Raman spectroscopy. Compared to pristine GNPs at the same region, Raman spectra of Cu-GNPs show clearly 2D and G signal shift after the ball-milling process; the signal 2D shifted to smaller cm<sup>-1</sup>, and the signal G moves to greater cm<sup>-1</sup>. Different Cu-GNPs concentrations (7, 10 y 15 % wt) were dispersed on DGEBA by extrusion process; the dispersion was evidenced trough scanning microscopy. The composites thermal conductivity was assessed by differential scanning calorimetric technique. The thermal conductivities of the composites with Cu-GNPs were enhanced compared to those without filler.

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## COMPARISON OF IONIC CONDUCTIVITY AND PHYSICAL PROPERTIES BETWEEN -OH AND -MET SUBSTITUENTS IN PPEGMA+MMT NANOCOMPOSITES

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RICARDO IVÁN RODRÍGUEZ RAMÍREZ, JUANA CUETO, GREGORIO GUZMAN, JUDITH CARDOSO MARTINEZ

Recent studies have shown that the nature of the polymer used as ion transporter affects directly in the electrodynamics of the Li<sup>+</sup> species in batteries ([Li-Po]bat), this means that by changing the substituents of the polymeric chain, the actual medium or by adding an extra supporting material, the charge yield can be modified. In this work we made a simulation of the relation that the [Li-Po]bat has with Poly(ethylene glycol)methacrylate (PEGMA), ionic liquid and montmorillonite (MMT) to measure the electrodynamics of the whole [Li-Po]bat and the possibility of using this materials to enhance the charge transfer of the battery. After realizing that the methylated form of PEGMA (mPEGMA) forming a composite with the MMT in ionic liquid will enhance the efficiency of [Li-Po]bat, we decided to make the experiment by using MMT, PEGMA and mPEGMA to make a nanocomposite via sonication before polymerization and adding ionic liquid to make the efficient charge transfer medium to compare the yield obtained with the methylated version of the polymer to analyze which of these variations has the best behavior in real life. The characterization was made by FT-IR analysis and X-Ray diffraction; the physicochemical behavior was tested by TGA and DSC analysis; the electrical behavior was measured by DEA analysis. We observed a decrease in the pPEGMA ΔCp after adding MMT. We also obtained an increase in the decomposition temperature (130 to 150°C). Its conductivity increased 4 orders of magnitude after the whole material was made (PEGMA+MMT+Li++Ionic liquid) compared to the pristine polymer.

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## MECHANICAL CHARACTERIZATION OF HYBRID COMPOSITE WITH NATURAL FIBERS (AGAVE/COIR) BY ROTATIONAL MOULDING

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ROSA GABRIELA LÓPEZ-GONZÁLEZNÚÑEZ, RUBÉN GONZÁLEZ-NÚÑEZ, PEDRO ORTEGA-GUDIÑO, JORGE RAMÓN ROBLEDO-ORTÍZ

Hybrid composites reinforced with agave and coir fibers were produced by dry blending and rotational molding. The effect on mechanical properties was studied for a 20%wt. with different weight ratio of agave and coir fiber (100-0, 70-30, 50-50, 30-70 and 0-100). The results showed improved tensile and flexural modulus (26% and 33% respectively) and impact strength (12%) was reached with a proportion of fiber was 70-30 (agave-coir) when compared to materials prepared only with agave fiber.

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## FAST AND FACILE FUNCTIONALIZATION OF GRAPHENE OXIDE ASSISTED BY MICROWAVE AND ITS USE AS A REINFORCEMENT IN NYLON-6

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EDGAR HOMERO RAMIREZ SORIA, JOSÉ BONILLA CRUZ, TANIA ERNESTINA LARA CENICEROS

Functionalization of graphene oxide (GO) with organic groups opens up a wide range of potential applications in different fields of knowledge. Scientific studies of how the new functional groups affect the interlayer d-spacing of function-alized GO (FGO) have not been adressed. On the other hand, the development of new methodologies to functionalize GO are highly demanded. In particular, the functionalization of GO with alkoxy silane compounds typically takes between 1 h up to 40 h and the FGO exhibit a low func-

tionalization yield. Herein, a new approach to functionalize GO with APTS assisted by microwave is presented, wherein the functionalization time is of only 20 min. The main advantage of functionalizing GO assisted by microwave over other techniques is the uniform heating of the sample, which leads to short reaction times and high reactions yields. Highly oxidized graphite was obtained modifying an improved Hummer's method. APTS was investigated to introduce free amine groups to GO. The functionalization mechanisms of GO with APTS are proposed, wherein a Schiff base to protect amine groups is formed, before of nucleophilic attacks between the oxygen atom from -OH groups and Si atom from alkoxy-silane group. The reduction of GO and the presence of chemical bonds C-N, C-O-Si and NH<sub>2</sub> (C1s, O1s and N1s, respectively), from APTS attached to GO, were observed by XPS. FGO exhibited a progressive increase in the interlayer d-spacing (obtained by XRD) as APTS concentration was increased. Also, a full coverage of GO was obtained following the atomic ratio of Si:C by XPS. Also, thermal analysis by TGA was obtained where FGO samples exhibited a more thermal stability in comparison with GO. Subsequently, the silane-FGO sheets were incorporated into Nylon-6 by electrospinning. These fibers were characterized their mechanical properties.

#### EFFECT OF THE CHEMICAL OXIDATION OF GRAPHITE IN THE PHYSICO-CHEMICAL AND RHEOLOGICAL PROPERTIES OF PLA / GO COMPOSITES

MONICA ELVIRA MENDOZA DUARTE, IVAN ALZIRI ESTRADA MORENO, SERGIO GABRIEL FLORES GALLARDO, ERIKA IVONNE LOPEZ MARTÍNEZ, ERASTO ARMANDO ZARAGOZA CONTRERAS, ALEJANDRO VEGA RIOS

This study is focused on investigate the effect of the inclusion of graphite oxide (GO) into a poly-lactide (PLA) matrix on the thermal, rheological and mechanical properties of the composite. The incorporation of GO fillers into PLA was carried out by means of an internal mixing chamber. Four formulations with GO concentrations of 0, 0.1, 1 and 3 wt% were prepared. The mixing temperature was 190°C. Thermal stability, thermo-mechanical behaviour and rheology of the composites were evaluated by means of TGA, DMA, Rotational Rheometry, respectively. It was found that degradation temperature (T<sub>5%</sub>), thermomechanical properties, and flux properties were modified with increasing amount of graphite oxide in the matrix.

#### SYNERGISTIC EFFECT OF 1D & 2D CARBON NANOSTRUCTURES FOR IMPROVEMENT OF IMPACT RESISTANCE OF EPOXY BASED NANOCOMPOSITES

JUVENTINO LÓPEZ BARROSO, CARLOS VELASCO SANTOS, ANA LAURA MARTÍNEZ HERNÁNDEZ, JOSÉ LUIS RIVERA ARMENTA

In this work, it was investigated the response of impact resistance properties of epoxy resin reinforced with both 1D and 2D carbon nanostructures. Hybrid nanocomposites were prepared with multi-walled carbon nanotubes (MWCNT) as 1D nano-reinforcement and graphene derivatives such as graphene oxide (GO) and reduced graphene oxide (RGO) as 2D nano-reinforcement. Nanocomposites with 1D, 2D, and blends of these nanomaterials were prepared in order to study the influence of adding different combinations of those nanomaterials over Izod impact resistance of nanocomposites. Additionally, the influence of oxygenated moieties created over MWCNT surface after two-step chemical modification (O-MWCNT) and inherent to GO and RGO was evaluated. The final mechanical properties of nanocomposites reflect an increment (138 %) on impact resistance in presence of two

nanostructures rich of oxygenated functional groups such as O-MWCNT and GO. This points not only to the formation of a better interface between 1D & 2D nanostructures and the matrix but also an improved dispersion state of the nano-reinforcements which was acquired due to the presence of these functional groups. Moreover, the SEM micrographs of fracture zones of the nanocomposites, show clearly the change on brittle nature of epoxy resin into a different toughness material by the addition of carbon nanostructures. Finally, based epoxy resin nanocomposites were synthesized by two different procedures in order to evaluate how the manufacturing method affects the final impact properties of nanocomposites.

#### INTERLAMINAR REINFORCEMENT OF GLASS FIBER/ EPOXY COMPOSITES WITH GRAPHENIC MATERIALS EXPANDED AND EXFOLIATED

LOURDES RAMOS GALICIA, CHRISTIAN DANIEL REYES VASQUEZ, JULIO A. RODRIGUEZ - GONZALEZ, CARLOS RUBIO-GONZALEZ, ANA LAURA MARTÍNEZ-HERNÁNDEZ, ARLOS VELASCO-SANTOS

Graphenic nanomaterials including those obtained by traditional Hummers method have resulted in good reinforcements in polymer composites. However, in spite of their properties, nanomaterials have could not to displace to micro reinforcements in laminated composites. Nevertheless one recent field in this context is focus to combine the properties of advanced fiber-reinforced polymers with nanomaterials in order to improve the interlaminar mechanical properties. Despite some carbon nanomaterials have improved this property in epoxy glass laminates, the dispersion and the disposition in major scale of these reinforcement materials limits their applications. This research is focus to obtain graphenic nanoplatelets by expansion and exfoliation, the method allows obtaining easily more quantities than other traditional. Graphenic nanoplatelets obtaining by this method after expansion and subsequently expansion and exfoliation are incorporated to glass fiber laminates. Also graphite and graphene materials obtaining by traditional hummers methods are incorporated to laminated polymers. Composites are fabricated using a spraying solvent procedure onto prepreg surface in each layer. Prepregs are grouped using the vacuum bag technique and then cured in an autoclave. The polymer composites are prepared to 0.05, 0.1 and 0.3 wt % of graphenic materials. The results of short beam strength show a clear improve in the interlaminar force with the graphenic nanoplatelets in comparison with the composite without interlaminar reinforcements and with the composites with graphene materials. Scanning Electron Microscopy show the differences in interlaminar separation with each graphenic reinforcements. Characterization of the graphenic materials incorporated to glass fiber/ epoxy laminates is also presented.

#### POLYMER FOAMS: INFLUENCE OF CROSSLINKING DENSITY ON THE MORPHOLOGY OF CELULAR COMPOSITE BASE ON LDPE/EVA/GTRP

LYNDON HUMBERTO, ISRAEL DURÓN SÁNCHEZ, JOEL AMADO SALAZAR ALVÁREZ, JOSÉ FRANCISCO HERNÁNDEZ GÁMEZ, FLORENTINO SORIANO CORRAL, MYRIAM LOZANO ESTRADA, RODRIGO CEDILLO GARCÍA

Crosslinking and foaming ratio of low density polyethylene (LDPE)/ethylene vinyl acetate (EVA)/ground tire rubber powder (GTRP) blends were studied. The influence of temperature and residence time on the elastic modulus of several compounds was analyzed using an oscillatory rheometer. First, all compounds were prepared by melt mixing in an internal mixer

(GW brabender) at a content of 3 wt-% of crosslinking agent, 5 wt-% of azodicarbonamide (ADC) and 10 wt-% of GTRP (200 mesh). As a crosslinking agent 2,5 dimethyl-2,5-di (tert-butylperoxy) hexyne-3 (Trigonox 145) by Akzo Novel was used. The results of oscillatory rheometer shown that higher temperatures and residence times increases crosslinking density and therefore stabilizes the cell morphology avoiding coalescence, such results were corroborated by optical microscopy and gel content. On the other hand, the presence of the GTRP increases the cellular density and decreases the average cell diameter through the nucleation process.

### **SYNTHESIS OF A LIGNIN-STYRENE-BUTYLACRYLATE COMPOSITE WITH PLASTIC WOOD APPLICATION**

MARIA GUADALUPE SANCHEZ

In the present work the synthesis of a copolymer from lignin - styrene - butylacrylate by mass free radical polymerization using benzoyl peroxide as the initiator was carried out. Experiments were carried out by varying the amount of lignin at 10 and 15%, the reaction time was 1.5 and 2 hours using a water bath at 85 ° C under constant magnetic stirring. Once the copolymer was obtained it was characterized by differential scanning calorimetry (DSC), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM). Additionally, hardness was measured using a Shore D durometer. The reaction between lignin, styrene and butylacrylate produces a material with a Shore D hardness 12.5, using 15% lignin with 1.5 h as reaction time. IR showed that the functional groups OH of lignin are those that mainly react with the styrene and through SEM it was detected that there is change in the morphology of the material with respect to the lignin. The composite has high thermal stability, which is evident in the thermograms obtained by DSC, this composite material has potential application in the manufacture of plastic wood.

### **Poster**

#### **COMP01-MULTILAYER COMPOSITE MATERIALS PRODUCED BY ROTOMOULDING**

ROBERTO CARLOS VÁZQUEZ FLETES, PEDRO ORTEGA GUDIÑO, FRANCISCO JAVIER MOSCOSO SANCHEZ, RUBEN GONZALEZ NUÑEZ

The multilayer composite materials (polymer-fiber / polymer-foam / polymer-virgin) was performed by rotational molding in a laboratory-scale biaxial rotational molding machine. The polymer that was used in all layers was a linear medium density polyethylene. For the composite material we used agave fiber as the natural fiber. Azodicarbonamide was used as a chemical blowing agent. The same amount of total weight was used for each layer. The density increased with fiber content while decreasing it with foaming agent concentration. This is observed in typical SEM micrographs of the materials produced. This factor is reflected in the flexural and impact properties. Another important factor was studied in this process, which is the measure of the air mold temperature that determines the cycle total for the realization of these type of materials.

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## COMP02-INFLUENCE OF NANOCLAY AND AGAVE FIBER ON THE MECHANICAL PROPERTIES OF POLYLACTIC ACID COMPOSITES

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ALAN SALVADOR MARTÍN DEL CAMPO-FLORES, JORGE RAMÓN ROBLEDO-ORTÍZ, MARTÍN RIGOBERTO ARELLANO-MARTINEZ, EDGAR JOSÉ LÓPEZ-NARANJO, AIDA ALEJANDRA PÉREZ-FONSECA

In this study, PLA-nanoclay/agave fiber hybrid composites were prepared in a twin-screw extruder with 30% of fiber and different clay contents of 3 and 5 wt%. Afterwards, these pellets were processed by injection molding to obtain samples for the evaluation of the effect fiber/nanoclay incorporation to PLA. The mechanical properties were evaluated by flexural, tensile and impact test. Although the samples were analyzed by XRD analysis in order to observe the fiber/nanoclay interaction with PLA. The mechanical tests results showed that addition of nanoclays slightly reduce the impact strength while using the combination nanoclay/agave fiber this property increases from 30 to 41 J/m. In tensile results, it was observed that the combination nanoclay/agave fiber increased the tensile modulus of PLA from 1561 to 2180 MPa (5% nanoclay/30% agave). By other side tensile strength results showed that, this property is reduced by the addition of both materials presenting more significant decreases due to agave fiber addition than for nanoclay; this behavior is attributed to the high content of agave used and the bad compatibility between PLA and natural fibers. Flexural strength values showed also decreases when nanoclay/agave is added, while flexural modulus increased from 3585 to 5486 MPa for PLA hybrid composites (5% nanoclay/30% agave).

## COMP03-SURFACE TREATMENT OF AGAVE FIBERS WITH MALEATED PLA AS COUPLING METHOD FOR PLA COMPOSITES

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MARTÍN ESTEBAN GONZÁLEZ LÓPEZ, ROBERTO JAVIER CASTAÑEDA FONG-CHOY, ALAN SALVADOR MARTÍN DEL CAMPO FLORES, RICARDO MANRÍQUEZ GONZÁLEZ, AIDA ALEJANDRA PÉREZ FONSECA, DENIS RODRIGUE, JORGE RAMÓN ROBLEDO ORTÍZ

In this study, agave fibers were surface treated in solution with maleated PLA (MAPLA) in order to improve interfacial adhesion in PLA composites. For this purpose, treated and untreated fiber composites were produced at 10, 20, 30 and 40 wt.% of fiber content and characterized in terms of density, morphology, mechanical properties (hardness, flexion and tension) and water sorption. <sup>1</sup>H-NMR analysis indicates that MAPLA was successfully prepared by reactive extrusion process and its further surface modification on agave fibers was confirmed by FTIR and SEM analyses. At low fiber contents (10 and 20 wt.%) the density of the composites decreased with the treatment since treated fiber density is lower than untreated fiber. However, at higher fiber content (30 and 40 wt.%) density increases in treated fiber composites as a result of improved compatibility which leads to less voids and interfacial gaps observed at SEM micrographs. Although the highest improvements of tensile strength (from 36.6 to 40.5 MPa) and modulus (from 1.08 to 1.22 GPa) were obtained for 40 wt.% fiber composites, improved interfacial adhesion also promoted slight increases at lower fiber contents and a similar trend was observed for hardness and flexural properties, confirming that surface treatment with MAPLA successfully improved compatibility. Finally, composites with treated fiber exhibited lower water sorption values (up to 13% lower at 40 wt. % fiber content) confirming better wettability of the fibers due to the treatment and suggesting that hydroxyl groups of the fibers were successfully esterified during the treatment.

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**COMP04-PHEMA HYDROGELS REINFORCED WITH PHA-PEG NANOGELS: NANOCOMPOSITES WITH IMPROVED MECHANICAL PROPERTIES**

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YADIRA CERDA, ARTURO ZIZUMBO, ANGEL LICEA, IVÁN ZAPATA

Hydrogels are crosslinked polymeric materials with great capacity of water absorption and therefore are soft materials with a wide range of applications, especially in the biomaterials arena. However, their poor mechanical properties are a major limitation. In the literature there are several strategies being tested to improve the mechanical properties of hydrogels. One is the addition of nanometric fillers (organic and inorganic) to reinforce their microstructures. Nanometric fillers may improve chemical, mechanical and thermal properties of fragile polymers, such as hydrogels. The aim of this work was to prepare nanocomposite hydrogels of crosslinked poly(2-hydroxyethyl methacrylate) (PHEMA) as matrix added with poly(n-hexyl acrylate)-core-poly(ethyleneglycol)-shell (PHA-PEG) nanogels of different sizes and PEG molecular weights. In the first step the PEG-PHA nanogels were prepared by a surfactant free emulsion polymerization method. The higher the PEG molecular weight used, the thicker the shell of the nanogels and also the lower the overall nanogels size. These new nanogel fillers were dispersed for the preparation of PHEMA hydrogels by a photochemical crosslinking reaction using ethyleneglycol dimethacrylate (EGDMA) as crosslinker. The nanogels impart PHEMA hydrogels improved mechanical properties in flexion and compression assays, and increased their thermal stability as compared with the hydrogel matrix without fillers.

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**COMP05-STUDY OF THE EFFECT OF THE ADDITION OF CHITOSAN AND POLY(LACTIC ACID) ON THE PHYSICOCHEMICAL PROPERTIES OF EXTRUDED POLYPROPYLENE FILMS**

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DORA EVELIA RODRÍGUEZ FÉLIX, LAUREN LUCERO LIZÁRRAGA LABORÍN, JESÚS MANUEL QUIROZ CASTILLO, MARÍA MÓNICA CASTILLO ORTEGA, JORGE ROMERO GARCÍA, TOMÁS JESÚS MADERA SANTANA

The mixture of natural and synthetic polymers is a simple and practical method of producing new materials with interesting properties and environmentally friendly. Films formed by blending two or more polymers usually have physicochemical properties different from those of the initial components. Polylactic acid (PLA) is the only polymer produced from natural resources at a large scale of over 140,000 tons per year. PLA can compete with non renewable petroleum based products; is biodegradable, compostable and recyclable. Chitosan is obtained of the chitin the second most abundant natural polysaccharide, after of cellulose; have interesting properties such as biocompatibility, biodegradability, non-toxicity and antimicrobial activity. On the other hand, polypropylene is one of the most widely used synthetic polymers due to its easy processing, excellent properties and low cost. In this work extruded films of polypropylene, poly(lactic acid) and chitosan were prepared. The effect of chitosan and poly(lactic acid) in the polypropylene matrix was analyzed as a function of thermal, mechanical and morphological properties using Polypropylene-graft-maleic anhydride as a compatibilizer and glycerol as a plasticizer. Keywords: polypropylene, biopolymers, extrusion

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**COMP06-SWELLING AND MORPHOLOGICAL BEHAVIOR OF NANOCOMPOSITE HYDROGELS BASED ON ALGINATE, POLYVINYLPIRROLIDONE AND CARBON NANOTUBES**

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MANUEL GUTIÉRREZ PORCHAS, DANIEL PUENTES CAMACHO, TERESA DEL CASTILLO CASTRO

The interest in development of polymeric hydrogels embedded with carbon nanotubes (CNTs) is growing rapidly owing to their useful applications in human health approaches such

as tissue engineering, actuators and drug delivery systems. CNTs have some outstanding properties; regular pore size structure, high electrical conductivity, electromechanical stability, well-defined one-dimension structure, low density, high specific surface area and high mechanical resistance. The inclusion of CNTs into hydrophilic polymeric networks allows obtaining nanocomposite hydrogels with superior properties compared with their individual counterparts. In this work, composite hydrogels were prepared by encapsulating multiwalled carbon nanotubes (MWCNTs) within a biocompatible hydrogel matrix of calcium alginate and polyvinylpyrrolidone in order to enhance the mechanical stability of the polymeric network. MWCNTs surface was modified by using an acidic HNO<sub>3</sub>/H<sub>2</sub>SO<sub>4</sub> treatment assisted with microwave irradiation to produce carboxylic groups, making them easier to disperse. The composite hydrogels were characterized by swelling kinetic measurements and scanning electron microscopy. These composite systems combine the mechanical and electrical properties of filler with the swelling capacity and molecular diffusivity associated to polymeric network, therefore they can be considered a potential stimuli-responsive platform for biomedical applications.

#### COMP07-COMPOSITES OF POLYPROPYLENE AND CELLULOSE FIBERS OF PAULOWNIA

MARCO ANTONIO ESTRADA RAMOS, JOSE MANUEL ROJAS GARCÍA, MARÍA DEL CARMEN DÍAZ NAVA

Currently, the research about new or improved polymeric composites using natural fibers such as coconut fibers and agave fibers is still in the state of the art to get enhanced properties but looking for lower weight materials. The present work aims in the production and evaluation of composites obtained from cellulose fibers of Paulownia (CFP) and a polymeric matrix of polypropylene (PP), included to validate their compatibility. 3-20 % by weight of CFP were investigated to elucidate the effect of the amount of CFP in PP/CFP composites using a maleic anhydride grafted polypropylene (MAPP). In agreement to literature, the results indicate that addition of MAPP in the PP/CFP composites improves the dispersion of the natural fibers in the matrix of PP. So, the increase of the amount of CFP in the composites yields: (i) both the tensile and flexural elastic moduli of the composites increase, (ii) the multiaxial impact resistance does not show significant change, (iii) the calorimetric analysis, determined by DSC, shows an improvement in the thermal stability of the composites; and (iv) the viscoelastic response, determined by DMA, shows that the thermal transitions of the amorphous and crystalline regions in the composites have some changes because it is assumed that the CFP works as a nucleating agent modifying the crystallinity of the composites.

#### COMP08-THERMAL AND MECHANICAL PROPERTIES OF DEGRADED TERNARY FILMS OF POLYETHYLENE/POLY(LACTIC-ACID)/CHITOSAN

LAUREN LIZÁRRAGA, DORA RODRÍGUEZ, JESÚS QUIROZ, JORGE ROMERO, JOSÉ ENCINAS

Nowadays polyethylene is a widely used material due to its dielectric properties, high durability, low cost, easy processing and good chemical resistance. Nevertheless, it has been caused environment problems because of the slow degradation process in the environment. The use of mixtures of synthetic and natural polymers have potential as an option to reduce the environmental problems caused by plastic waste, in this work were studied the effect of the accelerated degradation on the thermal stability and mechanical properties of ternary polymer films of polyethylene, poly(lactic-acid) (PLA) and chitosan. The films were prepared by the extrusion method with a composition of 70% polyethylene, 15%



chitosan, 15% PLA with and without polyethylene graft maleic anhydride as compatibilizer and were degraded on a QUV-se equipment at times of 50, 100, 150 and 200 hours. the films were characterized by TGA and DSC to study the thermal stability, also its mechanical properties were measure and the carbonyl index was obtained by FTIR.

#### COMP09- ROTATIONAL MOLDING OF POLYLACTIC ACID BIOCOMPOSITES BASED ON AGAVE AND COIR FIBERS

ERICK OMAR CISNEROS-LÓPEZ, AIDA ALEJANDRA PÉREZ-FONSECA, YOLANDA GONZÁLEZ-GARCÍA, DANIEL EDÉN RAMÍREZ-ARREOLA, RUBÉN GONZÁLEZ-NÚÑEZ, JORGE RAMÓN ROBLEDO-ORTÍZ

In this study, biocomposites of polylactic acid (PLA) reinforced with agave fibers (Agave tequilana Weber var. Azul) or coir fibers (Cocos nucifera) were produced by rotational molding. In particular, a simple dry blending technique was used to disperse the natural fibers in the biodegradable polymer matrix. Different fiber contents were used between 0 and 30% wt. The samples were characterized in terms of density, porosity, morphology and mechanical properties (tensile, flexion, hardness and impact). In general, it was possible to observe that low fiber contents (10% wt.) produced the best morphology and lower porosity, indicating that there is an optimum fiber content to get well-distributed fibers in the matrix, leading up to 24 and 26% increases on tensile modulus for agave and coir biocomposites, respectively compared to neat PLA. Tensile and flexural strength decreased with fiber content due to poor compatibility between the fibers and the matrix. In the case of impact strength, contrary to agave fibers, biocomposites with higher coir contents presented an increased impact strength (up to 8%) compared to PLA.

#### COMP10-EFFECT OF AGAVE FIBER ON THE MECHANICAL PROPERTIES OF PLA BIOCOMPOSITES USING FUSED DEPOSITION MODELING

VALERIA FIGUEROA VELARDE, YOLANDA GONZÁLEZ GARCÍA, LUIS CARLOS ROSALES RIVERA, JORGE RAMÓN ROBLEDO ORTÍZ

Among additive manufacturing technologies, fused deposition modeling (FDM) has appeared as a faster, cheaper and easier method for rapid prototyping. In FDM, a polymer filament is extruded layer by layer (X and Y axes) onto a movable plate (Z axis) until a tridimensional structure is obtained. Compared to former techniques, the processed figures are more precise produced with less waste products. This technique has been successfully applied in the development of prototypes for the biomedical and aerospace science and has increasing potential in different engineering fields. In the present work, biodegradable agave fibers (mesh 100 – 140) were used as a reinforcement material in a polylactic acid (PLA) matrix. Different weight percentage relation (0, 3, 5 and 10%) and deposition angles (45 and 90°) were tested in order to compare the fiber effect on the tensile properties t. The results showed that at high fiber contents, the mechanical properties decreased. The values for tensile stress ( $\sigma$ ) varied from 51.2 to 31.1 MPa, elongation percentage (%El) from 7.2 to 5.7% and modulus of elasticity (E) from 1084.1 to 852.2 MPa. Although deposition angle only affected the tensile stress and elongation percentage (%El), the maximum tensile properties were obtained for the deposition angle of 45°. Finally, tensile tests show minor differences between the 5 and 10% samples; while 0 and 3% fiber content showed a considerable difference on the elasticity modulus and elongation percentage.

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**COMP11-PROCESSING AND CHARACTERIZATION OF BIODEGRADABLE POLYMERIC COMPOSITES FORMULATED WITH AGAVE FIBER**

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JORGE INGA LAFEBRE, RUBÉN GONZÁLEZ NÚÑEZ, CARLOS JASSO GASTINEL

Biodegradable polymer composites were formulated with poly (lactic acid)/poly (butylene adipate-co-terephthalate) (PLA/PBAT) blends and agave fibers. For the composites, blends of 80/20 and 60/40 w/w of PLA/PBAT were used with 20 or 30 wt% of fiber on a polymer weight basis. Processing was done in a twin screw extruder, followed by injection molding to prepare the specimens for mechanical testing. For mechanical properties, as expected, tensile and flexural modulus increased with fiber content, while the values for the pure blends decreased with PBAT content. Nevertheless, for the composites, tensile and flexural strength suffered a slight decrease with fiber content and the increase in fiber or PBAT content, resulted in an increase in impact strength. Scanning electron microscopy (SEM) sample observations showed rigid fracture, denoting poor interaction between polymer blends and fiber. As shown by differential scanning calorimetry, fiber and PBAT promote a decrease in composite crystallinity. The increase in fiber-polymer blend interaction was also followed by the addition of a biodegradable coupling agent. The results show that the decrease in rigidity of PLA as matrix by the inclusion of PBAT, allowed an increase in elastic deformation and toughness, opening the field for tough biodegradable polymeric composites.

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**COMP12-BIMETALLIC CoO<sub>y</sub>-CuO<sub>x</sub> PARTICLES IN POLYFURAN FILMS, ELECTROMAGNETIC ABSORPTION AND ELECTRIC CONDUCTIVITY**

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MARÍA DEL ROSARIO MEJÍA CUERO, ELENA COLÍN OROZCO, GUILLERMO JESÚS CRUZ CRUZ, J. CUAHUTÉMOC PALACIOS GONZÁLEZ, LIDIA MARÍA GÓMEZ JIMÉNEZ, MARIBEL GONZÁLEZ TORRES, FRANCISCO GONZÁLEZ SALGADO, ROSARIO RAMÍREZ SEGUNDO, FERNANDO GABRIEL FLORES NAVA, MARÍA GUADALUPE OLAYO GONZÁLEZ

The influence of CoO<sub>y</sub>-CuO<sub>x</sub> bimetallic particles on the physical, chemical and electrical properties of polyfuran (PFu) films is analyzed in this work to be potentially applied in the absorption of electromagnetic energy in flexible solar panels. The syntheses of particles was by sol-gel, obtained with spherical profile, mean size in the 60-800 nm interval and O/Cu and O/Co atomic ratios in the 0.30-0.39 and 0.3-0.49 interval, respectively. The synthesis of PFu was by glow discharge plasmas at 13.56 MHz, 0.65-0.8 mbar and 150 W. The films have thickness in the 9-90 micrometer interval with a linear tendency as a function of the power of synthesis. Chemical analyses of the polymeric films were performed by IR and XPS spectroscopies relating the formation energy of the chemical groups with C1s and O1s atomic orbital energies. The results showed C-C=C-, C-O, C=O and other groups as ≈C≈, which are conjugated fragments of broken furan rings. However, the analysis indicated that almost all initial furan molecules joined to construct PFu structures. The combination of polymer films and metallic particles was by cryo-lyophilization with ethanol to produce pores in the polymer where the particles are housed. The hybrid films absorbed electromagnetic energy mainly in the UV wavelength interval, although it was observed an additive absorption of both, polymeric and metallic fractions.

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**COMP13-EFFECT OF THE PRESENCE OF SILICON NANOPARTICLES IN THE COEFFICIENT OF LINEAR THERMAL EXPANSION OF MAIZE**

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MAURICIO JIMÉNEZ-CALVO, MIGUEL CHÁVEZ-GUTIÉRREZ, ALICIA REYES-SAMILPA, ÁNGEL RAMÓN HERNÁNDEZ-MARTÍNEZ

Nanocomposite materials have great advantages compared to other plastics and composites, because when the properties of the polymers with a nano-sized reinforcement are combined there is an improvement in their specific properties. In the present work, maize starch was used as the matrix of the nanocomposite, because of its biodegradability and low costs. Nanocomposite specimens were obtained by the extrusion-injection method. For material extrusion DSM Xplore MC-5 equipment was used at 90 °C in the three heating zones for 3 minutes at 100 RPM. To obtain specimens, the DSM Xplore IM5.5 injector was used. Previously, corn starch was wetted with 20% by weight water for 24 hours, 10% by weight glycerol was used as plasticizer. Different amount of silica nanoparticles (Aerosil-vs Nis-silice) as filler were added to the maize starch base structure, these being 2.5, 5 and 7.5% by weight. Thermomechanical analysis was performed to determine the linear coefficient of thermal expansion and glass transition temperature in a TMA Q400, TA Instruments equipment under the standard ASTM E831-14 to evaluate dimensional changes of the test specimens due to exposure to different temperatures. Mean values of thermal expansion coefficient were 0.0598  $\mu\text{m}/\text{mm } ^\circ\text{C}$  for pure corn starch based plastic, and 0.0580, 0.1104 and 0.2196  $\mu\text{m}/\text{mm } ^\circ\text{C}$  for 2.5%, 5% and 7.5% silica nanoparticles concentration on the corn starch base matrix. Glass transition temperature mean values were 55 °C for pure corn starch based plastic, and 51 °C, 45 °C and 39 °C for 2.5%, 5% and 7.5% silica nanoparticles concentrations, respectively.

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**COMP14-RHEOLOGICAL DETERMINATION OF AGAVE FIBER AND HIGH DENSITY POLYETHYLENE COMPOSITES**

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RICARDO NAVARRO, MÓNICA FLORES, MERCY DZUL, IMELDA SAUCEDO, ERIC GUIBAL

Compound materials with polymeric matrix and natural fiber reinforcements have become of great interest for the industry and the academy because of their ecological potential and their economic advantages. The formulation of these materials requires a proper evaluation of their flowing behavior before they can be produced. As such, the objective of the present investigation is to present the rheological determination of the Agave Fiber and High Density Polyethylene (HDPE) composites. Said behavior has been analyzed by preparing materials with four different sizes of fibers at three different percentages. The measurements were made with a Capillary Rheometer, as well as applying the Power Law (Ostwald de Waele) to adjust the obtained data, thus obtaining the equations that defines the behavior of the materials. It was found that, at low fiber proportions the size of the fiber has a greater influence in the viscosity, while, at higher proportions of fiber, the effect of the size is almost imperceptible.

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**COMP15-ENCAPSULATION OF A THIOPHOSPHINIC ACID EXTRACTANT WITH ALGINATE-CARBOXYMETHYL CELLULOSE FOR PALLADIUM RECOVERY  
IMMOBILIZATION OF THIOPHOSPHINIC ACID EXTRACTANTS IN ALGINATE CAPSULES FOR Pb(II)  
EXTRACTION**

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RICARDO NAVARRO, MÓNICA FLORES, MERCY DZUL, IMELDA SAUCEDO, ERIC GUIBAL

Novel impregnated alginate beads were manufactured by encapsulating Cyanex 302 (bis 2,2,4-trimethylpentyl monothiophosphinic acid) with alginate-carboxymethyl cellulose. Alginate is a linear polysaccharide composed of variable amounts of D-manuronic acid and L-guluronic acid, which can be cross-linked by using calcium ions, whereas carboxymethyl cellulose consists of linear chains containing (1→4)-linked glucopyranose residues. For the fabrication of the beads, first an emulsion was prepared with different ratios of Cyanex 302, carboxymethyl cellulose, CaCl<sub>2</sub>, gelatin and water. The emulsion was then dropwise added into different sodium alginate solutions to form a shell film. Three kind of alginate was used (low, medium and high viscosity, at different concentrations). Finally, the obtained capsules were cured in the 0.5 M CaCl<sub>2</sub> solution. The resultant materials are mononuclear capsules constituted by a core (matrix type with very small extractant drops) covered by a thin calcium alginate film. The morphology of the capsules was examined with an optical microscope and mechanical resistance tests were performed by agitation of the beads in HCl solutions. Selected capsules were tested for Pd(II) extraction from HCl solutions. The HCl concentration influence on the extraction efficiency was investigated. The sorption isotherms were obtained and the Langmuir equation parameters were calculated. Sorption kinetics studies were also performed and the intraparticle diffusion coefficients were determined. The extraction efficiency and the stability of beads diminish with the HCl concentration. The increase in extractant loading enhances metal sorption capacity at equilibrium but slows kinetics of metal sorption.

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**COMP16-IMMOBILIZATION OF THIOPHOSPHINIC ACID EXTRACTANTS IN ALGINATE CAPSULES  
FOR Pb(II) EXTRACTION**

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IMELDA SAUCEDO, JANETTE ALBA, RICARDO NAVARRO, THIERRY VINCENT, ERIC GUIBAL

As an alternative to conventional metal extraction processes, new extractant impregnated resins (EIRs) were synthesized by the immobilization of thiophosphinic acid extractants in alginate capsules using two different procedures: matrix-type immobilization and mononuclear encapsulation. In the first case, the extractant was immobilized in the matrix of the polymer by emulsification and subsequent ionotropic gelation of alginate in the presence of calcium ions. In the case of mononuclear capsules, the extractant is immobilized as a mononuclear liquid core coated by a thin layer of alginate. The capsules were prepared with Cyanex 301 (bis 2,2,4-trimethylpentyl dithiophosphinic acid) and Cyanex 302 (bis 2,2,4-trimethylpentyl monothiophosphinic acid) and the extractant concentration in the organic phase of the capsules was varied. Selected capsules were tested for Pb(II) sorption from HCl aqueous solutions. The effect of HCl concentration was investigated before determining the sorption isotherms and evaluating the contribution of diffusion mechanisms in the control of uptake kinetics. Finally, lead desorption from loaded sorbents was carried out. The extractants are efficient for recovering Pb(II) in weakly acid solutions (i.e., 0.1 M HCl): Cyanex 301 is less sensitive to pH than Cyanex 302. The amount of extractant immobilized in mononuclear capsules is lower than in matrix-type beads; this leads to lower sorption capacities but slightly better mass transfer properties. The balance between the advantages and drawbacks of the different systems makes more promising matrix-type capsules. The desorption of Pb(II) is possible using 1 M HNO<sub>3</sub> solutions: metal ions were completely desorbed.

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#### COMP17-COMPOSITES BASED ON ELASTOMERS AND CHICKEN FEATHERS

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CAROLINA CASTILLO-CASTILLO, BEATRIZ ADRIANA SALAZAR-CRUZ, MARIA YOLANDA CHAVEZ-CINCO, JOSE LUIS RIVERA-ARMENTA

The use of waste material to prepare composites materials has get increasing interest, due it became in an option to obtain materials with improved physicochemical properties. The styrene-butadiene elastomers are copolymers with wide spectrum of applications since adhesives, plastic modifiers, asphalt modifiers, among others. Chicken feather main component is queratin, which has good thermal and mechanical stability. In present work, a composites based on chicken feather and a styrene-butadiene elastomer were prepared by means melt mixing. Thermal properties were evaluated by means differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and dynamic mechanical analysis (DMA), with the aim to evaluate the effect of elastomers structure (radial and lineal). The processing conditions, chicken feathers amount and compatibilizer were evaluated on composites properties.

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#### COMP18-PREPARATION AND CHARACTERIZATION OF COMPATIBILIZED PA6/LMDPE BLENDS BY ROTATIONAL MOLDING

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RUBÉN GONZÁLEZ-NÚÑEZ, FERNANDO RUIZ, ROSA GABRIELA LOPEZ-GONZALEZ NUNEZ, DENIS RODRIGUE

Blends of polyamide 6 (PA6) and linear medium density polyethylene (LMDPE) at different volume ratios with and without a compatibilizer (Surlyn 9020) were prepared by rotational molding. The blends were previously produced by two different methods: i) dry blending using a high shear mixer and ii) melt blending with a twin-screw extruder. The prepared blends were characterized in terms of morphology, mechanical (tensile, flexion and impact) and thermal (DSC) properties.

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#### COMP19-PREPARATION AND CHARACTERIZATION OF PLA/LMDPE BLENDS BY ROTATIONAL MOLDING

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EDUARDO RUIZ SILVA, LUIS CARLOS ROSALES RIVERA, JORGE RAMÓN ROBLEDO ORTÍZ, DENIS RODRIGUE, RUBÉN GONZÁLEZ NÚÑEZ

Blends of poly(lactic acid) (PLA) and linear medium density polyethylene (LMDPE) at different weight ratios were prepared by rotational molding using a laboratory scale biaxial machine. The blends were previously produced by two different methods: i) dry blending using a high shear mixer and ii) melt blending with a twin-screw extruder. The prepared blends were characterized in terms of morphology, mechanical (tensile, flexion and impact) and thermal (DSC) properties. The morphological results showed a clear incompatibility between the two polymers in which the domains of the minor phase have well defined spherical shapes and a broad size distribution. On the other hand, the results of the mechanical properties depend of the blend preparation method. In general, blends prepared with melt blending presented a slight increase in flexural and tensile properties compared with those blends prepared via dry blending. For impact (charpy) mechanical properties, it was seen an increase until a maximum value was attained, after which the value decreased.

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**COMP20-DEVELOPMENT OF A METHODOLOGY FOR CHEMICALLY MODIFY MALE PLANTAIN STARCH (MUSA PARADISIACA L.) AND IT'S INCORPORATION INTO POLYMERIC MATRICES**

MONTSERRAT CONTRERAS HERNANDEZ, JOSÉ MANUEL ROJAS GARCÍA, GEORGINA MONTES DE OCA RAMÍREZ

Current high consumption of synthetic thermoplastics is attributed to both the versatility of manufacture a lot of different products of daily life and their excellent processability. However, at the end of their useful life these materials are not very well disposed yielding bad environmental impact. Starch is one the most useful natural polymer because it offers low cost, high availability and high biodegradability. It has as disadvantages its very sensitive behavior to hydrolyze by water absorption and it has low degradation temperature. Therefore, its processability is compromised to get biodegradable polymeric materials having good mechanical properties compared to those synthetic polymeric materials. In Mexico, the variety of banana named as plantain or *Musa paradisiaca* L. is harvesting the most part of the year, so it represents a potential source of starch because in its no mature stage contains starch up to 70 % by weight on a dry basis. In this study, three methodologies were developed to modify this type of starch by chemical approach to improve thermal stability and decreasing its hydrophilic nature. So the modified starch is more compatible to synthetic polymer. Finally, blends of modified starch and polylactic acid (PLA) were prepared to elucidate their mechanical performance, and the usability as packaging material.

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**COMP21-DEVELOPMENT OF A METHODOLOGY FOR THE ELABORATION OF A POLYMERIC COMPOSITE MATERIAL WITH AGAVE CUPREATA FIBERS FOR THE MANUFACTURE OF SCHOOL FURNITURE**

PATRICIA NAYELY HERNANDEZ ACUÑA, JOSÉ MANUEL ROJAS GARCÍA, GEORGINA MONTES DE OCA RAMÍREZ, ADRIANA LÓPEZ LEÓN, ITALO MARTÍNEZ PONCE, MONTSERRAT CONTRERAS HERNANDEZ, JOSÉ ANTONIO ÁVILA ALFARO

Nowadays, better and lighter materials are required in the market, but also having excellent mechanical performance and environmental sustainability. So, many studies are focused on those issues by getting new natural fibers-based polymer composites. In this work we study the feasibility of produce scholar furnitures made by using a polymer composite material of a synthetic polymer such as polypropylene, and a natural fiber from *Agave cupreata* culture got as a by-product from the production of mezcal liquor in Guerrero State in Mexico. As a prior stage to use natural fibers in order to prepare the new composites, we required to use different processes such as washing, grinding, sieving and chemical functionalization of *Agave cupreata* fibers by using dicumyl peroxide or trimethoxysilane as coupling agent. Several experiments were made by using a ZK25T SD15 Dr. Collin co-rotatory twin-screw extruder to prepare the polymer composites having 20 wt.% of fiber, and three different particle size of natural fibers were used. Then, the composites were injected by using a Demag-Sumitomo Systec-100 injection molding machine. Finally, the mechanical performance was evaluated by using the tensile test, flexural test, and multiaxial impact test. In agreement to literature, modified *Agave cupreata* fibers showed lower thermal degradation in 200-250 °C range than the neat natural fibers. In addition, the new composites using the modified fibers showed better tensile, flexural and multiaxial impact resistances than the neat natural fibers. Therefore, these composites exhibit good mechanical properties suitable to use them as a raw material to manufacture school furnitures.

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### COMP22-POLYAMINE-MESOCELLULAR SILICA FOAMS: SYNTHESIS AND CHARACTERIZATION

HECTOR MELENDEZ-ORTIZ, BERTHA PUENTE-URBINA, GRISELDA CASTRUITA-DE LEÓN, ESMERALDA SAUCEDO-SALAZAR, LUIS ALFONSO GARCÍA-CERDA

Poly(vinylamine) (PVAm) derivatives have attracted attention for many applications including coatings, water purification, or gas membrane separation due to their affinity for many supports, pH responsiveness, metal binding capacity and polyelectrolyte complexation. However, PVAm cannot be prepared from vinylamine (VAm) due to its low stability and fast conversion into the corresponding imine through tautomeric equilibrium. On the other hand, the development of hybrid materials such as those based on mesoporous silicas and polymers have received much attention due to they have replaced a lot of polymeric materials in different applications. These materials combine the properties of their components giving as result composites with unique properties Here, we report the covalent grafting of PVAm onto mesocellular silica foams (MCF) via free radical polymerization. Firstly, MCF was functionalized with vinyltrimethoxysilane (VTMS) in order to obtain a silica with vinyl groups onto its surface. Then, the previously obtained MCF-VTMS silica was reacted with vinylformamide (NVF) through the free radicals generated from the thermal decomposition of initiator. The hybrid material MCF-PNVF was hydrolyzed in order to obtain the PVAm-modified silica. The hybrid materials were characterized by X-ray diffraction, infrared spectroscopy, and thermogravimetric analysis.

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### COMP23-TRIBOLOGICAL STUDY OF NATURAL FIBER FILLER FOR IMPROVEMENT LIFE-CYCLE HDPE COMPOSITES

CAROLINA HERNÁNDEZ-NAVARRO, GABRIELA MENDOZA-LEAL, ERNESTO GARCÍA-BUSTOS, JAIME NAVARRETE-DAMIÁN, LUIS ALEJANDRO ALCARAZ-CARACHEO, FRANCISCO JAVIER GARCÍA-RODRÍGUEZ, JOSÉ FRANCISCO LOUVIER-HERNÁNDEZ

There is a wide variety of different natural fibers which can be used as reinforcement or fillers, in fact, natural fibers are potential replacers for inorganic fibres such as glass or aramid fibres in automotive components such as door panels. Moreover, polymers are used increasingly for tribologically stressed components, whereby metallic bearings, gear wheels or sliding elements are replaced by plastic components. The fact that plastics are often rather economical to produce, especially in very complex shapes with good functional integration, explains this trend. In this work, a basic study is reported of composites of high density polyethylene (HDPE) filled with peanut shell fibers (PE/PE) and with nutshell (PE/NS), prepared by injection molding technique in different proportions. The composites were characterized chemically and structurally by Fourier transform infrared spectroscopy (FTIR) and X-Ray Diffraction (XRD). The influence of the fiber content of the composites on tensile, and wear properties of the composites have been evaluated. The tribological essays were carry out by the reciprocating sliding wear test with a 10 N load, employing a 10 mm diameter Al<sub>2</sub>O<sub>3</sub> ball as counter-body. Results show a shift of about 3 degrees in 2Theta when peanut is added to the polymer. Also, Young Modulus shows a slight increase of about 5 % as peanut content is increased up to 10 % in weight, while the tensile strength reduces in a similar fashion, showing a transition from ductile to brittle as the natural fiber is added.

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## Invited Presentations

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### THE ROLE OF SHAPE MEMORY IN SELF-HEALING POLYMERS

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MAREK URBAN

Among particularly impressive properties of stimuli-responsive materials that recently received significant attention are materials with the ability to self-repair. Recent studies have utilized a variety of non-covalent and covalent chemistries that resulted in the development of self-healing polymers. The main challenge is to maintain properties, while embedding self-healing components. This lecture will outline recent advances in self-healing of polymers as well as the role of catalysts in self-healing of polymer networks. Covalent incorporation of chemically modified poly and monosaccharides into crosslinked polymers offers another possibility that takes advantage of free radical stability. If properly designed, self-repairing can be achieved in the presence of atmospheric carbon dioxide and water. Unlike plants, these networks require no photo-initiated reactions, thus are capable of repairs in darkness under atmospheric conditions and lead to the formation of carbonate and urethane linkages. The last portion of this lecture will discuss recent developments in encoding shape memory components manifested by entropic energy increase as well as heterogeneities into polymer networks that result in self-healing.

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### PHASE CHANGE TRANSFORMATIONS WITH DYNAMICALLY ADDRESSABLE POLYMER GELS

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PETER BOUL, PETER JAROWSKI, CARL THAEMLITZ

Dynamic polymers assembled through hemiaminal and aminal functionalities reversibly fragment upon binding to trivalent metals. Gels produced with these dynamic polymers are broken down to liquids after the addition of metal salts. Nuclear magnetic resonance (NMR) spectroscopy studies of intermediates and density functional theory (DFT) calculations reveal that the presence of these metals causes shifts in the energetic landscape of the intermediates in the condensation pathway to render stable non-equilibrium products. These non-equilibrium products are liquids that remain stable liquids at room temperature but convert to gel upon heating. Thermal activation causes the fragmented ligands to transform catalytically into closed-ring products which are macroscopically observable as new gels with distinct physical properties. The interplay between equilibrium and non-equilibrium gels and liquids and the ligands responsible for these transformations has been observed rheologically to offer controlled gel times dictated by the thermodynamics and kinetics of the system. This constitutionally dynamic macromolecular system offers the possibility of harnessing an equilibrium / non-equilibrium system in tandem with its inherent self-healing and triggered release properties.

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### STOPPING FIRE AND REDUCING GAS PERMEABILITY USING AQUEOUS POLYELECTROLYTE COMPLEX-BASED NANOCOATINGS

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JAIME GRUNLAN

In an effort to impart flame retardant behavior to textiles and super gas barrier to plastic film, using few processing steps, a nanocoating deposited from a water-soluble polyelectrolyte complex (PEC) was developed. In the case of flame retardant fabric, the coating is



comprised of polyethylenimine and poly(sodium phosphate). This treatment imparts self-extinguishing behavior to cotton fabric, during vertical flame testing, in just two coating steps. Adding an aqueous melamine solution to the coating procedure renders nylon-cotton blends self-extinguishing. These blended textiles are widely used for apparel and upholstery in furniture and transportation. More recently, a PEC coating was developed for polyester-cotton, which passes vertical flame testing after five standard washes or 8 hours in boiling water. These environmentally-benign flame retardant treatments provide an alternative to bromine and antimony-based systems that carry significant health and environmental concerns. In regard to gas barrier, a 2  $\mu\text{m}$  coating prepared with an aqueous polyelectrolyte complex containing PEI and polyacrylic acid, reduced the oxygen transmission rate of a 127  $\mu\text{m}$  PET film by two orders of magnitude. This simple high barrier coating, that imparts commodity polymer film with high barrier, could be useful for various types of food pharmaceutical and electronics packaging applications. For more information, please visit: <http://nanocomposites.tamu.edu>

### THE BAIER CURVE AFTER 50 YEARS: PROGRESS IN ANTIFOULING AND FOULING RELEASE COATINGS

CHRISTOPHER OBER, AMANDA LEONARDI

Functionalized block copolymers allow for systematic control of surface chemistry and structure in environmentally benign antifouling coatings. Block copolymer structure can be used to control surface chemistry and morphology, mechanical properties, as well as temporal response to environmental conditions. Dynamic and chemically ambiguous surfaces which resist marine fouling are made by incorporating polar, non-polar, and chemically active components into a block copolymer design. Block copolymers produced using anionic polymerization can be modified via efficient chemistries such as thiol-ene "click" chemistry to create architecturally diverse materials with a wide range of properties. As an example, sequence controlled peptide chemistry has been utilized to precisely control chemical structure. These surfaces limit settlement behavior of a diverse range of marine organisms by employing protein-resistant components such as poly(ethylene glycol) (PEG) to deter settlement, low surface-energy materials including siloxanes and fluoro-oligomers to reduce adhesion strength, and targeted structures such as antioxidants to inhibit both settlement and biological adhesive curing processes by marine organisms. Surface chemical composition and structure has been investigated ex situ using X-ray spectroscopy techniques including X-ray photoelectron spectroscopy (XPS) and near-edge X-ray fine structure (NEXAFS) spectroscopy. Additionally, surface chemical rearrangement can be observed in real time using in situ time-resolved bubble contact angle measurements. Coatings were evaluated as antifouling coatings by studies of settlement and adhesion of marine algae, diatoms, and barnacles, which each have significantly different mechanisms of attachment. Correlation of this biological response to surface properties and copolymer design allows for rational design of antifouling coatings based on chemical structure.

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Oral

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**THE ROLE OF AIR PLASMA AND SILANE SURFACE TREATMENTS OF ARAMID FIBERS ON THE SYNTHESIS OF ZNO NANOPARTICLES ONTO THEIR SURFACE**

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LUIS ANGEL ORTEGA FLORES, GRACIELA MORALES, FLORENTINO SORIANO CORRAL,  
GUSTAVO SORIA ARGÜELLO, ROSA MARTHA JIMÉNEZ BARRERA, JOSÉ DE JESÚS KU HERRERA

Aramid fibers are structural fibers extensively used for armor protection and as polymer reinforcement due to their outstanding mechanical properties. However, these fibers are highly susceptible to UV degradation and exhibit poor adhesion with most polymers. A strategy recently explored to overcome such drawbacks involves coating the fibers with ZnO nanoparticles. Even though this strategy has shown adhesion improvements between the ZnO-coated fibers and the polymer matrix, further enhancements through functionalization of the fibers prior ZnO synthesis has not been investigated. Given this motivation, in this work aramid fibers are treated by air plasma and/or surface-modified with a silane-coupling agent prior to ZnO synthesis in order to promote chemical interaction. The synthesis of ZnO onto the fibers involves two sequential growing process; ultrasound and subsequently microwave heating using methanol as suspending medium. The morphology of the ZnO-modified fibers was characterized by scanning electron microscopy and atomic force microscopy. Physicochemical analysis of ZnO-modified aramid fibers was carried out by Raman and Fourier transform infrared spectroscopy. Results of this work evidenced that surface modification of aramid fibers by using air plasma and/or a silane coupling agent plays a dominant role on the homogeneous coverage of the fiber with ZnO with respect to the pristine counterparts. The increased surface roughness upon ZnO synthesis onto the fibers can provide enhanced adhesion with polymer matrices. The ZnO-modified fibers developed in this work are excellent candidates to manufacture structural polymer composites with enhanced UV protection and mechanical properties.

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**MULTIFUNCTIONAL SHAPE MEMORY NANOCOMPOSITES**

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LAURA PEPONI, VALENTINA SESSINI, MARINA P. ARRIETA

Shape-memory materials are smart materials able to change reversibly their shape in response to an external stimulus, such temperature, humidity, etc. In order to offer shape-memory behaviors, polymers present permanent domains formed by chemically or physically cross-linked structures, and switching domains able to respond to the external stimulus. When the external stimulus is the temperature, depending on the amorphous or crystalline nature of the switching phase, the transition temperature can be provided either by its glass transition or its melting temperature. So, in this work, we present different systems based on biodegradable and/or biocompatible polymers reinforced with bio-nanoparticles such as cellulose nanocrystals, hydroxyapatite and cloisite with shape memory behavior.

## Poster

**SMART01-DEVELOPMENT OF A NEW CLASS OF STIMULI-RESPONSIVE POLYMERIC FLOCCULANTS IN COMBINATION WITH ELECTROCOAGULATION PROCESSES FOR REMOVAL OF HEAVY METALS AND ANTIBIOTICS FROM CONTAMINATED WATER**

MONICA GUADALUPE AGUILAR AGUIRRE, JUAN ANTONIO PIÑA ACOSTA, MOISES SALAZAR GASTELUM, ROSA MARÍA FELIX NAVARRO, ANGEL LICEA CLAVERÍE

Nowadays, the presence of heavy metals in wastewater is one of the most important pollution problems, due to its high toxicity and its cumulative properties. In addition, contamination with drugs (classified as emerging pollutants) is considerable and increasing; therefore actions are required to treat them because of the potential risk to human beings and aquatic living organisms, in addition to the necessity to increase water sources for domestic use. The present work focuses on the development of new generation polymeric flocculants, meaning biocompatible polymers with response to stimuli (temperature or pH) for flocculation of contaminated water, in combination with an electrocoagulation process. The methods chosen are efficient, economical and environmentally friendly, well suited for the treatment of water contaminated with drugs and heavy metals, such as ciprofloxacin and cadmium, respectively. Chitosan based polymers grafted with poly(N-vinylcaprolactam) (PNVCL), grafted with polyacrylic acid (PAAc), and doubly grafted (PNVCL + PAAc) were synthesized, characterized and evaluated as flocculants. The optimal dosage for turbidity removal was 0.01 mg mL<sup>-1</sup> at 60 min and at a pH interval from 3 to 9. Chitosan containing PNVCL grafts exhibited a phase transition temperature of 41 °C. Water contaminated with ciprofloxacin, cadmium and, an additional turbidity contaminant (kaolinite), were treated by three processes: 1st-flocculation with polymers, 2nd-electrocoagulation without polymers and 3rd-sequential treatment, by which flocculation with polymers was carried out in the first instance and then the clarified water was subsequently treated by electrocoagulation. The most effective process was the sequential treatment with high ratio of removal of turbidity, cadmium and ciprofloxacin (> 99%).

**SMART02-KINETIC STUDY OF THE COPOLYMERIZATION OF 2-(DIETHYLAMINE) ETHYL METHACRYLATE WITH PEG-METHACRYLATE**

MARIA PRISCILA QUIÑONEZ-ANGULO, IVÁN ZAPATA-GONZÁLEZ, ÁNGEL LICEA-CLAVERÍE

Due to the temperature and pH sensibility exhibited by poly(2-(diethylamine) ethyl methacrylate) (PDEAEM), several works have focused in the development of nanocarriers of drugs containing DEAEM; some of them incorporate poly(ethyleneglycol) (PEG) to improve the transport of the drug and to provide the nanocarrier with stealth properties. In order to improve the performance of the nanocarrier in the bloodstream and the interaction with the drug, it is necessary to know its copolymer composition and microstructure. However, the kinetic information available in the literature to predict these characteristics for DEAEM polymers containing PEG is scarce. The aim of this work is the kinetic analysis of the system DEAEM/PEG-methacrylate (PEGMA) and the determination of reactivity ratios based on the terminal model compared with other methods. The solution free-radical copolymerization of

DEAEM/PEGMA using 4,4'-Azobis(4-cyanovaleric acid) (ACVA) as initiator, was carried out in ethanol at 70°C. The copolymer composition and the overall and partial conversion have been obtained by 1H-NMR measurements, varying the feed composition in 10 mol% steps. Results show that the polymerization rate of both monomers is similar, the copolymer composition is close to the feed composition and it looks like there is an azeotropic composition, which needs to be determined. The values of copolymerization parameters are now being consolidated by several different methods of determination.

#### SMART03-A NOVEL GREEN METHOD FOR THE SYNTHESIS OF POLYPYRROLE/ ALGINATE/ CARBON NANOTUBE COMPOSITES

REINA VIANEY QUEVEDO ROBLES, TERESA DEL CASTILLO CASTRO, MARÍA MÓNICA CASTILLO  
ORTEGA

Conducting polymers are frequently applied for the development of new multifunctional nanomaterials[1]. Polypyrrole (PPy) is particularly interesting due to its biocompatibility, good electrical conductivity and stability in atmospheric conditions, which has promoted its use in biomedical applications[2]. However, the brittle nature and limited processing capabilities of PPy bring about the need for blending it with other materials[3]. In this work, PPy was synthesized in aqueous solution using a combination of chemical oxidative polymerization and microemulsion technique. The method involves the use of H<sub>2</sub>O<sub>2</sub>, an environmentally friendly oxidant, and sodium dodecyl sulfate (SDS), an anionic surfactant. Moreover, polymerizations were carried out in the presence of alginate (ALG), pristine carbon nanotubes (pCNTs) and functionalized-carbon nanotubes (fCNTs) for improving the mechanic and electrical properties of the new composites. The composites were characterized by electric conductivity measurements, IR-FT, UV-VIS and cyclic voltammetry. The presence of ALG and pCNTs improved the mass yield and the electroactive properties of PPy obtained in micellar media with H<sub>2</sub>O<sub>2</sub> oxidant. This green-derived polymer composite can be considered a suitable platform for some biomedical applications. [1] K. Leonavicius, A. Langmuir 27 (2011) 10970-10976. [2] S. Ravichandran, Langmuir 28 (2012) 13380-13386. [3] S. Sahoo, S. Express Polymer Letters 6 (2012) 965-974.

#### SMART04-EFFECT OF GRAPHENE AND CARBON NANOFIBERS ON THE THERMAL SHRINKAGE BEHAVIOR OF LIQUID-CRYSTALLINE ELASTOMER NANOCOMPOSITES

ROSA JULIA RODRÍGUEZ-GONZÁLEZ, HIRAM BARUCK ARIGUZNAGA-CASTILLO, LETICIA  
LARIOS-LÓPEZ

Liquid-crystalline elastomer (LCE) nanocomposites doped with 0.15, 0.45, 0.75 and 1.05 wt% of graphene or carbon nanofibers (CNF) were prepared, and the effect of the carbon nanostructures on the thermal shrinkage behavior was evaluated. Nanostructures were characterized by RAMAN Spectroscopy and XRD. Uniaxial stretching and photopolymerization processes were used in order to prepare monodomain LCE films. Thermotropic liquid-crystalline behavior of the LCE nanocomposites was studied by DSC, POM and XRD. Results revealed that both type of carbon nanostructures induce a decreasing of the temperature of the thermal transitions; and the biggest change (up to 23°C) was observed in the elastomer with the highest concentration of CNF. Furthermore, thermal shrinkage analysis showed good thermal-responses in both systems. The higher shrinkage ratio (around 50%) was observed in nanocomposites with graphene, being similar to the thermo-contraction reached by the LCE without nanostructures. In contrast,

nanocomposites with CNF showed lower percentages of contraction, ranged from 46 to 26%, depending on the concentration of CNF. These results indicate a certain relationship between the phase transition temperature and the shrinkage behavior of the LCE nanocomposites. RAMAN spectroscopy and optical microscopy of nanocomposites with the lower concentration (0.15%) of nanostructures showed that CNF were better dispersed into the elastomers than graphene. Moreover, micrographs showed a good alignment of CNF induced by the uniaxial stretching process; and also that they were embedded into the polymer elastic matrix. This work was supported by the CONACYT, México (Project CB-258195).

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**SMART05-THERMAL AND LIGHT-INDUCED DEFORMATIONS OF LIQUID- CRYSTALLINE ELASTOMERS CONTAINING AZOBENZENE MOITIES**

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LETICIA LARIOS-LÓPEZ, EDUARDO JOEL LÓPEZ-TORRES, ROSA JULIA RODRÍGUEZ-GONZÁLEZ

Main-chain liquid-crystalline azo-containing elastomers (azo-LCE) were synthesized via a two-stage method. In the first stage a thiol-acrylate Michael addition reaction was used, obtaining aggregates LC in polydomains. In order to align the domains, in a second stage a uniaxial stress was applied, followed by a photo-initiated or thermal-initiated crosslinking reaction. The optical anisotropy in monodomain films was confirmed by measuring the transmittance of a probe light through crossed polarizers as a function of the rotation angle. Thermal and light-induced behaviors were investigated in the aligned samples. DSC results indicated that both the isotropic and glass transition temperatures decrease as the content of the azocompound in the LCE increases. Upon heating, elastomers exhibited contraction percentages around 50%, showing the highest values in those LCE having 1mol% of azocompound. Light-induced deformation of LCE at room temperature showed a slight shrinkage and/or bending distortion in the films under irradiation with 405nm light, proving that these elastomer are photo-responsive materials.

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**SMART06-MECHANICAL AND TRIBOLOGICAL CHARACTERIZATION OF POLYETHYLENE/MAPE/CARBON NANOFIBER COMPOSITES PREPARED BY ROTATIONAL MOLDING**

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ZENEN ZEPEDA RODRIGUEZ, MARTÍN ARELLANO MARTÍNEZ, RUBÉN GONZÁLEZ NÚÑEZ, EMILIO CRUZ BARBA, ERNESTO GARCÍA BUSTOS, MILTON OSWALDO VÁZQUEZ LEPE

In this work, we measured properties and characterized composites with and without addition of maleic anhydride grafted polyethylene (MAPE) into carbon nanofibers (CNFs) in a lineal medium density polyethylene (LMDPE) as matrix. The carbon nanofibers threated with MAPE (M-CNFs) was obtained by oxygen cold plasma treatment to increase hydroxyl, carboxyl and ether groups on CNFs surface. The obtained plasma functionalized CNFs (p-CNFs) was immersed in xylene-MAPE solution. Subsequently M-CNFs was homogenized and dispersed in LMDPE by dry blending and processed by rotational molding. The mechanical properties such as tensile, flexure and impact resistances were performed according to ASTM D790-03, ASTM D638-03 and ASTM D6110-04. Whereas, the wear coefficient, micro hardness and scratch resistance, were studied by wall cratering, with a reciprocating tribometer and using nanoindentation respectively. The glass transition, melt and degradation temperature was analyzed by DSC. FTIR, RAMAN and XPS techniques was used to study the chemical environment and structural default induced by functionalization of M-CNFs. While the

morphology nanocomposites were observed by SEM. The mechanical, tribological, thermal properties and morphology was modified due to the addition of M-CNFs in the matrix, this behavior is related to the matrix-fiber interface adhesion promoted by functional groups in MAPE, which results in strength and heat transfer to the stiffness and high thermal resistance CNFs.

#### SMART07-BIODEGRADABLE POLYURETHANES FUNCTIONALIZED WITH COUMARIN AND REINFORCED WITH SILICA FOR COATIN APPLICATIONS

DANIEL LÓPEZ, CÁSTOR SALGADO, MARINA PATRICIA ARRIETA, LAURA PEIONI, MARTA FERNÁNDEZ-GARCÍA

The aim of this work is the synthesis and characterization of coumarin-based nanocomposites for application in coatings, capable of self-repair by photochemical cycloaddition reactions. For this, linear polyurethanes (PUs) based on hexamethylene diisocyanate (HDI), coumarin diol (CD) (5 mol%) and polycaprolactone with two different molecular weights ( $M_n = 530$  and  $2000$  g / mol) as matrices have been synthesized. As reinforcement, unfunctionalized and functionalized silica (1 and 3% by weight) ( $SiO_2$ ) nanoparticles were incorporated. PUs were obtained by formation of a CD-HDI prepolymer for further chain growth with PCL and HDI. In this manner, high molecular weight polymers were obtained. The silica nano particles were functionalized with a coumarin derivative in the presence of (3-aminopropyl) triethoxysilane (APTES) and dispersed in the polymer matrix by sonication. The polymer matrices were structurally characterized by NMR spectroscopy, FTIR and size exclusion chromatography (GPC). The good dispersion of the nanocomposites was analyzed by FE-SEM. The thermal stability of the systems has been studied by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Tensile stress tests have been performed to determine Young's modulus, stress, and elongation at break of samples. The kinetics of photo-crosslinking and photo-excision of the samples were evaluated by irradiating the saamples at 365 and 254 nm, respectively. It has been observed a higher yield in the nano-compounds reinforced with coumarin-functionalized silica than in those of unmodified silica. Also, a greater interaction of silica with the hard segments of the PU for samples with PCL530 was observed, causing a decrease in the degree of cross-linking. While the PCL2000-based samples admit larger amounts of nano-silica as reinforcement, favoring higher degrees of photo-dimerization. The incorporation of nanofiller increases the thermal stability of the nanocomposites; the materials being reinforced with functionalized silica having the highest degradation temperatures. With irradiation the Young's modulus increases as well as the thermal stability of the nano-compounds, due to cross-linking. Therefore, such materials may be employed as coatings

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## Invited Presentation

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### EFFICIENT SIMULATION OF THE FULL MOLECULAR WEIGHT DISTRIBUTION IN LOW DENSITY POLYETHYLENE AUTOCLAVE REACTORS

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ENRIQUE SALDIVAR-GUERRA, BRUNO LÓPEZ-CARPY, IVÁN ZAPATA-GONZÁLEZ, CÉSAR GARCÍA-FRANCO

The production of low density polyethylene via free-radical polymerization at high pressure is still a topic of academic and industrial high interest. The highly branched structure of LDPE and its molecular weight distribution (MWD) confer this material its unique rheological properties which are not matched by polyethylenes synthesized by any other polymerization technique. This has led to significant efforts dedicated by several research groups to the mathematical modeling of the MWD and branching distributions (BD) of LDPE generated in these processes. Recently, different mathematical techniques, deterministic and stochastic, have been discussed for the description of the full MWD and BD, but they are usually very demanding in terms of computing power, resulting in very long simulation times. This is further complicated when processes involving multizone autoclave reactors are to be modeled. In this paper we present a relatively simple and very efficient technique for the modeling of the full MWD multizone autoclave reactors for the production of LDPE operating at steady state. Several simulation examples will be presented and discussed.

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### ENERGY SATURATION AS AN ALTERNATIVE GLASS TRANSITION MECHANISM

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ISAAC SANCHEZ

Treating monomer-monomer energetics of a tangent sphere chain model as a square well potential in a quasi-chemical (QC) approximation yields configurational energy saturation prior to reaching zero temperature. At saturation, a balance exists between repulsive and attractive forces that stabilize the polymer model liquid density, which thereafter becomes effectively temperature independent. These low temperature, force stabilized states are identified as ideal glass states. Near complete energy saturation at the glass temperature  $T_g$  appears to obtain in 23 of 25 polymers analyzed. Among 14 polymers for which fragility indices have been measured, a good correlation between fragility and saturation degree was found; fragile polymers tend to be less saturated. The repulsion-attraction force balance raises the question as to whether it defines a unique repulsive state. To address this question, electron density was used to measure the strength of repulsive forces; global electron densities were determined at  $T_g$  and averaged 0.61 mol/cc for 15 polymers that contain oxygen and 0.53 mol/cc for 7 hydrocarbon polymers. This experimental observation suggests that  $T_g$  is a near isoelectronic state for certain polymer types. Using experimental internal pressures measured at  $T_g$ , number of electrons associated with a QC monomer was determined. These theoretically calculated electron monomer densities strongly correlate with  $T_g$ . In comparing 2 polymer liquids of similar structure at the same temperature, one expects the polymer with the higher electron density to have the higher  $T_g$ .

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**ON THE HOMOGENEITY OF POLYMER NETWORKS SYNTHESIZED BY FRP AND RAFT  
COPOLYMERIZATION OF VINYL/DIVINYL MONOMERS IN SUPERCRITICAL CARBON DIOXIDE**

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EDUARDO VIVALDO-LIMA

In this contribution, the differences in homogeneity of polymer networks synthesized by conventional free radical (FRP) and reversible addition-fragmentation chain transfer (RAFT) copolymerization of 2-hydroxyethylene methacrylate (HEMA) and ethylene glycol dimethacrylate (EGDMA) in supercritical carbon dioxide (scCO<sub>2</sub>), using Krytox 157 FSL as the dispersing agent, are quantitatively addressed. The combined results of differential scanning calorimetry (DSC), swelling index (SI), infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) measurements show that the hydrogels synthesized by FRP and RAFT are significantly different, with apparently less heterogeneity present in the materials synthesized by RAFT copolymerization. A ratio of experimental ( $M_{cexp}$ ) to theoretical ( $M_{ctheo}$ ) molecular weight between crosslinks, recently proposed by our group, was used as a quantitative tool to assess the degree of heterogeneity of a polymer network. The findings presented in this presentation have been already reported in the literature (Processes, 5, 26, 2017).

Oral

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**ON THE PULSATING FLOW OF A BIOLOGICAL FLUID: BLOOD WITH CHOLESTEROL.  
PERTURBATION AND ANALYTICAL SOLUTIONS**

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EDTSON EMILIO HERRERA-VALENCIA, MAYRA LUZ SANCHEZ VILLA, VICENCIO FAUSTO CALDERAS, LUIS MEDINA TORRES, DOMINGA ORTIZ BAUTISTA, FERNANDO ALDO VARELA, CESAR SAUL VELASCO

In this work, analytical predictions of the rectilinear flow of a non-Newtonian liquid under a combined pulsating, time-dependent pressure gradient and a random longitudinal vibration flow is analyzed. The fluctuating force component of the combined pressure gradient and inertial oscillating mechanism is assumed to be of small amplitude and can be adequately represented by a weakly stochastic process, for which a steady-homogeneous perturbation scheme is suggested, in terms of a small parameter. The rheology and flow is analyzed with the BMP constitutive equation. In the regimen of linear viscoelasticity the complex fluidity display three mean peaks associated to the cholesterol content in the sample. In the regimen of large deformations (non-linear viscoelasticity) the system is analyzed using a regular perturbation scheme. To zeroth order in the small parameter epsilon, the fluidity function can be separated in two contributions associated to the slip conditions and the non-Newtonian behavior. To first order, the fluidity is related to the monotony of the wall stress derivative of the volumetric flow to zeroth order. To second order, the fluidity function is associated to the convexity through the second wall stress derivative of the volumetric flow pounded by the square of the wall stress. The effect of the slip mechanisms is to decrease the fluidity enhancement. According to the BMP model, the fluidity enhancement can be separated in two contributions (pulsatile and oscillating mechanism), which depend on the square of the amplitude of the oscillations, amplitude of the perturbations, the Reynolds and Weissenberg numbers and, the characteristic dimensional numbers relationship to the shear-thinning and non-Newtonian mechanisms (Thixotropy) to the material properties in the system.



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## POWER LAW RELAXATION (PLR) ANALYSIS OF "ORIGIN OF THE STRAIN HARDENING IN BRANCHED METALLOCENE POLYETHYLENES"

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RUBÉN HORACIO LÓPEZ BAÑUELOS, RUBEN SALDIVAR GUERRERO, JAVIER GUDIÑO RIVERA, CESAR A. GARCÍA FRANCO

Molecular architecture is of paramount importance in the dynamics and properties of polyolefins. The presence of short chain branching (as a consequence of comonomer incorporation) affects the magnitude of the plateau modulus, thus the magnitude of the entanglement molecular mass. Crystallization and morphology as well as mechanical and physical properties also exhibit a dependence on the presence, type and amount of comonomer incorporation. On the other hand long chain branching (LCB) also exhibits a remarkable effect on both, linear and non-linear viscoelastic behavior of molten polyolefins (shear thinning and strain thickening). In practice, the level of LCB incorporation is quite small to prevent "the point of diminishing returns" concerning physical and mechanical properties. As a consequence of these small amounts of LCB, traditional characterization techniques such as size exclusion chromatography, scanning calorimetry and light scattering find limited application in the characterization of LCB. On the other hand rheology exhibits unique sensibility to the presence of small amount of LCB. Based on Costeaux et. al. interesting work and data, on a series of long chained branched polyethylenes in which the branching level was varied on a systematic way, we used the Power Law Relaxation (PLR) approach for the characterization of Costeaux materials. We will demonstrate that the parameters of PLR namely  $S$  and  $n$  correlate with the amount and type of branching underlining their potential as characterization tools.

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## OPTIMAL POLYMER GRADE TRANSITION POLICIES USING A DERIVATIVE-FREE OPTIMIZATION APPROACH

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MIGUEL ANGEL GUTIERREZ-LIMON, ANTONIO FLORES-TLACUAHUAC, ENRIQUE SALDIVAR-GUERRA

During start-up, shut-down or normal operation, optimal dynamic transitions among products are normally required to achieve an operation target in the best possible way. Such a target can be related to desired values of processing variables such as temperature, composition, flowrates, etc. Therefore, in these sort of problems the aim consists in computing the time domain values of the control variables  $u(t)$  such that the system response  $y(t)$  attains a desired value embedded in an objective function  $\Omega(y, u)$  which can be either maximized or minimized. Optimal product transitions can be systematically calculated by setting the product transition problem as a dynamic optimization problem. Several optimization techniques for handling the solution of dynamic optimization problems assume that the gradient of the objective function and related constraints are somehow available. On the other hand, there are some practical optimization problems where derivatives are not available or are not reliable making impossible or undesirable to use gradient-based optimization techniques. Derivative-free optimization (DFO) algorithms have been proposed to deal with optimization problems with no gradient information. In this work we propose a methodology for the efficient on-line control of optimal grade transition policies in polymerization reactors without deploying a dynamic mathematical model of the polymerization systems. All what is required to compute the optimal grade transition policies is a black-box simulation model. In this case we use the Aspen Dynamics simulation

environment as our black-box system. Using only input-output information and a DFO code all the grade transition policies have been successfully computed. The methodology has been applied to the polystyrene and high density polyethylene manufacturing processes.

#### RAFT POLYMERIZATION MODELING: THE CASE OF THE MISSING REACTION STEP THEORY

IVAN ZAPATA-GONZALEZ, ENRIQUE SALDIVAR-GUERRA, ANGEL LICEA-CLAVERIE

The reversible addition-fragmentation chain transfer (RAFT) polymerization via dithiobenzoates with regeneration of the 2-arm intermediates in the kinetic mechanism, proposed by Buback and Vanna in the Missing Step theory, was modeled for the first time via the Reduced Stiffness by Quasi-Steady State Approximation (RSQSSA) methodology. The methyl acrylate (MA) and the styrene (Sty) polymerization were analyzed by a comparison of the theoretical solution with the experimental data collected in the literature. The Quasi-Steady State was valid for the 3- arm intermediates only when the kinetic rate constant of regeneration of these species was close or above to the values of the addition rate coefficient. For both MA and Sty polymerizations, the simulations demonstrated a good agreement between the model solutions and experimental values, in the evolution of conversion with time,  $M_n$  and  $M_w$ . Also, the full-molecular weight distribution predicted by the model indicated a very good match with the experimental data. A symmetric bivariate population of 2-arm intermediates was obtained, resulting in a high probability to find species with the same chain length in both arms. Similarly, the results showed that the 3-arm intermediates with the same chain length in each arm could be mostly generated, but in this case an asymmetric multivariate population was found. The findings presented in this work have been already reported in the literature (Chem. Eng. J., 2017, 326, 1242).

#### AQUEOUS SOLUTIONS OF DEEP EUTECTIC SOLVENTS FOR PREPARATION OF CO-CONTINUOUS POROUS CARBONS VIA SPINODAL DECOMPOSITION PROCESSES

FRANCISCO DEL MONTE, MARIA LUISA FERRER, MARI CONCEPCION GUTIERREZ, MARIA DE LAS NIEVES LOPEZ-SALAS, RAFAEL JIMENEZ-RIOBOO, ELENA POSADA

Spinodal decomposition (SD) processes have proved effective for the synthesis of macro- and mesoporous materials. Despite the theoretical aspects of SD processes are well understood, finding the proper experimental conditions - both the components as well as the ratio in which they have to be combined - to attain co-continuous structures is a non-predictable and quite tedious process, typically based on trial and error. The challenge is finding a "tool" capable to predict the suitability of a particular starting solution to undergo SD processes. Here in, we used aqueous solutions of deep eutectic solvents (DESs) for the preparation via SD of co-continuous porous carbons, the morphologies of which ranged from spinodal- to aggregates-of-particle-like just depending on dilution. Despite the starting DES/H<sub>2</sub>O binary was macroscopically homogeneous, Brillouin spectroscopy revealed the occurrence of certain nanostructural rearrangements within a dilution range that coincided with that used for preparation of carbons with morphologies transitioning from spinodal- to aggregates-of-particle-like.

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## DEVELOPMENT OF ACRYLONITRILE TERPOLYMERS AND THEIR EVALUATION AS CARBON FIBERS PRECURSORS

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DANIEL ALCALÁ SÁNCHEZ, JUAN CARLOS TAPIA PICAZO

In the process of producing carbon fibers (CFs), the thermal stabilization of polyacrylonitrile (PAN) fibers is a most important step. The thermal behavior of PAN fibers is governed by their physicochemical characteristics. A detailed analysis of the effect of control parameters on the polymerization and spinning process of FC precursor polymers leads to high performance FC with minimum structural imperfections. In this work, two types of precursor terpolymers from PAN have been synthesized with different chemical characteristics. The effect of two types of comonomers (vinyl acetate and methyl acrylate) on the spinning process, mechanical properties and thermal behavior of PAN fibers obtained from these terpolymers has been investigated. FT-IR and optical microscopy have been used to analyze structural changes of PAN fibers in the thermal stabilization process. It has been observed that the chemical composition of the precursor polymers affect the physicochemical characteristics of PAN fibers and their behavior in the thermal stabilization process. That is, the presence of different types of comonomer affects the mechanical properties of PAN fibers, as well as the initiation temperatures of the cyclization, dehydrogenation and oxidation reactions.

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## POLYMERIZATION REACTOR MONITORING BY ON-LINE RAMAN SPECTROMETRY

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RAMIRO INFANTE, LUIS ALBERTO VILLARREAL, JOSÉ ALEJANDRO DÍAZ, RICARDO LÓPEZ, ESTHER TREVIÑO, BEATRIZ REYES, MAYKY OLIVOS

Monitoring polymerization reactors by in-line RAMAN spectroscopy is a recent development which applied by itself, allows a fine control of the operation and that in conjunction with feedback control techniques (field of future studies in this case), opens the possibility to the synthesis of polymers of highly controlled properties such as conversion, length of chain and microstructure (chemical composition distribution). Some polymer reaction engineering laboratories begin to implement online spectroscopy techniques for the monitoring and control of reactors, and this trend will increase in the near future. In order to compare results obtained in this study, we selected chemical systems of practical/commercial interest that form the current benchmark for in-line optic spectrometry. Additionally, the myrcene monomer was selected due to its natural and renewable origin with potential to be produced on a large scale for the synthesis of bio-elastomers. The application of portable Raman spectrometry was also studied and results are compared with the in-line high resolution Raman spectrometer.

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## NEW COMPUTATIONAL TOOLS TO AID THE DESIGN OF PROFILE EXTRUSION DIES

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ANANTH RAJKUMAR, LUÍS FERRÁS, CÉLIO FERNANDES, OLGA CARNEIRO, ALBERTO SACRAMENTO, JOÃO NÓBREGA

The forming flexibility of thermoplastic polymers, induced a large range of applications for extruded profiles. However, the usual methodologies employed in industry to design profile extrusion dies, based on experimental trial-and-error procedures, comprise high resources consumption, which significantly increase their cost and time to market. In this work we present and assess experimentally a new design methodology for complex profile extrusion dies with the aid of OpenFOAM computational library.

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**ELUCIDATING MECHANISMS IN BARE AND SURFACE MODIFIED PICKERING SiO<sub>2</sub>-SUPPORTED STYRENE EMULSION POLYMERIZATION KINETICS: INTERPRETING THE SILANOL/PHENYL  $\pi$ -INTERACTIONS BY RAMAN SPECTROSCOPY**

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B FOUCONNIER, FRANCISCO LÓPEZ-SERRANO

Some mechanistic events, occurring in the Pickering styrene emulsion polymerization, using a SiO<sub>2</sub> dispersion, are evaluated. Three levels of a water soluble initiator polymerizations were performed at 80°C. The emulsion polymer content was ca. 15% with conversions close to 90%. Measuring conversion and particle size, the particle density was estimated for bare and surface modified, with hexadecyltrimethylammonium bromide (CTAB), SiO<sub>2</sub> particles. Then, the average number of radicals per particle was inferred, resulting in a pseudo-bulk type polymerization. Even though, bare SiO<sub>2</sub> nanoparticles do not participate in the nucleation mechanism they, along with the initiator, promote an enhanced oligomer coagulation. On the other hand, the CTAB modified SiO<sub>2</sub> nanoparticles do participate in the nucleation and coagulation mechanisms, yielding more stable and smaller poorly covered polymer particles. The experimentation, along with the inferred average particle radicals, allowed untangling some events such as: particle nucleation, radical entry to particles, coagulation and vitreous and Trommsdorff effects. On the other hand, a different internal reference band in Raman spectroscopy, to monitor SiO<sub>2</sub>-supported styrene Pickering emulsion polymerization kinetics, is also presented. Raman spectroscopy allowed detecting silanol/styrene-aromatic ring interactions yielding a non linear relationship, against conversion, in the 1630/1000 wave number ratio, commonly used for monitoring styrene polymerizations. The detection of silanol/aromatic-ring interactions allowed supporting the proposal for the continuous nucleation during Pickering polymerization, this was realized without requiring a more sophisticated analysis such as NMR.

Poster

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**ENG01-CONTROL OF COMPOSITION IN REACTIONS OF COPOLYMERIZATION ANIONIC AND NMP<sub>co</sub> USING MATHEMATICAL MODELS THAT EMPLOY OPEN-LOOP CONTROL**

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JAIME GONZÁLEZ VILLA, ENRIQUE SALDÍVAR GUERRA, RAMON DÍAZ DE LEÓN GÓMEZ, HÉCTOR RICARDO LÓPEZ GONZÁLEZ

In this work, we use mathematical models (based on the well-known polymerization kinetics of anionic polymerization and NMP) that employ open-loop control for get feeding trajectories optimal of one of the monomers for the synthesis of a copolymer of controlled composition. The feeding trajectories optimal were experimentally verified in anionic copolymerizations and NMP<sub>co</sub>. By way of example, the manner in which the work for the case of anionic copolymerization was developed is given below. For the case of anionic copolymerizations we worked with  $\beta$ -myrcene (MYR) and 4-methylstyrene (4MES) as a pair of comonomers; first we carry out homopolymerization reactions of each monomer to determine its propagations coefficients ( $k_p$ ), then copolymerizations with different initial ratios of feed of these monomers were carried out with the purpose of determine its reactivity ratios ( $r$ ) using of the terminal model copolymerization. Subsequently, we use the mathematical model (using the kinetic information determined previously, i.e.  $k_p$ 's and  $r$ 's) for get feeding trajectories optimal of  $\beta$ -myrcene, and we verified experimentally this optimal trajectory of feeding. The copolymer was characterized GPC, and RMN (of proton and

carbon 13) for determine to determine its composition and microstructure. The results show that a copolymer of MYR and 4MES of controlled composition was synthesized.

#### **ENG02-KINETIC APPROXIMATION OF THE RAFT COPOLYMERIZATION OF STYRENE-GLYCIDYL METHACRYLATE WITH DIFFERENT INITIATION SYSTEMS AND TEMPERATURE**

NORMA GARCÍA NAVARRO, JUAN JOSÉ BENVENUTA TAPIA, JOSÉ ALFREDO TENORIO LÓPEZ, EDUARDO VIVALDO LIMA, ENRIQUE SALDÍVAR GUERRA

Bulk copolymerization via RAFT of styrene with glycidyl methacrylate at different feed ratios ( $f_{GMA} = 0.1-0.6$ ) was performed in the presence of allyl tritiocarbonate as a RAFT transfer agent with Azobisisobutylnitrile, 1,10 Azobis-(cyclohexanecarbonitrile) and 1,1-di(tert-butylperoxy)-cyclohexane as initiators over a wide temperature range (90-120 °C), similar to those used under industrial conditions. In order to synthesize a number of well-defined S-GMA copolymers useful in various applications as compatibilizers and chain extenders. The total reaction time was 3 to 4 hours, reaching conversions of 80 to 95%. The copolymers were characterized by NMR and GPC. The copolymerization proceeded in a first order controlled way according to the monomer concentration, and the polydispersities of the copolymers were relatively narrow to high conversions in all cases ( $<1.4$ ). The reactivity of the system was determined by the extended Kelen-Tudos method:  $r_S = 0.4$  and  $r_{GMA} = 0.6$ . With a kinetic model of RAFT copolymerization the values of the kinetic constants of the copolymerization system:  $k_r$  and  $k_{raft}$  were approximated. The model allowed to calculate the conversion, monomeric composition and made use of the method of moments to determine  $M_n$  y  $M_w$ . Due at high conversions presents gel effect, the free volume parameters were determined for the kinetic constants of the propagation and termination stages. The UWAUS programs were used for optimization, and DDASSL to solve the system of differential equations. The results showed a better fit at the lower temperature and with the trigonox initiator.

#### **ENG03-MODELING OF ATOM TRANSFER RADICAL COPOLYMERIZATION USING ARGET PROCESS. THE PSEUDO-HOMOPOLYMERIZATION APPROACH AND THE MOMENTS METHOD**

IVAN ZAPATA-GONZALEZ, JESUS RUIZ-VILLEGAS, ANGEL LICEA-CLAVERIE

In the last two decades, Reversible-Deactivated Radical Polymerization (RDRP) has been one of the most developed techniques in the polymer engineering, being the Atom Transfer Radical Polymerization (ATRP) the most widely employed. The benefits of ATRP are: flexibility, ability to synthesize polymers with specific and often complex architectures and controlled structural properties, such as narrow molecular weight distributions (MWDs). Recently, Activators ReGenerated by Electron Transfer (ARGET) method has emerged as a way that uses low levels of catalysts (ppm) in the polymerization, which has been very important in order to synthesize medical devices, products for food and also for industrial scaling up. The prediction of the full-MWD, copolymer composition and microstructural conformation of the copolymer produced in ARGET ATRP is transcendental to estimate the final properties. However, to solve the mathematical system, which involves a large scale and stiffness, is a challenge in the field of Polymer Reaction Engineering. In this work, we present the development of two mathematical models in order to predict the  $M_n$ ,  $M_w$ , dispersity, polymerization rate, and the full-MWD. The Moment method has been used estimate the kinetic rate constants via a fitting with the experimental data, obtained in the literature. The other model, Pseudo-Homopolymerization approach, is used to predict the partial and the full-MWD. The results are in agreement with the experimental data presented in the synthesis of poly[(butyl methacrylate)-co-(butyl acrylate)].

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**ENG04-VISCOELASTIC STUDY OF WATER-SOLUBLE ASSOCIATING MULTIBLOCK  
COPOLYMERS OBTAINED VIA RAFT POLYMERIZATION**

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AMERICA ANABEL ISLAS-SANCHEZ, ENRIQUE JAVIER JIMENEZ-REGALADO, CLAUDE ST THOMAS

Herein, we report the synthesis and rheological evaluation of different water soluble associating polymers. It worth noting that water-soluble hydrophobically associating polymers have gained in interest in the last year due to their unique rheological properties in an aqueous solution and the stability in dispersion media as well as their applications in a large technologies areas such as: cosmetics, enhanced oil recovery, coatings, paints etc. These polymers are constituted with a long hydrosoluble chain usually polyacrylamide and a hydrophobic segments formed through derivative of acrylamide which are inserted to the polymeric chains. In an aqueous solution, the hydrophobic moiety tend to associate and lead to inter o intramolecular interactions. Previous report presented the preparation of PAM-co-DHAM via micelar polymerization. This investigation pretends to synthetize multiblock copolymers (tri, pent, hepta or nonablock) with 1 to 4 hydrophobic block. The chain extension by incorporation of novel hydrosoluble or hydrophobic block confirms the RAFT functionality of the polymers. Polymers from macroagent toward nonablock copolymers were characterized by NMR and DLS for determining their structure and the molecular weight of each polymers. Furthermore, rheological study was carried out a different concentration of polymers. The results exhibit the incorporation of each block to the polymer final and viscosity of polymers increases from macroagent to nonablock.

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**ENG05-INJECTION MOLD CYCLE TIME REDUCTION BY A SIMULATION ANALYSIS USING  
CIRCULAR AND SQUARE CROSS SECTIONS IN THE COOLING SYSTEM.**

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JONATHAN SALVADOR LÓPEZ LÓPEZ, JESÚS ENRIQUE RAMÍREZ MORALES, FRANCISCO JAVIER CERVANTES VALLEJO, KARLA CAMARILLO GÓMEZ, JOSÉ FRANCISCO LOUVIER HERNÁNDEZ

Design of cooling channels in an injection mold is crucial to obtain a good quality molded part in the shortest cycle time. Using software simulation, four different cooling channels design are compared for a non-planar HDPE part. The first two designs (type I) include circular and square cross-section straight channels, while the other two are circular and square cross-section non-straight channels (type II), which follow the path along the non-planar part at a constant distance. Cavity mold to cooling channel distance is 16 mm. Diameter of circular cooling channels is 8 mm, and side size for square cooling channels is 6.283 mm in order to have the same surface area value for both. Results show that type II channels reduce significantly the cooling time about 25 %, and a more uniform heat flux distribution. Comparison among circular, square and rectangular channel design for type II, shows no significant difference. Simulation was done using Moldex3D.

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**ENG06-RING-OPENING POLYMERIZATION OF THE L-LACTIDE USING BISMUTH COMPOUNDS AS  
CATALYSTS**

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MARÍA ORTIZ, JOSÉ JIMÉNEZ, JOSÉ BÁEZ, GERARDO GONZÁLEZ

In this work, a joint computational and experimental study for the ring-opening polymerization (ROP) of L-lactide (L-LA) using citrate, subsalicylate and acetate of bismuth as catalysts is presented. The initiator of the reaction was 1-octanol and the reaction temperature was set up to 170 °C. We performed DFT calculations at the SMD[D3-PBE0/LANL2DZ]pd,6-31G(d)] level for proposing the reaction mechanism in the initiation for

all these catalysts. The experimental and computational results showed an excellent agreement. The bismuth acetate is the most active catalyst in the presence or absence of initiator. Computationally, the lowest energy barrier was found for this catalyst and experimentally high conversions and moderate number average molecular weights ( $M_n$ ) were observed. On the other hand, bismuth subsalicylate was the second more active catalyst but this yielded a larger conversion and high molecular weights when using it without the alcohol. Finally, bismuth citrate is poorly active with or without alcohol to polymerize the L-LA.

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#### ENG07-STUDY OF THE LINEAR COEFFICIENT OF THERMAL EXPANSION OF HIGH DENSITY POLYETHYLENE MATRIX COMPOSITE MATERIALS REINFORCED WITH AGAVE BAGASSE

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FERNANDO PÉREZ, AXEL RUIZ, MAGDALENO CABALLERO, MIGUEL CHÁVEZ

In this research, the influence of the agave bagasse fibers on the linear coefficient of thermal expansion of high density polyethylene matrix composites was studied. The fibers were treated with NaOH, and they were used at three different concentrations: 5, 7.5, and 10% by weight.

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#### ENG08-APPLICATION OF COMPUTATIONAL-EVOLUTIONARY TECHNIQUES FOR THE OPTIMIZATION OF THE PLASTIC INJECTION PROCESS.

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CLAUDIA GABRIELA ANGUIANO, JESÚS ZAVALA GUTIÉRREZ, VÍCTOR ALFONSO ALCÁNTAR CAMARENA, GUILLERMO RANGEL SANCHEZ, RICARDO FLORES MEDINA

This work presents a method of optimization of plastic injection process, for the control of quality variables. A radial artificial neural network is used to model the process, later heuristic techniques are used to evaluate the volumetric contraction of plastic parts. Two optimization strategies are used: genetic algorithms (GA) and differential evolution. The technique of differential evolution according to the results shown, is appropriate to our particular case of analysis.

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#### ENG09-MECHANICAL CHARACTERIZATION OF STYRENE - ACRYLONITRILE (SAN) COPOLYMER OBTAINED BY NANOEMULSION POLYMERIZATION USING THE PIT METHOD

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RODRIGO GUERRERO BRAVO, ABRAHAM GABRIEL ALVARADO MENDOZA, ROSAURA HERNÁNDEZ MONTELONGO, LOURDES ADRIANA PÉREZ CARRILLO, CESAR A. REYNOSO GARCÍA, JOSÉ NIEVES CARRILLO CASTILLO, MARTIN RABELERO VELASCO

The styrene-acrylonitrile copolymer (SAN) is one of the most important at industrial-level by the wide range of applications, such as impact modifiers and to improve the mechanical properties. In this work, the synthesis of the SAN copolymer is reported by using an alternative low energy emulsification method: phase inversion temperature (PIT). A great advantage of this method is that the copolymerization reactions were carried out at room temperature using a polyethoxylated nonionic surfactant and a pair-redox system as the initiator. To obtain a broad spectrum of mechanical properties, different mass ratios of styrene-



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acrylonitrile were prepared. The synthesis produced stable latexes with 90% conversions and particle diameters smaller than 100 nm. Differential scanning calorimetry and infrared spectroscopy were used to confirm the formation of the copolymer and stress tests were performed on the various copolymers prepared to determine their mechanical properties, obtaining a broad spectrum thereof, depending on the composition.



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Poster

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**GT01-POLYPYRROLE COATED CELLULOSE ACETATE MEMBRANES AND THEIR  
POTENTIAL APPLICATION IN METAL RECOVERY**

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DIEGO HERNANDEZ

Cellulose acetate membranes made by electro-polishing technique (controlled variables) and coated with polypyrrole (PPy) in situ synthesis. Were characterized and used to remove gold complexes. The membranes were characterized by SEM, EDS, electrical conductivity, FTIR and mechanical tests. The membranes mentioned above were applied to adsorption tests with two gold complexes (AuI- and AuBr-). Adsorption efficiencies were compared for each of the complexes. For the AuI complex the efficiency at 12 Hr was 91.2% and for the AuBr-a 12 Hr complex was 91%. The Langmuir model suggests the formation of a monolayer.

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**GT02-DEGRADATION OF POLYMER ADDITIVES FROM DRINKING WATER BY AN ADVANCED  
OXIDATION PROCESS USING ELECTROGENERATED ACTIVE CHLORINE**

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MÓNICA ESPERANZA VELÁSQUEZ TORRES, JORGE VAZQUEZ ARENAS, JUDITH CARDOSO MARTÍNEZ

Phthalic acid derivatives are widely used in the polymer industry to produce esters such as plasticizers. These compounds are commonly employed to modify the physical and mechanical properties of poly (vinyl chloride) and poly (ethylene terephthalate) during their processing. Thus, phthalic esters can migrate to food and drink and act as endocrine disruptors. Other environmental hazards and health effects are known due to their high chemical stabilities that hamper their degradation. In the present study, an advanced oxidation process is proposed to abate a phthalic acid derivative (phthalic anhydride and phthalic ester) in water, using a dimensionally stable anode (Sb<sub>2</sub>O<sub>5</sub> doped Ti/RuO<sub>2</sub>-ZrO<sub>2</sub>), synthesized via the Pechini method. Graphite and Ag/AgCl/KCl (3M) electrodes were used in the electrochemical cell as cathode and reference electrodes, respectively. The microelectrolysis and degradation studies were conducted in synthetic solutions containing 0.6 mM phthalic anhydride and 0.05 M NaCl. UV-VIS spectra indicated that the degradation of phthalic anhydride was performed between 40-45 minutes of electrolysis applying 6.5 mA/cm<sup>2</sup>, while an iodometric study revealed that the active chlorine formation responsible of the degradation process relies on the chloride concentration in the electrolyte, and higher degradation rates of phthalic derivative are reached as the concentration of the active species is increased on the catalyst surface.

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**GT03-GEOPOLYMERS FROM AGROINDUSTRIAL WASTES**

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CLAUDIA A. HERNÁNDEZ-ESCOBAR, RURIK FARIÁS-MANCILLA, SERGIO G. FLORES-GALLARDO, E. ARMANDO ZARAGOZA-CONTRERAS

The use of agroindustrial wastes such as wheat or oats husks, corn or sugar cane bagasse, or walnut shells, is extremely attractive since their components such as cellulose, lignin, and aluminosilicates make them a biorenewable source of raw materials. Geopolymers are a

new class of inorganic aluminosilicate polymers. These materials have a wide field of application, where the uses as a substitute for cement, refractory bricks, or ceramic precursors, are the main uses. In this research, the fly ash from the wheat husk was extracted by a calcination process at 1100 °C. The thermogravimetric analysis revealed that the ash amount in this source was 16 wt%, whereas the atomic ratio of silicon and aluminum was evaluated by elemental analysis (EDAX), indicating 97% silicon and 3% aluminum. With these ashes, geopolymers were obtained by an alkaline activated reaction, with sodium hydroxide in concentrations of 8 M, 12 M, and 16 M. Subsequently, the compressive strength was evaluated in specimens made with curing times of 7, 14, 21, and 28 days, at 20 °C. The compressive strength indicated that at a constant temperature, the resistance increased directly related to the alkaline activator concentration and with the curing time, obtaining the best results with the alkaline solution of 16 M. These results suggested that the wheat husk as a source of aluminosilicates can be equally competitive compared to traditional sources in Asia, where the main source of aluminosilicates is rice husk.

#### GT04-SYNTHESIS AND CHARACTERIZATION OF CHITOSAN-COLLAGEN-HYALURONIC HYDROGEL FOR CARTILAGE REGENERATION

JORGE ALFONSO TAVARES NEGRETE, J. GABRIEL LUNA VÁRSENAS, B. ARGELIA ROSILLO DE LA TORRE, JOSÉ JORGE DELGADO GARCIA, LAURA EDITH CASTELLANO TORRES, ARTURO VEGA GONZÁLEZA, IRAIS AMARANTA QUINTERO ORTEGA

Degenerative osteoarthritis affects approximately 15% of the third age people due to the increase in life expectancy and as a result of mechanical overload due to daily activities. This disease is promoted by the degradation of the cartilage extracellular matrix secreted by chondrocytes and formed mainly by collagen and glycoproteoglycans as hydrogels: The more extracellular matrix is lost, the less available health chondrocytes are. A three polymer crosslinked hydrogel is proposed as a extracellular matrix scaffold, using chitosan as the main component providing good biocompatibility, antibacterial properties and structural strength. Collagen is incorporated for their flexibility and tensile strength and finally, the glycoproteoglycan hyaluronic acid is added due to their role in cellular adhesion in the native cartilage, as nutrient for chondrocytes and as collagen precursor. The synthesis of this biomaterial was performed by a Schiff base reaction using the amino groups present in the natural state of the polymers, varying the concentration of collagen and hyaluronic acid to have different ratios of crosslinking. The rheological properties of the hydrogels were studied and the storage and loss moduli reported for different crosslinking ratios. Those properties were discussed in the context of a larger characterization using infrared spectroscopy, scanning electronic microscopy and shear and stress resistance.

#### GT05- ANTIFUNGAL PROPERTIES OF POLYCAPROLACTONE-CINNAMON OIL MIXTURES

ALFONSO BARAJAS CERVANTES, MAYRA ELIZABETH GARCÍA SÁNCHEZ, OSCAR ROBLES VÁZQUEZ, INÉS JIMÉNEZ PALOMAR, PEDRO ORTEGA GUDIÑO

In recent years the interest of the industry to develop films of biodegradable polymers with antifungal and antimicrobial characteristics for its application in the food packaging and in the development of nontoxic dermal patches has increased, this has promoted the investigation of polymers incorporating agents which can inhibit growth of cell and also based on natural products, among the various alternatives, emphasize the use of essential oils such as some kinds of cinnamon. Cinnamon essential oil (*Cinnamomum zeylanicum*) it

has been shown to be able to combat bacterial contamination, as well as the ability to inhibit the growth of a wide variety of yeasts and fungi, has been reported to be used in the protection of food. In addition, are considered of low danger and of low risk to the human being, are commercialized in Mexico of economic form. This work focused on identifying the effects on the mechanical properties of the incorporation of cinnamon oil in polycaprolactone (PCL) and determining the diameter of long-term fungal inhibition for dermal applications.

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#### GT06-POROUS WHEAT GLUTEN MICROPARTICLES OBTAINED BY ELECTROSPRAY: PREPARATION AND CHARACTERIZATION

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FRANCISCO RODRÍGUEZ FELIX

Currently, microporous polymer materials are being studied extensively due to their attractive properties which allow for a wide potential of applications, such as Prolonged Release Systems (PRS). The objective of the present work was to prepare and characterize porous microparticles of Wheat Gluten (WG) using the electrospray technique. The effect of the physicochemical parameters of the solution and electrospray technique parameters on the morphology and size of the materials obtained was studied. For all of the concentrations of WG, porous microparticles with sphere geometry were obtained. At higher concentrations of WG (8% w/v), higher values of viscosity ( $0.32405 \pm 0.002 \text{ Pa} \cdot \text{s}$ ), density ( $0.997 \pm 0.0005 \text{ g/cm}^3$ ), and particle size ( $1.42 \pm 0.71 \mu\text{m}$ ) were obtained while at lower concentration, high stability rheological is presented exhibited Newtonian fluid behavior. Characterization by Scanning Electron Microscopy (SEM), Fourier Transform Infrared spectroscopy (FT-IR) and x-ray diffraction indicated that the material obtained has a potential application in the PRS industry.

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#### GT07-ELECTROSPUN FIBERS OF BIODEGRADABLE POLYURETHANE OBTAINED BY LIPASE BIOCATALYSIS

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MARINA P. ARRIETA, KARLA A. BARRERA RIVERA, DANIEL LOPEZ, ANTONIO MARTINEZ RICHÁ, LAURA PEPONI

Electrospinning is a very interesting technique used to obtain polymeric micro and nanofibers. However, the optimization of the "processing-window" is required in order to obtain homogeneously fibers. Electrospun fibers can be used in many application fields, even if biomedicine is one of the more frequently one. Therefore in this case, it is necessary to use biopolymers, biocompatible and/or biodegradable, depending on the final use. For this reason, polyurethanes based on PCL are considering very good candidates for electrospinning. In particular, in this work we used, oligomeric PCL diol was synthesized starting from CL using diethyleneglycol as initiator and immobilized *Yarrowia lipolytica* lipase as biocatalyst. The obtained bifunctional monomer was reacted with HDI in 1,2-dichloroethane (OH:NCO ratio = 1:1), at 80°C 1h and 30 minutes in order to synthesize the corresponding polyurethane. The electrospinning "processing-window" has been optimized in order to obtain the polyurethane electrospun nanofibers.

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#### GT08- INTRINSIC VISCOSITY OF METHYLCELLULOSE TO DETERMINE ITS MOLECULAR WEIGHT

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GABRIELA ESCOBAR VÁSQUEZ, ANTONIO MARTÍNEZ RICHÁ

In this work, we will try to determine the intrinsic viscosity  $[\eta]$  experimentally. We will use methylcellulose as the solute and the DMSO (Dimethyl sulfoxide) as the solvent, with the determination of  $[\eta]$  will allow us to know the molecular weight  $M$  of such polymer. The knowledge of molecular weight is very important, since it depends on a large number of physical and structural properties. To determine the  $[\eta]$ , the Cannon-Fenske viscometer will be used to produce the curve between the specific viscosity ( $\eta_{sp}$ ) versus concentration. The extrapolation to infinite dilution of this curve will allow us to determine the value of  $[\eta]$ . The intrinsic viscosity  $[\eta]$  of a polymer is related to the molecular weight  $M$  according to the Mark-Houwink-Sakurada equation. The values of  $K$  and  $a$  for a given polymer depend on both the solvent and the solute. Thus, the intrinsic viscosity of a polymer sample is different in different solvents. In a dilute solution of polymer in a mixture with poor solvent can be expected to exhibit lower intrinsic viscosity, otherwise the solution of the same polymer would be with a good solvent. Therefore, the interaction produced between the solvent and polymer does not depend on the nature of both, but on the temperature as well.

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#### GT09-SUPRAMOLECULAR PHOTO-RESPONSIVE LIQUID CRYSTAL AZOPOLYMERS

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DÁMASO NAVARRO-RODRÍGUEZ, CINTHYA VALESKA CASTRO PÉREZ, ROSA JULIA RODRÍGUEZ-GONZÁLEZ, LETICIA LARIOS-LÓPEZ, NAYELY TREJO-CARBAJAL

Supramolecular chemistry based on halogen bond (XB) interactions is becoming a new source of liquid crystals (LC). Differently to LC complexes formed by hydrogen bond (HB) interactions, LC complexes formed by XB interactions show directionality and hydrophobicity, among other unique characteristics. In this work, the synthesis and properties of new complexes (small molecules and polymers) bearing highly anisotropic azo-compounds (azobenzene-coupled-pyridine and perfluoroyodo compounds) are presented and discussed. These new supramolecular structures combine liquid crystal and photo-induced properties, a combination that has been scarcely explored in supramolecular structures auto-assembled through XB bonds.

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#### GT10-GROWTH OF THIN FILMS AND DOPED WITH IONIC LIQUID

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We present the result of controlled conditions for grow a thin film using the sol-gel method, and the aid of dip-coater; furthermore, the optical characterization of the thin films is presented. The sol-gel was doped with an ionic liquid (1-butyl-3-methylimidazolium hexafluorophosphate and 1-butyl pyridinium tetrafluoroborate). The room temperature to avoid breaking was controlled. The optical characterization of thin films using an optical microscope and FTIR, shows a good optical transparence and the preservation of IL respectively

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### GT11-EFFECT OF TERPENES AND ALKYL GROUPS ON THE CRYSTALLINITY OF POLY( $\epsilon$ -CAPROLACTONE)

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The effect of different types alkyl groups on the poly( $\epsilon$ -caprolactone) (PCL) was studied. The ring-opening polymerization (ROP) of  $\epsilon$ -caprolactone was initiated by terpene-derived alcohols, such as geraniol, farnesol, nerol and prenol and using ammonium decamolybdate as a catalyst. The effect of diols with voluminous groups such as 1,3 Propanediol, Diethyl-1,3-propanediol, 2,2-Dimethyl-1,3-propanediol and 2,2-Dibenzyl-1,3-propanediol was also analyzed. The PCLs were characterized NMR, FT-IR, mechanical properties, GPC and DSC. The alkyl groups as part of terminal groups or diols affected the crystallinity of the PCLs.

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### GT12-EFFECT OF CU(II) IN THE ADSORPTION OF MAXILON BLUE ON MOLECULARLY IMPRINTED PET

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The effect of Cu (II) on the adsorption of maxilon blue on PET grafted with acrylic acid (PET-g-AA) and on molecularly modified PET (MIP) was evaluated using the maxilon blue dye as molecule Template in a watery system. The synthesis of the grafted PET and modified PET was performed by molecularly imprinting, in both cases the synthesis was by radical free polymerization, the products were characterized by infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and differential scanning calorimetry (DSC). A factorial experiment 23 design was used to determine the effect of pH (3 and 5.5), initial copper concentration (10 and 30 mg / L) and contact time (240 and 480 min) on copper adsorption in PET grafted with acrylic acid and molecularly modified PET for an individual component system, the concentration of Cu(II) was evaluated by atomic absorption spectroscopy (EAA). The unretained dye concentration was assessed by visible spectroscopy. At pH 3, 10 mg / L of Cu(II) and 240 min of contact it was found that the Cu(II) is less adsorbed, allowing a greater adsorption of the maxilon blue.