Polymat Contributions

Abstract Book

Volume 2

MESOSCOPIC STUDY OF THERMORESPONSIVE POLYMERIC MEMBRANES: CONTROL OF PORE SIZES VIA TEMPERATURE EFFECTS

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Abstract: The applications of thermoresponsive amphiphilic copolymers as synthetic membranes have great potential in areas such as for medicine, catalysis, environmental sciences, and technology. The thermoresponsive membranes of planar type are generated by self-assembly of one or more amphiphilic copolymer, where one of its block segments exhibits a solution critical upper or lower temperature. In this work, the DPD approach was employed to explore the dynamic diffusion process and control the pore size of thermoresponsive membrane. The dynamic behavior that exhibits the thermoresponsive membranes of planar type in aqueous environment was explored in detail on temperature interval of 293K-333K, Figure 1.

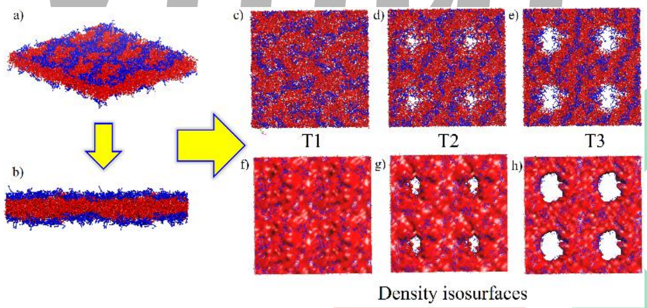

Figure 2. Pictures of thermic behavior on control pore size of thermoresponsive membranes of planar type during the thermal study: (a-e) evolution of pore size of thermoresponsive membranes at different temperatures; (f-h) density isosurface of thermoresponsive membranes at different temperatures to visualize of pore size.

The numeric simulation outcomes reveal that the polymeric membrane can modulate the pore size by effect temperature. Finally the polymeric membrane it may control the process of diffusion of specific molecules depending on their size.

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PREPARATION OF NOVEL DENDRITIC MOLECULES BEARING DONOR-ACEPTOR GROUPS (PYRENE-BODIPY) AS POTENTIAL ENERGY TRANSFER DEVICES

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In this work, we propose the synthesis of a novel series of dendritic molecules bearing donor-acceptor groups (pyrene-bodipy) for future applications in energy transfer.

Initially, first and second generation Fréchet type dendrons (Py_2-G_1OH and Py_4-G_2OH) were prepared 1-pyrenylbutanol and 3,5-dihydroxybenzylic alcohol. These compounds were further linked to a bodipy unit via classic reaction to obtain the desired products (Bodipy-G_1Py_2) and Bodipy-G_2Py_4).

In order to study the spectroscopy properties of this kind of compound, a bodipy contain a anisole group on the para position were synthesized.

The spectroscopic study of this compound show a very interesting absorption band at 340-370 nm.

The obtained compounds were fully characterized by FTIR and ^1H and ^{13}C NMR spectroscopy and their molecular weights were determined by MALDITOF. The optical and photophysical properties of these molecules will be further studied by absorption and fluorescence spectroscopies

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Analysis of optical and structural properties of polymorphous silicon thin films for applications in solar cells .

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It has been shown that thin film of polymorphous silicon (pm-Si:H) materials have considerable adventages in absorption, photoconductivity and photostability with respect to conventional amorphous silicon, because pm-Si:H has nanometer sized crystalline Si inclusions embedded in an amorphous silicon matrix. These are attractive properties for the photovoltaic industry. The structure of pm-Si:H improves the transport properties with respect to amorphous silicon, even after being in a prolonged exposure to solar radiation. In this work pm-Si:H was synthesized by plasma enhanced chemical vapor deposition PECVD. Dichlorosilane was used as silicon precursor gas diluted in H_2 and Ar. In order to obtain different structural configurations of pm-Si:H films, the H_2 flow rate was varied from 20 to 100 sccm and the deposition temperature was varied from 150°C to 300°C. The films were characterized by Raman spectroscopy and UV-visible transmission/reflection. Transport properties were also studied by photoconductivity measurements. The crystalline fraction, the size of the Si nanocrystals and the optical gap was obtained for each sample. These structural and optical properties were correlated to the observed transport properties. The possible application of these materials to solar cell structures is also discussed.

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Obtaining and characterization of the hetero junction of ITO/PEDOT:PSS/PANI/Al for its application on organic solar cells

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Organic based composite photovoltaic (PV) cells have attracted much attention as one of the promising futuro energy efficient devices [1]. Organic solar cells offer the potencial of low cost fabrication and large area aplication when comparing the technology to the silicon based solar cells [2]. We investigate the optics, electric and structure properties of the PEDOT:PSS/PANI mixing about glass, ITO and FTO sustrates, for organics application. Also it is proposed the fabrication of organic solar cells (OSCs) using the next architecture ITO/PEDOT:PSS/PANI/Al indicate in fig. 1 and using as PANI layer active. The technics using for deposition of the PEDOT:PSS transparent layer is spin coating about glass on the initial way. For active layer and catod terminal evaporated for obtain it.

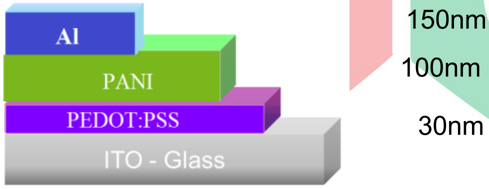

Figure 1. Estructure OSCs

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Vip. and. CIDS-BUAP

Obtaining and characterization of the hetero junction of ITO/PEDOT:PSS/PANI/Al for its application on organic solar cells.

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We investigate the optics, electric and structure properties of the PEDOT:PSS/PANI **mixing about glass, ITO and FTO substrates, for organics application. Also it is proposed the fabrication of organic solar cells (OSCs) using the next architecture** ITO/PEDOT:PSS/PANI/Al indicate in fig. 1 and using as PANI layer active. The technics using for deposition of the PEDOT:PSS transparent layer is spin coating about glass on the initial way. For active layer and **catod** terminal evaporated for obtain it.

Workeys: organic solar cells, poly(3,4-ethylenedioxythiophene), polystyrene sulfonate (PEDOT:PSS), polianiline (PANI).

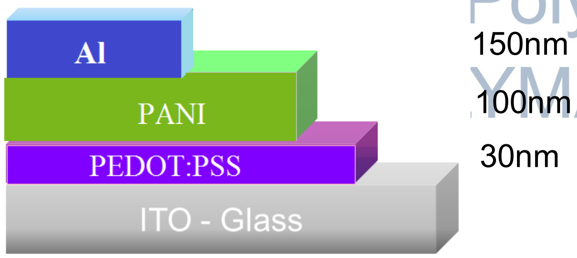

Figure 1. Estructure OSCs

One–step aqueous synthesis of cadmium sulfide nanoparticles with different soluble polymers

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Abstract

In the last years, semiconductor nanoparticles have emerged as an important class of materials that offers great promise to a diverse range of applications ranging from energy conversion to biomedicine. The synthesis of these nanoparticles is an important aspect of the research, due their water-solubility, simple chemical modification well dispersed and stabilized nanoparticles by utilizing soluble polymers, surfactant or capping agent. In comparison with the original organometallic synthesis, the resulting alternative routes are safe, simple, inexpensive, reproducible, versatile, and yield nanoparticles with well-controlled size, shape, and size/shape distribution.

Cadmium sulfide nanoparticles were prepared with one-step aqueous synthesis method. Different soluble polymers, i.e. dextrin, maltodextrin and polyethylene glycol, were used and the effect of different concentrations was analyzed for their effectiveness in limiting the particle growth. The morphology and the crystalline structure were measured by transmission electron microscopy (TEM) and x-ray diffraction (XRD), respectively. Particle size of the particles obtained from these experiments correlates well with the optical absorption spectroscopy and Scherrer´s formula from XRD patterns. Thus the presence of polymer on the surface of cadmium sulfide plays a significant role in reducing the size of the particle. XRD analysis revealed single crystal cadmium sulfide nanoparticles of size 3 nm in case of dextrin capping.

“SYNTHESIS, CHARACTERIZATION AND STUDY OF THE THERMAL AND OPTICAL PROPERTIES OF NEW POLYMER FILMS OF PORPHYRIN, MESO-SUBSTITUTED PORFPEG4-AC-g-PE-nKGy”

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A new porphyrin derivative: meso-substituted porphyrin tetratraphenyl bearing a tetra (ethylene glycol) side chain (PORFPEG4) was synthesized. This new photoluminescent chromophore is characterized by FTIR, 1H and 13C NMR spectroscopies.

A precursor polymer was synthesized by reaction of commercial low density polyethylene (PE) films in the presence of acryloyl chloride using gamma radiation at different doses of radiation (2 to 8 KGy). In addition, a flexible tetralhylene glycol spacer (PORFPEG4) was esterified with a new porphyrin molecule to obtain a series of PORFEGEG4-AC-g-PE-nKGy grafted poliform films. These films were characterized and studied their thermal and optical properties.

Development of a robust and recyclable laccase preparation via covalent immobilization on poly(glycidyl methacrylate) microspheres

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Enzymatic immobilization is a useful method to improve biocatalytic processes, due to the increase in operational stability, thermostability and enzyme recyclability [1-2]. Despite many advantages, the ranges of pH and temperatures in which the immobilized enzymes show an optimal activity are still narrow and specific for each type of enzyme, therefore limiting potential industrial applications. The immobilization of oxidative enzymes, in particular, is a very challenging topic that needs to be further investigated.

In this work, three different types of oxidoreductases, namely laccase from *Trametes versicolor* (*Tvl*), *Agaricus bisporus* (*Abp*) and *Myceliophthora thermophila* (*Mtl*) were covalently immobilized on poly(glicidyl methacrylate) (P(GMA)). P(GMA) microspheres were synthesized by dispersion polymerization and characterized *via* NMR, FTIR and Scanning Electron Microscopy. In a second step the single biocatalysts were immobilized *via* covalent coupling to the epoxy groups of the polymer and the co-immobilization of *Tvl* and *Abp* was also carried out. Finally the immobilized enzymes were characterized in terms of activity at different pH and temperature values, reusability, storage stability, and bound protein.

The results show that each immobilized enzyme has an optimal activity at different pH and temperature ranges. Remarkaly all obtained preparations show improved storage stability and reusability. For the co-immobilization, a broad pH and temperature activity range was achieved with the optimum activity corresponding to the *Tvl* and *Abp* maximum. These results suggest that immobilization and co-immobilization of those enzymes on P(GMA) microspheres are an excellent option for the development of a efficient biocatalyst with potential applications in pesticides degradation, dyes decolorization and waste water purification.

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Nucleosides as Organizing Architectural Moieties.

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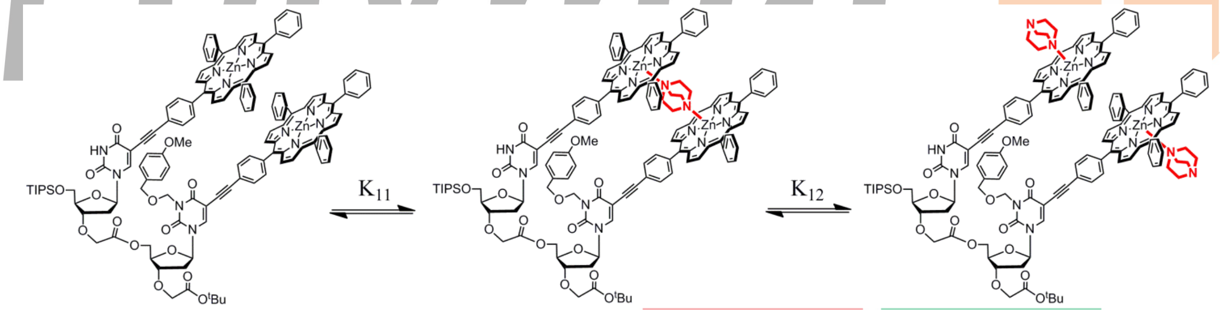
Chemistry "beyond the molecule" is epitomized in nature by a plethora of relatively weak noncovalent interactions. The three-dimensional structures of most biopolymers are controlled with noncovalent interactions, either between different parts of the same strand (as in protein α-helices) or between two separate strands (as in the DNA duplex and protein β-sheet). While nature has refined the construction of biopolymers, our mastery of the subtle noncovalent interactions as synthetic tools is in an early stage of development. Only in the past two decades people begun to develop ways of mimicking the natural light-harvesting complexes by noncovalent assembly of porphyrin units aiming to obtain favored spacing and orientation between the chromophores. The construction of multi-chromophoric assemblies has led to resurgence of interest in coordination chemistry due to formation of ordered arrays directed through molecular recognition events. As a module in the construction of supramolecular assemblies, porphyrins and metallo-porphyrins can be exploited in two different ways: porphyrins can behave as donor building blocks insofar as they comprise meso-substituents, such as pyridyl groups, which can act as ligands that can suitably coordinate to metal cations, while metalloporphyrins can act as acceptor building blocks as soon as the metal atom inside the porphyrin core has at least one axial site available for coordination.

For the last years, we have focussed on cofacial bis-porphyrin tweezers for host/guest interactions and investigated the possibilty to obtain self-coordinated molecular systems with predictable spectral and redox characteristics. We report here the synthesis of a di-nucleotide bearing pendant porphyrins dedicated to adopt a pre-organized coformation with face-to-face porphyrins, and capable to self-organize in a stable sandwich type complexe with bidentate base such as DABCO.[1] Using a similar strategy as the one used in antisense research, an artificial nucleotidic backbone was built from modified deoxy-uridine units linked with a more rigid linker than the phosphodiester moieties found in natural oligonucleotides. Antisense research uses modified oligonucleotides, less flexible than natural strands, to pre-organize the system toward the obtaining of stable double



The films of SrAl2O4 were synthesized by using the Spray Pyrolytic Technique on quartz at temperature of 550 °C. Subsequently, the samples was annealed during 16 hours at 800 °C in a muffle. The incorporated dopant is europium (Eu3+) and was handled with the following concentrations: 2, 4, 6, 8 and 10 at.%, the best percentage was 6 at.% of the ion europium. The emission of the films are in the colors red, green and yellow corresponding to the electromagnetic spectrum in the visible region. The characterization of these films was carried out by means of XRD, SEM, XPS, photo and cathodoluminescence helices between synthesized and natural oligonucleotides. A modified oligonucleotidic backbone was here used to target a parallel conformation of the porphyrins appended to each deoxy-uridine moiety. To provide a rigid environment for the porphyrins, the uridine units were coupled in 3'-5' stepwise fashion using ether-ester type of spacer of suitable length, and porphyrins were anchored to the uridine by means of robust carbon-carbon bonds. Earlier studies demonstrated that a peptidic linker doesn't provide sufficient pre-organization to enhance significantly the association constant with bidentate bases such as DABCO on the contrary of some flexible linkers such as uridine or 2'-deoxyuridine. We document herein that the gain in stability for the formation of sandwich type host-guest complex with DABCO can be even greater when a dinucleotide linker is used. Such pre-organization increases the association constants by one to two orders of magnitude when compared to the association constants of the same bidentate ligands with a reference Zn(II) porphyrin. Comparison of these results with those obtained for rigid tweezers shows a better efficiency of the flexible nucleosidic dimers. We thus document the fact that the choice of rigid spacers is not the only way to pre-organize bis-porphyrins, and that some well-chosen nucleosidic linkers offer an interesting option for the synthesis of such devices. Furthermore, the chirality and enantio-purity of the nucleosidic linkers paves the way toward the selective complexation of enantio-pure bidentate guests and the resolution of racemates.

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π-Conjugated Covalent Organic Frameworks

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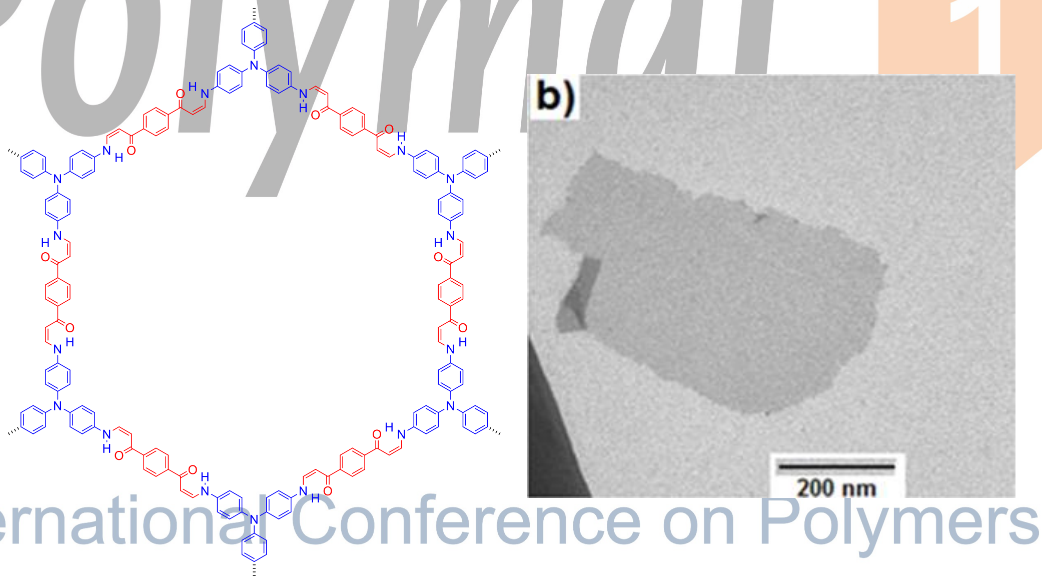
Two-dimensional (2D) polymers have recently emerged as an intriguing new materials. When built entirely from sp2-hybridized atoms, 2D polymers could combine the optoelectronic characteristics of conventional π-conjugated polymers and 2D inorganic materials, such as graphene, thereby leading to novel set of properties and applications. In this lecture, I will discuss the current state of art in synthesis of 2D polymers and highlight our recent progress in this direction, using (i) dehalogenative coupling polymerization on metal surfaces and (ii) dynamic covalent polycondensation in solution[1]. The novel properties resulting from the π-electron delocalization (conjugation) in 2D systems will be also be discussed.



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EFFECT OF SEVERE PLASTIC DEFORMATION ON PRECIPITATION HARDENING ALLOY AFTER ANNEALING

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The equal Channel Angular Pressing (ECAP) process has been reported to improve several mechanical properties, such as the yield strength, UTS and hardness in some ductile alloys. The high dislocation density produced by this technique and the rearrangement of such defaults into tangles, generate subgrains of some tenths of nanometers. In this work, the annealed Al-2017-T4 alloy was processed up to 5 ECAP by route BC. Residual stress and the crystal texture characterization was carried out by X-ray diffraction. Scanning and transmission electron microscopies were employed for observing the grain refinement and dislocation tangles formation. Vickers microhardness profiles were measured for evaluating the strain homogeneity induced by the ECAP process. The results showed a grain reduction of 81% from zero to fifth ECAP passes. Residual stress values start as compressive kind and after third pass increases up tensile values on external face. The resulting low values of residual stress analysis were due to the initiation of possible cracks in the material. Macrotexture evoluted continuously during the first stages of ECAP and after the third pass a stabilization was observed ($A^{*}_{2\theta}$). Vickers microhardness increase after the first stages but also stabilize after the third ECAP passes.

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Incorporation of Conjugated Diines in Hybrid Perovskites for Enhanced Optical and Electronic Properties

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Solar energy is the most promising clean energy sources for the future. Currently, most solar panels are made of crystalline silicon, this represents high costs owing to the energy intensive processes required to manufacture these devices, which in turn has significant economic and environmental consequences [2]. Is for these reason that new photovoltaic technologies are highly desirable. One of the most promising technologies are perovskite-based solar cells, which could be a good alternative, due to great versatility, ease of processing, high conversion efficiency and its potential to decrease the cost of production and the environmental impact associated with it [1].

Despite the great promise of perovskite solar cells, there are still concerns regarding its stability towards light and water. As an alternative, two-dimensional (2D) hybrid perovskties have shown increased stability albeit at lower conversion efficiencies, mainly due to its limitations in terms of conductivity and light absorption. Herein, we will discuss the incorporation of conjugated diines in the structure of 2D lead halide perovskites with the objective of increasing and improving its stability, electronic conductivity, charge separation and/or mechanical properties.

In particular, we will discuss the design and synthesis of a conjugated diene , its incorporation into 2D hybrid perovskites and finally, we will elaborate on the postsynthetic modification of such materials and the implications of such transformation on the optoelectronics properties of these materials.

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Synthesis and application of lithium zirconate in a mixture CO_2-CH_4 to capture CO_2.

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Ceramic materials have been of interest in recent years due to their ability to capture gases such as carbon dioxide (CO2), which is one of the components of biogas and is also a greenhouse gas [1]. This work proposes the use of lithium zirconate to capture CO2 to purify a biogas [2] produced from grass residues. Lithium zirconate was synthesized by the combustion method in a 1.1: 1.0: 0.2 ratio of lithium carbonate (LiCO3), zirconium oxide (ZrO2) and potassium carbonate (K2CO3). In the first capture tests, a flow of 52 mL / h of the CO2-CH4 mixture in 1 g of lithium zirconate was circulated at room temperature, getting in a variation of 3% by weight of the lithium zirconate before and after Passing the gas mixture, indicating that the capture of one of the components of the gaseous mixture used was carried out. These results indicate that zirconate can be useful to purify a biogas by capturing one of the gases that compose it.

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LO IMPORTANTE DE UNA EMPRESA DE BASE TECNOLÓGICA

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Una empresa de base tecnológica basa sus actividades en las aplicaciones de nuevos conocimientos científicos o tecnológicos generando nuevos productos, procesos o servicios que ayudan a tener una mejor calidad de vida para quienes los necesitan o consumen. Estas empresas favorecen la creación de empleos para gente altamente calificada, capaz de añadir un alto valor agregado a los productos generados por dichas empresas. Cuando salen de una universidad u organismo público de I+D se denominan Spin-Off.

Se expondrán los entes mas importantes para que estas salgan adelante con éxito.

IMPLEMENTACIÓN DE UNA FUENTE PULSADA DE ALTO VOLTAJE PARA EL TRATAMIENTO DE MATERIALES POLIMÉRICOS EMPLEADOS EN LA REMOCIÓN DE COLORANTES AZOICOS DE SOLUCIONES ACUOSAS.

Juan Nabor Balderas Gutiérrez, Celso Hernández Tenorio, Rosa Elvira Zabala Arce, Miguel Villanueva Martínez.

Resumen

El presente trabajo describe el diseño e implementación de una fuente pulsada de alto voltaje en configuración flyback, capaz de operar en un rango de frecuencia de 500 – 5.5 kHz, y voltajes superior a 1.5 kilo volts, produciendo descarga de plasma luminiscente a presión atmosférica y en vacío. El sistema está constituido a partir de un circuito de control SG3524 capaz de operar a alta frecuencia. Cabe mencionar que, el incremento del voltaje se lleva a cabo mediante un transformador elevador con relación 1:10, implementado en un núcleo de ferrita para evitar corrientes parasitas y la saturación del núcleo al trabajar a altas frecuencias. El sistema es empleado al tratamiento superficial de material polimérico y primordialmente al tratamiento de esferas y películas de quitosano, los cuales son empleados en la remoción de colorantes tipo azoicos de soluciones acuosas. Por otra parte, cabe mencionar que el material modificado con plasma de descarga luminiscente posee mayor capacidad de adsorción en comparación al material sin modificar y a pH cercanos al neutro entre 4-6.

Palabras claves- Fuente pulsada, plasma luminiscente, Transformador elevador, tratamiento de polímeros.

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Lignin-Derived Alternative Thermoplastics

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Presently, most high-performance commercial polymers are derived from petroleum-based compounds (petrochemicals). The worldwide consumption of plastic between the years 2014 and 2020 is predicted to increase by 29%.[1] As the world consumption of petroleum-based products increases, there is a growing concern that the world's main energy source will be unable to meet the demands. Along with the potential depletion of fossil fuel source, is the concern for the environmental as the products produced from fossil fuel results in hazardous waste and greenhouse gas emission. As the world seeks solutions to these problems, no overarching resolution has been found. One obvious solution to this problem would be to engineer biodegradable polymers that are produced from sustainable raw materials (biomass).[2] One could imaging a green life cycle for these polymers that would avoid the production of hazardous waste and excess greenhouse gas pollution since they wouldn't require combustion practices in their demise. Actually, the Biomass R&D Technical Advisory Committee commissioned by congress, proposed to replace the current U.S. petroleum consumption up to 30 % with biofuels by 2030.[3] In this regards, lignin, which is in the second most abundant polymer on earth has been identified as a major feedstock for biofuels and chemicals. Lignin is the largest bio-based source for aromatic compounds and as such many groups, including ours are interested in building bio-based replacement polymers for petroleum-based ones.[4]

In this presentation, we will describe the design, synthesis and properties (thermal and physical) of a new series of alternative poly(ether-amide) thermoplastics from lignin-based raw materials. Our results show that our polymers' glass transition temperatures (Tg) range from 96 ºC – 100 ºC, which is similar to hard plastic polymers such as polystyrene and poly(methyl methacrylate) with Tg ~ 100 ºC. The melting points (mp) (245 ºC – 255 ºC) were more similar to polystyrene ~ 240 °C and higher than poly(methyl methacrylate) at 160 °C. In essense, the porperties are inbetweem polyesters and polyamides. We will also discuss some very important structure/property relationship with respect to hydrogen bonding and its effects on the thermal, physical, and mechanical properties properties of these polymers.

Acknowledgements (10 pt)

We would like to thank the Mississippi State University and the Department of Chemistry for financial support for this work.

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IMPLEMENTATION OF A HIGH VOLTAGE PULSED SOURCE FOR THE TREATMENT OF POLYMERIC MATERIALS USED IN THE REMOVAL OF AZOQUE COLORS FROM AQUEOUS SOLUTIONS.

Juan Nabor Balderas Gutiérrez, Celso Hernández Tenorio, Rosa Elvira Zabala Arce, Miguel Villanueva Martínez.

Summary

The present work describes the design and implementation of a pulsed high voltage source in flyback configuration, capable of operating in a frequency range of 500 - 5.5 kHz, and voltages higher than 1.5 kilo volts, producing discharge of luminescent plasma at atmospheric pressure and in vacuum, in addition it is able to work with different geometries of reactor maintaining the homogenous discharge. The system consists of the control circuit SG3524 capable of operating at high frequency and generate the desired control pulse, which is coupled to a current boosting circuit to avoid voltage deflections and reverse currents. It is worth mentioning that the voltage increase is carried out by means of a 1:10 ratio transformer implemented in a ferrite core to avoid parasitic currents and the saturation of the core when working at high frequencies. The system is employed for the surface treatment of polymeric material and primarily for the treatment of chitosan spheres and films, which are employed in the removal of azo dyes from aqueous solutions. On the other hand, it is possible to mention that the material modified with luminescent discharge plasma possesses greater capacity of adsorption in comparison to the unmodified material and to pH near neutral between 4-6.

Keywords - pulsed source, luminescent plasma, elevator transformer, treatment of polymers.

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CCC pincer complexes with fluorine fragments

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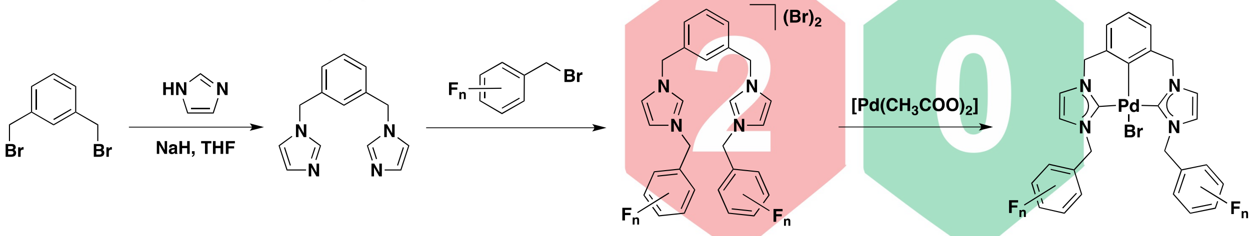
The applications of pincer complexes have increased in the last decade. Among them, the most important is their use as catalysts. In this sense, pincer complexes were employed to catalyze a wide range of reactions, e.g. cross-coupling, alcohol oxidation, among others.[1-3] The design of the pincer ligands is very important because they may control the catalytic activity of their related complexes.

Recently, the design of ligands has involved the addition of extra features. For instance, some ligands incorporated redox centers or showed a proton response. More interestingly, the functionalization of ligands with groups able to forming non-covalent interactions has been developed.[4] In this regard, we designed a series of pincer complexes that incorporates polyfluorinated substituents. As **Scheme 1** shows, the synthesis of the complexes was performed in three steps. The first one consist in the reaction of 1,3-bis(bromomethyl)benzene with imidazole in the presence of a base. Secondly, the formation of the bis(azolium) salts was performed. Finally, the synthesis of the complexes was carried out by the reaction of the bis(azolium) with [Pd(CH_3COO)$_2$]. The studies of the catalytic influence of the fluorinated substituents are currently being developed in our laboratory.



Scheme 1

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A Novel Mo-Alkylidene Catalyst Facilitates Olefin Metathesis in the Presence of Functional Groups

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Synthesis of highly functionalized polymers is an ultimate goal in chemistry because it allows for design of materials with tailored properties. Molybdenum catalysts (e.g. of the Schrock type) have successfully been used for polymerization of olefins but these catalysts are very sensitive to functional groups at the monomers. However recently, an N-heterocyclic carbene Mo-alkylidene catalyst has been reported that does tolerate functional groups and polymerizes olefins with hydroxyl, carboxyl, or carbonyl functionalities. [1]

We employed density functional theory to investigate the reaction mechanism of this catalyst and to explore the origin of its functional group tolerance at the example of the bicyclo[2.2.1]hept-5-en-2-carbaldehyd monomer. Energetics of the polymerization reaction as well as of the deactivation reaction are presented and regional selectivity of the polymer formation is explained. Compared to Schrock type catalysts, this novel Mo-alkylidene catalysts shows significantly reduced reactivity towards carbonyl coordination.

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Non-functional and Functional Co-substituted Poly[(amino acid ester)phosphazene] Biomaterials

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Polyphosphazenes are a class of versatile materials that can be functionalized with a variety of bioactive substituents including steroids, carbohydrates, amino acid esters, *etc*. These materials are typically biocompatible and biodegradable, producing non-toxic and non-acidic degradation products. Thus, substituted polyphosphazenes have been studied for a variety of biomedical applications ranging from drug delivery to tissue engineering. However, the synthesis of the respective polymers still presents a challenge relative to more conventional degradable biomaterials. The classical approach to prepare polyphosphazenes starts with the ring opening polymerization of the cyclic trimer hexachlorocyclotriphosphazene to poly(dichlorophosphazene) under inert conditions at high temperature, followed by purification of the product and nucleophilic substitution at the phosphorus atom. The process is cumbersome and affords materials with high polydispersity. We have recently developed a variation on this approach by allowing the ring opening polymerization to occur to a limited extent under non-inert atmosphere in an airtight container. This was followed by a one-step substitution with a single amino acid ester hydrochloride or a mixture of two esters, to afford co-substituted poly[(amino acid ester)phosphazene]s. Three functional materials were prepared, substituted with 10 mol % glutamic acid and 90 mol % alanine, phenylalanine or methionine, respectively. Adequate molecular weights (160 – 300 kDa) and low polydispersity (M_w/M_n = 1.3 to 1.8) were achieved. The materials were biocompatible, showing no cytotoxicity towards fibroblasts in both metabolic activity assays (using MTT) and morphological examination (performed by confocal microscopy). Furthermore, while successful electrospinning of the pure materials was difficult, a blend with 50 wt. % polycaprolactone produced relatively uniform fiber diameters with a bead-free morphology and good porosity. Further research will focus on scaffold preparation using the co-substituted poly[(amino acid ester)phosphazene]s for application in vascular tissue engineering.

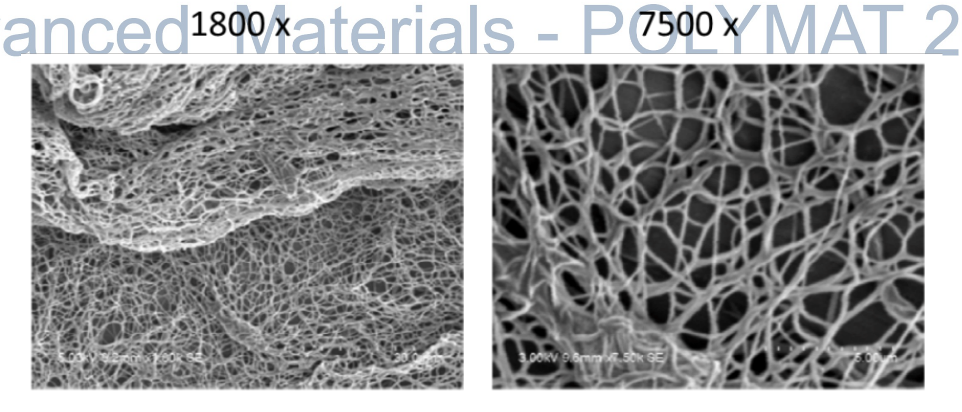

Fig. 1: Electrospun fibers of 5% w/v polymer solution in dichloromethane, containing 50% poly[bis(ethyl alanto)phosphazene] and 50% polycaprolactone

Metal-Free Catalysts for the Borylation of Heteroarenes

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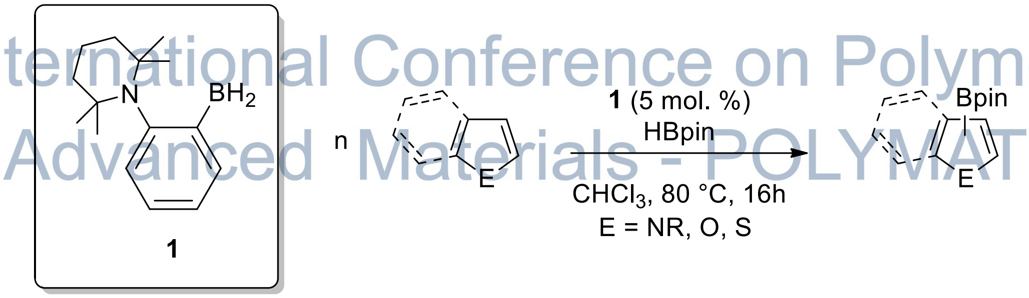
In the past decade, “frustrated Lewis pairs” (FLPs) have been shown to be excellent candidates to replace transition metal complexes in many important chemical transformations.[1] The combination of geometrically or sterically hindered Lewis acid and base pairs leads to very active sites that can activate several types of bonds. We demonstrated recently that species 1-TMP-2-BH_2-C_6H_4 can be used as a catalyst for the borylation of heteroarenes. Experimental evidences suggest that the rate determining step is the activation of a C_{sp2}-H bond by the FLP.[2] This presentation will describe the influence of the catalyst structure on the borylation of furanes, pyrroles and thiophene derivatives, the discovery of air- and water-stable precatalysts for this reaction, and the possibility of such species to activate C_{sp3}-H bonds.



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Solvatomorphism: the inclusion of unexpected guests. An interesting case of study of different solvates in the tecton [Pd(1,10-*phen*)(2,3,5,6-S-$C_6F_4H)_2$]

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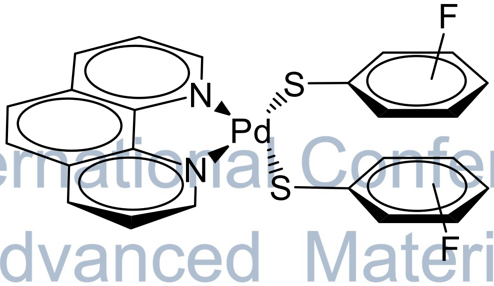
In this work is described the crystalline structures of a non-solvated tecton [Pd(1,10-phen)(2,3,5,6-S-$C_6F_4H)_2$] (**1**) (phen = 1,10-phenanthroline) and three different solvatomorphs [Pd(1,10-phen)(2,3,5,6-S-$C_6F_4H)_2$]·S, S = C_6H_6 (**2**), S = C_6H_6-Cl (**3**) and S = C_6H_6-Br (**4**). In addition is described the formation of the crystalline solvate [Pd(1,10-phen)(2,3,4,5,6-S-$C_6F_5)_2$]·C_6H_6-Br (**5**) for comparison purposes with the former compounds. In this case we are interested in getting deeper in the knowledge of the fascinating phenomena of solvatomorphism. Thus, we performed computational studies in order to elucidate the energetics involved of the non-solvated tecton and their solvatomorphs in attempt to establish how these unexpected guests are encrusted within the unit cell.



Tectons

(**1**) SR_F = 2,3,5,6-(C_6F_4H)
(**2**) SR_F = 2,3,5,6-(C_6F_4H)·C_6H_6
(**3**) SR_F = 2,3,5,6-(C_6F_4H)·C_6H_6-Cl
(**4**) SR_F = 2,3,5,6-(C_6F_4H)·C_6H_6-Br
(**5**) SR_F = 2,3,4,5,6-(C_6F_5)·C_6H_6-Br

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Synthesis and Characterization of Thermoresponsive Starch Nanoparticles

Starch, a polysaccharide produced by most green plants as an energy store, is one of the most abundant natural polymers. Its natural abundance as well as its biodegradability, biocompatibility, nontoxicity and low production cost, makes it an attractive base polymer for the development of novel materials. Recently, starch nanoparticles (SNPs) have gathered considerable attention and numerous reports have appeared on their preparation, characterization, and potential applications. However, only a few studies have been conducted on the development of thermoresponsive starch nanoparticles (TRSNPs). Thermoresponsive polymers exhibit a sudden transition in solubility in aqueous solution upon heating. Here we report that TRSNPs can be obtained by reacting SNPs with 1,2-epoxybutane, a small hydrophobic molecule. The resulting hydroxybutylated SNPs (HBSNPs) exhibited cloud point temperatures (T_c) ranging form 32-52 ^{o}C depending upon the molar substitution (MS). For HBSNPs to exhibit thermoresponsivity, the MS had to be greater than 1. The T_c values could be manipulated by varying the dispersion concentration and by the addition of salts. Dynamic light scattering studies showed that there was a substantial increase in the particle size of HBSNPs at the T_c. High resolution mass spectrometry of hydrolyzed HBSNPs indicate that some oligomerization of the hydroxybutyl groups was occurring on the individual anhydroglucose units of the SNPs.

Technological capabilities of Instituto de Investigación en Metalurgia y Materiales for services to the mining and metallurgical industries.

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ABSTRACT

Instituto de Investigación en Metalurgia y Materiales was founded in 1972 and was the first Institute at Universidad Michoacana. The creation of the Institute was in order to provide with services and consulting to the mining and metallurgical industries of the region. Master and doctorate programs in Metallurgy and Materials Sciences started in 1982 and 2002, respectively. After 44 years of existence, the Institute is composed by 7 departments with 21 researchers. The infrastructure of the Institute is accommodated in 6 buildings. Microscopy facilities are outstanding, there is a transmission electron microscope, a field emission scanning electron microscope, a scanning electron microscope and an atomic force microscope. The chemical analysis laboratory is another strength of the Institute, equipped with state of the art atomic absorption, optical emission and x-ray fluorescence spectrometers and other complementary techniques such as X-ray diffraction, it effectively provides service to the mining and metallurgical industry. Mechanical behavior of materials in quasi static or dynamic conditions may be also analyzed. Besides, within the diverse departments there are a number of instruments, rigs and equipments to perform, for example, nondestructive evaluation and thermal analysis of materials.

Coupling between graphene and intersubband collective excitations in quantum wells

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Abstract

Recently, strong light-matter coupling between the electromagnetic modes in plasmonic metasurfaces with quantum-engineering electronic intersubband transitions in quantum wells has been demonstrated experimentally [A. Benz et.al., ACS Photonics **1** (2014) 906, J. Lee et.al., Nature 511 (2014) 65]. These novel materials combining different two-dimensional electronic systems offer new opportunities for tunable optical devices and fundamental studies of collective excitations driven by interlayer Coulomb interactions. In this work, our aim is to study the plasmon spectra of a hybrid structure consisting of conventional two-dimensional electron gas (2DEG) in a semiconductor quantum well and a graphene sheet with an interlayer separation of *a*. This electronic bilayer structure is immersed in a nonhomgeneous dielectric background of the system. We use a simple model in which the graphene surface plasmons and both; the intrasubband and intersubband collective electron excitations in the quantum well are coupled via screened Coulomb interaction. Here we calculate the dispersion of these relativistic/nonrelativistic new plasmon modes taking into account the thickness of the quantum well providing analytical expressions in the long-wavelength limit.

Effect of heat treatments and small addition AL-Ti-C alloy in aluminum foams.

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Abstract

In the last years, aluminum-based alloys have been widely studied in order to improve their physical and mechanical properties. The Al-Ti-C alloy was used as a grain refiner for aluminum and magnesium alloys [1]. The Al-Ti-C alloy exhibits particles of TiC, which are precursors of nucleation during the solidification. In the present work, the effect of the addition of nanocarbon on the microstructure of the Al-Ti -C alloy was studied. The Al-Ti-C alloy was prepared using an arc-melting furnace, under an argon atmosphere. Subsequently, the ingot was heat treatment at 1000 ºC for 40 minutes in order to inoculation of nanocarbon. The microstructure of the alloy was analyzed by means of X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The main results showed a needle shaped morphology $TiAl_3$ phase, with nanometric TiC, homogeneously distributed within the aluminum matrix. It is worthy of note that the formation of TiC with an average diameter of 100 nm and an equiaxial shaped morphology was successfully produced. The formation and size of the TiC particles could be attributed to the addition of nano carbon as precursor, following the reaction: $[Ti] + [C] \rightarrow TiC_{(s)}$ y $TiAl_3 + [C] \rightarrow TiC_{(s)} + Al_4C_3$.

Keywords: Aluminum alloys; Al-Ti-C Alloys; Nucleation; Microstructure; TiC; Nanocarbon

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Thermal Analysis of ladder type polymers: evaluated stability and degradation in different atmospheres

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A novel series of ladder type polymers (1a-1f)(1-4) was characterized by thermogravimetric analysis (TGA) technique to determine the thermal stability of polymers in different atmospheres (oxygen and nitrogen), analyzing the effect generated by substituents in the structure of the material. The molecules of the substituents (methyl, trifluoromethyl and phenyl) are highly stable at decomposition temperatures (≥ 400 ° C) and normal behavior under nitrogen and oxygen. However, when ladder polymers contain a voluminous substituent (isatin, methylisatin and phenylisatin), the behavior under nitrogen atmosphere is unstable (≤ 380 ° C) compared to the process in the presence of oxygen when it has a better stability (≥ 480 ° C). Infrared spectroscopy (IR) studies were performed to observe changes in functional groups. These results allow the possibility of creating intelligent polymers

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RHEOLOGICAL DETERMINATIONS SAOS, LAOS, PARALLEL and ORTHOGONAL SUPERPOSION FOR MATERIALS

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With questions like: how does flow start? how is flow defined (steady, transient, oscillatory, superimposed, turbulent …)?, when is flow considered linear and when non-linear?, how are microstructural changes characterized in any type of flow ? how close are those characterizations to real life conditions? and others, the science of rheology continues revealing powerful characterizations of flow conditions through interpretations of the viscoelastic nature of materials. Theoretical advances continue to be supported with advances in rheometry which allows accurate control and/or measure of force (shear linear, shear oscillatory, step, shear non-linear, superimposed, counter rotating, orthogonal…), displacement (shear linear, shear oscillatory, step, shear non-linear, superimposed, counter rotating, orthogonal..), temperature, environmental conditions (including experimental time), to quantify the viscoelastic nature of materials. Current testing protocols are accurately designed for SAOS, LAOS, PARALLEL SUPERPOSITION, COUNTER ROTATING FLOW and ORTHOGONAL SUPERPOSITION in SMT Rheometers. Concepts, data samples and data interpretations is the focus of this presentation.

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POTASSIUM DOPED MATERIALS AS CATALYSTS FOR TRANSESTERIFICATION REACTION

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As public concern about polution increases and world petroleum reserves decreases, biodiesel is becoming more and more suitable alternative to fosil diesel fuel [1,2]. However, the current cost of biodiesel production is higher than that of petroleum-derived diesel [3]. The use of heterogeneous catalysts in the transesterification of vegetables oils or animals fats with a short chain alcohols has the potential to simplify the purification of products, reduce the operational cost and obtain high quality methyl esters and glycerol [4,5]. In the present work, we reported results obtained in the transesterification of soybean oil with methanol in presence of sodium trititanate nanotubes doped with different amounts of potassium as catalysts. Nanostructured sodium trititanate (NTNa) was synthesized by an alkali hydrothermal treatment of TiO_2 with sodium hydroxide as it was reported previously by Kasuga et al [6] . In order to inquire into the effect of potassium addition on the catalysts' properties, different amounts of potassium were added to the samples by a simple impregnation method. Prepared catalysts were characterized by N_2 physisorption, X-ray diffraction, SEM-EDX, transmission electron microscopy (TEM) and temperature-programmed desorption of CO_2 (TPD-CO_2). Catalytic activity tests were performed in transesterification of soybean oil with methanol in a 100 mL stainless steel batch reactor (Parr) equipped with a stirrer and temperature controller in presence of 0.5 g of the catalyst. For all experiments, a temperature of 80 °C and reaction time of 0.5 h were fixed. The biodiesel yield was calculated based on ^1H NMR as described in [7]. Crystalline structure of NTNa was confirmed by powder XRD as $Na_2Ti_3O_7 \cdot xH_2O$. No changes in the crystalline structure were observed after the incorporation of potassium by impregnation. TEM and SEM characterizations of the samples corroborated the presence of nanotubular structures in the catalysts. TPD-CO_2 results showed that the incorporation of potassium increased the total amount of basic sites in the catalysts that produced a noticeable increase in their catalytic activity in transesterification reaction. Obtained results showed that high yields of biodiesel (92-95%) were obtained with the synthesized catalysts in a short reaction time, in mild reaction conditions. An increase in the samples' potassium loading resulted in an increase in catalytic activity and biodiesel yield.

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Pyridine-based derivatives for potential use as chromophores for Dye-sensitized solar cells

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In this research the photophysical properties of 7 electron donating pyridine systems with possible applications in the design of solar cells sensitized by dyes (DSSCs) were studied. The fundamental objective of this research project is the design of new materials and the characterization of its luminescent properties of the systems ligand initially and as work later their metal-organic complexes, where the process of electron transfer to nanoparticles of oxide Titanium (TiO2) is highly efficient. Specifically, the characterization of the luminescent properties of each ligand system was performed based on computational calculations developed using the DFT methodology, as well as its time-dependent counterpart (TD-DFT)..

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Materials for downconversion in solar cells: Perspectives and challenges

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Solar energy has an enormous potential to solve society energy needs in a sustainable way. Notably, photovoltaic systems (PV) permit to obtain electricity based on solar energy. However, some issues must be addressed to establish PV as a reliable source of electrical power, for example, its low energy density. One of the approaches to improve the performance of PV systems is to utilize the solar spectrum in solar cells efficiently. Downconversion (DC) is a process where a high energy photon is converted into two or more photons with lower energy. Trough downconversion is possible to use a wider portion of the solar spectrum raising the efficiency in different kinds of solar cells. The present paper reviews the state of the art of materials and methods used to take advantage of downconversion processes in solar cells. Here we discuss some of the pros and cons of different designs in solar cells as well as the main characteristics of the materials utilized.

FORMATION OF RHOMBOHEDRAL PHASE IN GRAPHITE UNDER ITS BALL MILLING IN THE PRESENCE OF N,N-DIMETHYLFORMAMIDE

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High-quality graphene can be produced by means of mechanical splitting of single crystals of graphite [1], however, this method is unsuitable for mass production. The methods of graphite grinding using ball-mills and ultrasound irradiation of graphite in liquids [2-6], which allow production of graphene in large quantities, gained recently high popularity. N,N-dimethylformamide (DMF) is often used in the method of ultrasound irradiation of graphite (3, 7-9].

Primary attention was paid to the yield and characteristics of graphene obtained by these two methods. Residual graphite not converted to graphene was usually considered as waste. In our opinion, this residual material deserves to be studied because this can allow one to obtain new data on the mechanism of graphite splitting or about graphite, which is unsuitable for graphene production.

This report is devoted to an experimental observation of the formation of a rhombohedral phase in products of graphite grinding using a vibrational ball-mill in the presence of DMF. For comparison, we studied also products formed under ultrasound irradiation of graphite in DMF and not found a rhombohedral phase in its.

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COMPOSITE MATERIALS BASED ON STYRENE-BUTADIENE COPOLYMER AND CHICKEN FEATHERS

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The main component of chicken feathers (CF) is keratin, a protein that posses good properties asi durable, insoluble and provides high mechanical and thermal resisstance, which make i tan interesting material to be used as reinforcer of polymeric matrix. The present work was focussed to obtain a composite material base don styrene-butadiene copolymer (SBS) and CF. First, CF were washed with wáter, acetone and etanol to sanitize, and then dryed. From CF the part used in present work was the quill, the central component of feather, which was milled, and sieve to obtain a particle size of 707 μm.2 types of SBS copolymers were used, one with linear structure and second one with radial structure, with the aim to evaluate the effect of copolymer structure in composite. Composites SBS/CF were prepared by melting mix and ZnO was added to composites as compatibilizer trying to improve the physical performance of materials. CF was added in 2 concentrations, 1 and 3 phr, and temperature in mixing was 90° C for linear and 130°C for radial copolymers, with 3 different speed: 30, 50 and 70 rpm, keeping the mixing time constant in 20 min. The SBS-CF composites were evaluated by thermal thecniques as TGA, DSC, and DMA. For DMA analysis materials were compacted by press with 350°F with 10 Tons during 15 min. The thermal decomposition and dynamic mechanical behavior increase with addition of ZnO.

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PANI/OMMT BASED SEMICONDUCTING COMPOSITES

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The development of polymer nanocomposites has been extensively studied during the last years in order to get an improvement on conventional polymer properties [1]. To enhance polyaniline (PAni) electrical conductivity and mechanical stability, the formation of polyaniline/clay nanocomposites (PCNs) has been proposed by several authors [2,3].

This study deals with PCNs synthesis by in situ oxidative polymerization in the presence of clay as previously reported [4–8]. The effect of the preparation conditions, such as the agitation technique and the type of doping acid, on the morphological configuration and electrical conductivity of PCNs was studied by X-ray Difraction (XRD), Scanning Eletron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Four Probe method.

It is found that PCNs morphology is strongly influenced by the doping acid, but not by the agitation treatment. The formation of nanofibers around 50-100 nm thick and the intercalation and exfoliation of clay is observed on the micrographs. On the other hand, electrical conductivity appeared to be affected by both doping acid and agitation treatment.

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Fluoride adsorption on Mg-Fe and Mg-Al-Fe hydrotalcite

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The water pollution is a current problem, it is result of acelerate human development [1]. Among these contaminants are fluorides, which are used in aquaculture. This work proposes the adsorption method to reduce the concentration of fluoride ions in aqueous solution [2]. Two hydrotalcite compounds MgAlFe and MgFe were synthesized by coprecipitation (HTAlFe and HTMgFe). The laminar structure of hydrotalcites and the mixture of oxides after calcination at 500 ° C (HTCAlFe and HTCMgFe) was confirmed with FTIR and XRD. The memory effect of these materials allowed to carry out the adsorption process; when the adsorption capacity of the materials, provenient from the adsorption kinetics calculus, was compared. The most adsorb capacity of fluorides is of the solid HTCMgFe with 2.0 mg F - / g of HTCMgFe owing to it contain a greater amount of Fe, which has shown a great affinity towards fluoride ion [3], while HTAlFe has fewer FeOH surface groups to interact with fluoride. Therefore, the proposed material HTCMgFe is an adsorbent suitable for the removal of fluorides in aqueous solution.

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Depósito de nano-cúmulos de silicio embebidos en nitruro de silicio para aplicaciones fotovoltaicas.

Durante mi estancia con la Dra Marel Monroy, se realizaron depósitos de películas delgadas de nitruro de silicio (SiN_x) con nano-cúmulos de silicio (nc-Si) utilizando la técnica PECVD, cuyos precursores fueron amoniaco, argón, diclorosilano e hidrógeno. Se hicieron diversas corridas. En la primera se controló el flujo de hidrógeno, mientras que en la segunda se varió el flujo de amoniaco, y por tanto, se controle la relación de nitrógeno/silicio. Esto con el propósito de conocer el efecto del flujo de cada uno de ellos sobre sus propiedades ópticas.

Se observó que al variar el flujo de hidrógeno, hay una disminución en el espesor de los depósitos. Para la corrida en donde se controló la relación nitrógeno/silicio, se observó un incremento en la tasa de depósito, así como del índice de refracción y en el corrimiento del pico de emisión observado por fotoluminisciencia. De los depósitos realizados, se eligieron dos; uno que tuviese emisión en la región azul y un depósito cuya emisión se encontrara en la región roja del espectro visible, y así hacer una película TANDEM. Se observaron dos picos de emisión, que corresponden a los picos de las películas depositadas individualmente.

A partir de los resultados obtenidos, se observó que el efecto del hidrógeno sobre la fotoluminiscencia está más relacionada con la forma del espectro que con el máximo de la emisión. De acuerdo a la teoría de confinamiento cuántico esto significa que la cantidad de hidrógeno utilizada durante el depósito determina la distribución de tamaños de los nano-cúmulos dentro de la película. Además, también se pudo concluir que la variación del flujo de amoniaco permite obtener películas más enriquecidas en silicio para flujos pequeños y viceversa. Para las películas enriquecidas en silicio la emisión de fotoluminiscencia ocurre en el extremo cercano al rojo y la banda de absorción óptica se corre a energías menores. Esto se puede asociar con el tamaño de los nanocúmulos de silicio que se forman dentro de la capa de nitruro de silicio mediante la teoría de confinamiento cuántico.

Para continuar con el trabajo, también se estudiaron los mecanismos de relajación que ocurre en los nanocristales de silicio, utilizando la técnica de fotoluminiscencia resuelta en tiempo. Se hizo una corrida variando el flujo de amoniaco. En este trabajo, se observó un corrimiento del pico de PL hacia el azul conforme se incrementó el flujo de amoniaco, al medirse en el régimen de excitación continua. Además, se observó que el pico de PL se corre hacia menores longitudes de onda conforme aumenta la diferencia temporal entre excitación y detección (gate-widh de la ICCD).

El decaimiento de la PL en función del tiempo también fue consistente con la recombinación a través de estados de cola de bandas en nitruro de silicio, tanto en el tiempo de recombinación del orden de ns, como en el comportamiento de exponencial extendida. Se observó una contribución entre 460-475 nm que se atribuye a recombinación a través de estados de oxidación de tipo Si=O por la posición espectral y el tiempo de recombinación del orden de µs. Esto fue particularmente notable en la muestra más oxidada (10 sccm de amoniaco).

La única muestra que resultó rica en silicio (20 sccm de amoniaco) presenta una dinámica de recombinación completamente distinta a las otras dos. Esta muestra podría tener nc- Si y la PL podría ser debida a recombinación radiativa por confinamiento cuántico.

HYBRID SYNTHESIS OF HIERARCHICAL POROU STRUCTURES FOR THE OBTENTION OF FUNCTIONAL BIOCERAMIC SCAFFOLDS

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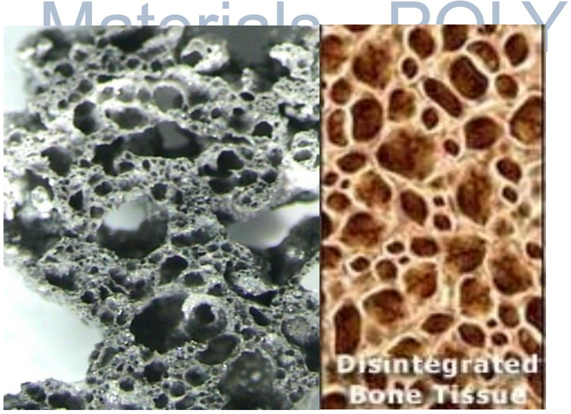
Since the 1960s there has been a continued interest in the development of substitute biomaterials for bone, cartilage and cutaneous grafts to perform the repair of different sections of human tissue, especially for the correction of post-traumatic or even congenital defects. Although methodologies have been designed to perform very efficient autologous grafts, there is a considerable limit regarding the small amount that can be obtained to cover a large bone defect, in addition to the recovery that results in obtaining this. Thus, the development of an osteogenic and antibiotic matrix in which osteoconduction, osteoinduction and osseointegration are simultaneously potentiated for the biological repair of such defects is necessary. The design of ceramic matrices from bioceramics such as bioglass, titania and ceria in conjunction with cell therapy have offered a wide panorama of tissue replacement, although there are certain problems to overcome such as the production and compatibility of cells in the biological area and the development of interconnected networks in the field of material. In this work we propose the development of reconstruction matrices of different tissues whose bioactivity is superior to that obtained in other work groups with this type of materials that present a simple structure, developing hierarchical porous structures from the hybrid synthesis, allowing the formation of three-dimensional structures such as biomimetic scaffolds. By using reaction systems such as sol-gel in conjunction with spray-drying techniques it is possible to produce active bioglass whose composition and mechanical properties comply with the parameters established by different institutions such as the FDA. In addition, the use of these methodologies allows the design of aggregates of nanoparticles with controlled porosities, determined diameters and with modifying agents as silver atoms or biopolymers, facilitating the experimental design and the analysis of variables in it, also helping to overcome the limitation of the design of interconnected three-dimensional structures. The biocompatibility of scaffolds obtained was tested in chicken embryos and in vitro cell cultures. The following optical photographs compare the disintegrated bone tissue structure with the structures of the obtained bioceramic scaffolds.



Visible luminescence of silicon quantum dots: an experimental and theoretical approach

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The impact of the surface reconstruction of the density distribution and photoluminescence of silicon quantum dots (QDs) embedded in a silicon oxide matrix (SiO_x) has been studied. Annealing treatments carried out on the as-deposited samples provoked the effusion of hydrogen species. Moreover, depending on the surrounding density and coalescence of QDs, they resulted in a change in the average size of the particles depending on the initial local environment. The shift in the luminescence spectra all over the visible region (blue, green and red) shows a strong dependence on the resultant change in the size and/or the passivation environment of QDs. Density functional theoretical (DFT) calculations support this fact and explain the possible electronic transitions (HOMO–LUMO gap) involved. Passivation in the presence of oxygen species lowers the band gap of Si_{29} and Si_{35} nanoclusters up to 1.7 eV, whereas, surface passivation in the environment of hydrogen species increases the band gap up to 4.4 eV. These results show a good agreement with the quantum confinement model described in this work and explain the shift in the luminescence all over the visible region. The results reported here offer vital insight into the mechanism of emission from silicon quantum dots which has been one of the most debated topics in the last two decades. QDs with multiple size distribution in different local environments (band gap) observed in this work could be used for the fabrication of light emission diodes (LEDs) or shift-conversion thin films in third generation efficient tandem solar cells for the maximum absorption of the solar spectrum in different wavelength regions.

Celdas solares de silicio con heterouniones de óxido de molibdeno (MoO_x)

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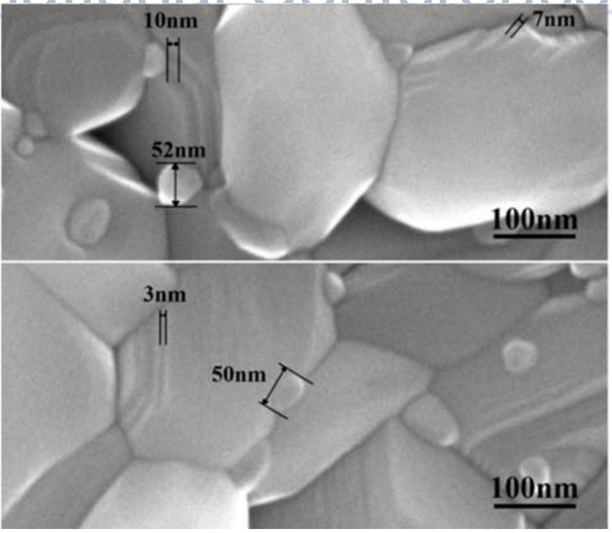
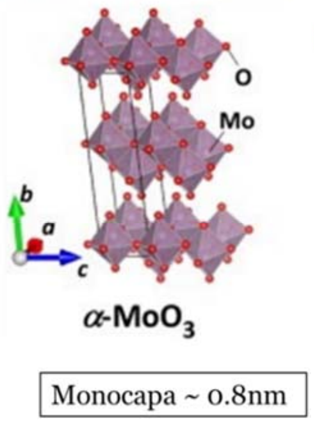
En el presente trabajo, se obtuvieron películas delgadas de MoO_x, crecidas mediante la técnica de sputtering a partir de un blanco de molibdeno. Se realizó difracción de rayos X (XRD), microscopía de fuerza atómica (AFM) y UV-Visible (UV-VIS) con el fin de investigar las propiedades estructurales, morfológicas y ópticas de las muestras. Optimizando las diferentes condiciones de depósito, las películas delgadas de MoO_x se crecieron con espesores que variaron desde 15 nm hasta 240 nm. El análisis realizado utilizando la espectroscopía XRD mostró la presencia de MoO_x (donde x, podría variar de 1 a 3). Especialmente, se observaron muestras con un valor de estado de oxidación ($x = 2$) antes del tratamiento térmico en aire y que cambia a 3 después del tratamiento. Adicionalmente, se encontraron cambios en la respuesta de fotoconductividad de las películas delgadas debido al tratamiento térmico. Las películas delgadas crecidas en este trabajo fueron usadas para la fabricación de celdas solares sobre substratos tipo n y p; lográndose un aumento importante en la eficiencia final de los dispositivos, cuando el MoO_x fue utilizado como campo eléctrico posterior en las celdas solares de silicio monocristalino.





ANALYSIS OF THE OPTOELECTRONIC AND STRUCTURAL PROPERTIES OF A DSSC WITH UNION ZNO / TIO_2 AND ITS EFFECT ON CONVERSION EFFICIENCY.

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The growing demand for energy and the large amount of waste generated worldwide makes the current energy model unfeasible where non-renewable sources of energy are paramount. There is no doubt that a new paradigm is required where the supply of energy for global development is based on environmentally friendly, renewable, economic and for all sources. Solar energy still presents challenges in the technological and economic aspects that can only be solved as the arduous task of the researcher is bearing fruit.

Nanoparticles of zinc oxide and titanium dioxide were synthesized by precipitation and forced hydrolysis methods, respectively. The influence of the optical, electronic, structural and electrochemical properties of the ZnO / TiO_2 bond on the performance of photovoltaic efficiency was studied. The synthesized samples have been characterized structurally, morphologically, optically and electrochemically using XRD, MEB, UV - Vis spectroscopy and electrochemical impedance and their application in a dye - sensitized solar cell (DSSC) based on the N719.

The average size of the zinc oxide crystal is in the range of 17-24 nm while the average size of the titanium dioxide crystal is between 50-60 nm. The optical banned band of these materials is 3.5% lower than that reported for zinc oxide and 1.5% lower for titanium dioxide. The DSSC based on N719 showed an increase in conversion efficiency (50%) due to the interfacial structural change in ZnO / TiO_2 binding.

Increasing the conversion efficiency of photovoltaic cells translates as a better use of solar energy, as long as the costs of materials and processes involved are cheap and their toxicity is relevant.

PREPARATION AND CHARACTERIZATION OF POLYLACTIC/POLYCAPROLACTONE/BIOGLASS COMPOSITE

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Currently, there is a great interest on the development of biodegradable and biocompatible materials suitable for a variety of biomedical applications, such as temporary scaffolds that facilitate tissue regeneration. In this sense, polymer/ceramic biomaterials have been considered as potential application as these. Some of the most promising ceramic are hydroxyapatite, calcium phosphates, and bioactive silicate glasses. Bioactive glasses are amorphous silicate-based materials which bond to bone and can stimulate new bone growth while dissolving over time, making them candidate materials for tissue engineering.

In this work, novel composite for tissue engineering Polylactic/Polycaprolactone/bioglass (PLA/PCL/G5) were prepared with different contents (wt%). It was found that the polymer was possible to load up to 30 wt % bioglass. Polylactic acid (PLA) synthesis was realized by polycondensation technique. Bioglass were synthesized by the sol–gel technique and then mixed with synthetic polylactic acid (PLA) and polycaprolactone. The morphology and compositional properties of the composites with different content of bioglass was investigated by X-Ray Diffraction (DRX), Fourier transformed infrared spectroscopy (FT-IR), and Scanning Electron Microscopy (SEM) characterization.

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Design of heterocyclic-based privileged ligands

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Catalysis is the most powerful tool in organic synthesis, for this reason, almost 70% of compounds used in our daily lives are prepared using at least, a catalytic step in their obtainment. Nowadays, the design and synthesis of new catalysts is an area in constant development and is focused on improving processes, to avoid special reaction conditions, such as, the use of inert atmosphere, deoxygenation, or dryness conditions.

For this reason, many researchers around the world are interested in the rational design and development of modular ligands, for obtaining catalytic precursors capable to achieve a quite range of catalytic applications. These privileged ligands, normally have a rigid structure with different functional groups to bind strongly to reactive metal center, as well as, generate a highly active and selective catalytic system.

In this seminar, we will discuss about the design and synthesis of novel bidentate ligands and their applications as part of different catalytic precursors used in a variety of carbon-carbon coupling reactions in a microwave enhanced protocol,[1] catalytic hydrogen transfer, asymmetric allylic alkylation,[2] C-H direct functionalization of arenes,[3] among others.[4] Additionally, some of these complexes work well in presence of moisture and oxygen with high TON and TOF values.

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New Pt(II) Complexes with fluorinated ligands for Alzheimer Disease

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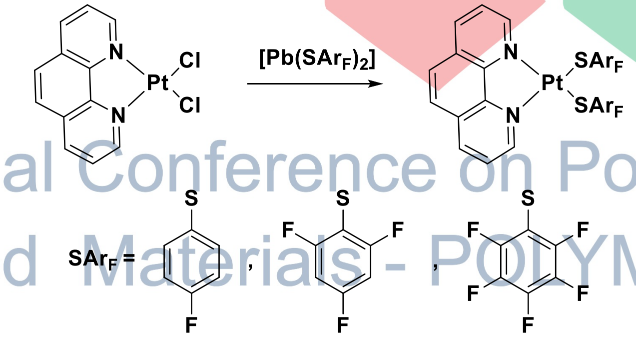
The interest on the chemistry of Pt(II) complexes in biological and medical applications has flourish since the discovery of the cytotoxic activity of cisplatin. Due to the mechanism through which cisplatin works scientists have extended his potential use for the treatment of Alzheimer's disease.

Alzheimer's disease (AD) is a progressive neurodegenerative condition, characterized pathologically by the presence of extracellular amyloid plaques in the brain. Anti-AD therapeutic strategies have focused, on the inhibition of the production of Aβ, on the inhibition of aggregation of Aβ, among others.[1]

It has been seen that the aggregation and neurotoxicity of Aβ is modulated by the addition of $[PtCl_2(phen)]$ and similar complexes. These Pt(II) complexes target the metal binding site of Aβ by exchange of the monodentate chloride ligands followed by coordination of the Pt(II) ion to the imidazole functional group in the histidine residues to give $[Pt^{II}(phen)–A\beta]^{2+}$ adducts. The coordination of the $[Pt(phen)]^{2+}$ complexes to Aβ inhibits the aggregation of the peptide and leads to precipitation of amorphous aggregates rather than amyloid fibrils.[2]

Knowledge of the atomic structure of the complexes made by Pt(II) compounds with Aβ would facilitate Aβ-specific therapeutic and diagnostic development.

Following our interest in the development of new Pt(II) complexes we decided to prepare a series of platinum complexes with fluorinated thiophenol fragments, shown in **Scheme 1,** these may help to enhance the activity of the complexes since aromatic fluorinated functionalities favored both π-π interactions and transporting through the membrane cell.



Scheme 1

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Silicone polymer composite with graphene.

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Polymers have been used because of their outstanding properties, sometimes even better than other materials as metals. Another type of materials which have remarkable properties are nano particles of carbon, as nanotubes of carbon, graphene and graphene oxide. Nowadays the use of nanoparticles of carbon has raised due to their properties and wide range of application on many disciplines, owing to this, researchers are working on the development of new materials and improving of others. Previous researches report that, by incorporation of these nano particles of carbon such as graphene oxide in polymer´s matrix improve their properties. This research aims at the developing of a silicone polymer where their mechanical properties and thermal properties are enhanced by adding of graphene oxide. Graphene oxide was dispersed by ultrasonication to an appropriate incorporation to the polymer´s matrix. On this research, composite of silicone polymer-graphene oxide is characterized by Atomic Force Microscopy (AFM), Raman microscopy and Thermogravimetric analysis.

STABILITY STUDY OF COMPLEX MIXTURES LIPOSOME-HYDROCOLLOIDS.

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Among the different techniques of microencapsulation, is the formation of liposomes, which are spherical structures, composed of amphiphilic phospholipids forming a lipid bilayer within which an aqueous phase with soluble molecules inside can be contained [1]. These structures are used in the pharmaceutical, molecular biology and food areas, for the protection by microencapsulation of molecules such as proteins, vitamins, minerals, dyes, flavorings, DNA and RNA among others. The important problems that limit the commercial use of liposomes are the ease these structures present to fusion, aggregation, flocculation and precipitation, which contributes to the destabilization and destruction of liposomes. These problems are the result of changes in temperature, pH, and concentration of divalent cations and ionic strength of the medium [2]. In order to counteract the effects of instability, the research has been directed to three main areas [3]: 1) manipulation of the lipid composition of the vesicles to produce particles with less release of their contents; 2) lyophilization in the presence of sugars of low molecular weight; and 3) addition of cholesterol, which increases the rigidity of the bilayer membrane [4].

In our research, the stabilization of the liposomal structure has been tested by the presence of polymeric additives of hydrocolloidal type. For this reason, the objective of this work was to develop a methodology to obtain complex mixtures of liposomes and polysaccharides, whose stability was studied against factors such as temperature (0, 3, 25 y 50 ºC), concentration and pH (acid, neutral and basic). Three polysaccharides were studied: xanthan (branched polysaccharide), guar and algarrobo (linear polysaccharides), at three concentrations (0.05, 0.5 and 1%), for their microscopically characterization and functional studies used protein BSA. The study of transmission electron microscopy evidenced the stability of the self-structured liposomal system in complex media. Mainly, xanthan hydrocolloid maintain the stability of liposomes to release of BSA at temperature and pH studies.

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EFFECT OF SOY PROTEINS IN THE THERMAL BEHAVIOR OF GLYCOPROTEINS (CRUDE AND PURIFIED MUCINS)

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Mucin is a biopolymer of proteins and carbohydrates, are importance in mammals; mucins are secreted in the gastrointestinal, respiratory, and reproductive organ of mammals [1]. Due to the complex structure of mucins, is difficult to explain how these molecules are associated, which *in vivo* are essentially resistant to proteolytic enzymes. Also, the protective function in the stomach mucose has been associated with the viscoelastic properties of mucin. It is believed that aggregation/gelation in the mucose has a critical role in the stomach capacity of not being attacked by the gastric juices. The mucin has a molecular weight of ≈ 2 x 10^6 Da, and consists of four units of glycoprotein.Each unit is composed of two regions; one is rich in aminoacids linked to oligosaccharides in a branched structure. The other region is composed of aminoacids characteristic of globular proteins [2, 3]. The study of the interactions of this glycoprotein is of great importance due to the protective functions and the recent interest in the study of mixtures with proteins; within these, the proteins of vegetable origin such as soy. Soy proteins have acquired great interest due to their functional properties, excellent nutritional values and their effect on health. They consist of four main components, globulins 2S, 7S, 11S and 15S [4].

The aim of this study was to determine the thermal behavior of crude (MC) and purified (MP) mucin mixtures with 1:1 blended soy protein. A differential scanning calorimeter (TA Instruments, USA) was used, samples were placed in hermetically sealed aluminum trays, a ramp of 5 °C/min was used in a range of 25 - 260 °C under an inert atmosphere of N_2. According to the obtained thermograms, glass transition values greater than 6-10% in the MC-protein mixtures are probably due to the higher carbohydrate content in the system. The enthalpies and heat capacity obtained were ΔH (2.5-136 J/g) and ΔCp (0.1-35 J/g °C) in MC-soy proteins, ΔH (1.9-158 J/g) and ΔCp (0.05 -23 J/g °C) in MP-soy proteins. It presents a 16-19% higher ΔH in mixtures of MP-proteins than in MC-proteins; However, ΔCp are 52% higher in the MC mixtures, so higher heat of reaction is required to denature the proteins in the MP mixture.

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IMPEDANCE SPECTROSCOPY OF POLYVINIL ALCOHOL AND MULTI-WALL CARBON NANOTUBES COMPOSITE MEMBRANES

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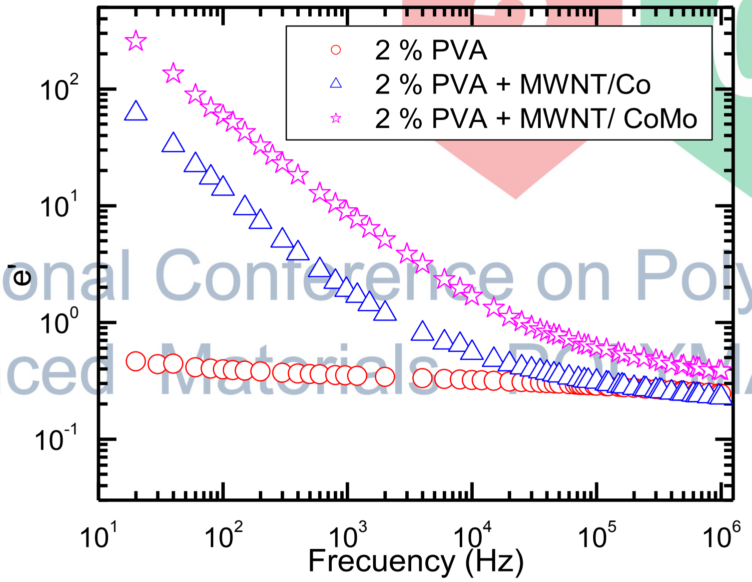
The dielectric response of composite membranes formed by multiwall carbon nanotubes (MWNT) synthesized by microwaves [1], and polyvinyl alcohol (PVA) were measured in the 20Hz to 1MHz frequency range at room temperature. In the synthesis of MWNT, cobalt (Co) and cobalt-molybdenum (Co-Mo) particles were used as catalysts and remain attached to the synthesized MWNTs. Both these two types of MWNT were used to prepare the composite PVA/MWNT membranes. The membranes are 2 cm in diameter, 100 µm thick, and with 1 wt% concentration of MWNT. Figure 1 shows curves of the real part of the dielectric constant (ε') as a function of frequency. The observed behavior show evidence of a dielectric relaxation mechanism occuring around the measured frequency range which is adscribed to MWNT-PVA polarized interactions. The Havriliak-Negami model is used to describe the measured behavior.



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DEVELOPMENT OF COORDINATIVELY AND ELECTRONICALLY UNSATURATED ZINC AND SCANDIUM LACTIDE POLYMERIZATION CATALYSTS

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Polylactide (PLA) is a biodegradable, biocompatible polymer that can be synthesized *via* the ring-opening polymerization of lactide. Since corn, beets or other plant material can be used as the feedstock for the production of lactide monomers, polylactide has become an attractive alternative to conventional polyolefins. In fact, it is increasingly being touted as a viable alternative to conventional petrochemically derived plastics. One of the main reasons for this is that the physical properties of PLA are similar to those of traditional polyolefins.[1]

The most common initiator used to synthesize polylactide for commodity applications on an industrial scale is stannous octoate. Unfortunately, this system suffers from poor molecular weight and stereocontrol, and ever increasing public concern over potential toxicity. As such, there is need for new types of catalysts that polymerize lactide. Although a variety of discrete single-site metal complexes promote the ring-opening polymerization of lactide, the scope of available catalyst systems remains limited, as do the properties of the polymeric materials produced. Furthermore, the relationship between catalyst structure, and both catalyst activity and polymer microstructure, is very poorly understood.

To this end, we have developed a diverse family of coordinatively and electronically unsaturated cationic zinc and scandium complexes.[2] The metals are supported by neutral dibenzofuran and pyrrole-based pincer ligands. These complexes are prepared by a route whereby the neutral bisphosphinimine ligand is first protonated with an appropriate Brønsted acid. The resultant protonated ligand is then reacted with an organometallic precursor to afford the corresponding cationic zinc or scandium alkyl, alkoxide, or aryloxide species via a simple and efficient alkane elimination pathway.

The evolution of these systems, from proof of concept to highly active catalysts, will be presented with emphasis upon polymer synthesis and characterization. Elucidation of the mechanism of polymerization will also be discussed. Notably, the steric and electronic properties of the ligand framework can be readily fine-tuned, including introduction of chiral functionalities, by modification of the N and P substituents. Such modifications have proven to have a profound impact on the catalytic properties of the complexes, ultimately providing access to living catalyst systems that exhibit extremely high activity at ambient temperature and low catalyst concentration.

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Castor oil (*Ricinus communis*): renewable resource for cross-metathesis degradation of *cis*-1,4-polybutadiene.

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Nowadays, sustainable development demands researches that promotes the conservation of natural resources and environment protection. In this regard, the recycling of waste materials is a fundamental task. For example, in 2016, natural and synthetic rubber worldwide consumption was $27x10^6$ tones[1]. In recent years, it has been reported several studies about *cross*-metathesis degradation of both natural and synthetic rubber with functionalized olefins [2] and essential oils [3]. In this work, castor oil (*Ricinus communis*) a renewable resourse of low toxicity, was used as both chain transfer agent (CTA) and green solvent in the *cross*-metathesis degradation of *cis*-1,4-polybutadiene (PB) with (1,3-dimesityl-4,5-dihydroimidazol-2-ylidene)(PCy_3) Cl_2Ru=CHPh (**I**). Castor oil is not a edible oil and it has special properties compared to the conventional vegetable oils [4]. According to results, PB was degraded in a controlled manner into oligomers, variying the molar ratio rubber/CTA, even with low molar ratio of catalyst ([C=C]/(**I**)= 10,000). Thus, molecular weight of PB decreased from $M_n= 10^6$ to $M_n= 10^3$ g/mol. Degradation oligomers were transesterified in the same batch reactor by basic homogeneous catalysis (NaOH-methanol, 45 °C, 3 hours) to obtain the mixture of products: hydrocarbons with low molecular weigtht and methyl esters ($M_n= 10^2$ g/mol). These products have a remarkable potential aplication as biofuels.

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Study of the behavior of casting 70Cu-30Zn alloy in ammonium hydroxide assisted cracking.

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Abstract

The present work is a study of the effect of susceptibility to stress corrosion cracking (**SCC**) of an alloy of **70Cu-30Zn** as cast (weight %). The testing medium employed was ammonium hydroxide solution (**NH_4OH**). The electrochemical and stress corrosion tests were performed at different concentrations of the electrolyte (**1, 0.5 and 0.1 M NH4OH**). The SCC tests were performed on compact stress samples, applying an initial axial load of 90% of the yield strength of the cast alloy. The charged samples were subjected to the corrosive agent until arrest of crack growth. The crack growth was monitored as a function of time. Subsequently, the surfaces of the specimens and their fracture surfaces were analyzed by scanning electron microscopy (**SEM**). The results obtained showed that the susceptibility to corrosion is function of the concentration of the electrolyte, since it is related to the process of rupture of the passive layer of the material.

Keywords: Cu base alloy, electrochemical tests, SCC.

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REPRODUCIBLE AND VERSATILE PROCESS TO OBTAIN CHITOSAN-TRIPOLYPHOSPHATE BEADS

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Chitosan and tripolyphosphate are biocompatible compounds that together can form beads suitable for several functions such as a carrier, a spherical surface to anchor molecules with different characteristics, a resin for the treatment of wastewater, etc [1]. Many parameters in the elaboration process of these chitosan-tripolyphosphate beads (CTPP-beads) can be varied and controlled to obtain particles with different diameters, swelling degrees and roundness [2]. These response variables influence the applicability of the CTPP-beads, and for that reason a well-established making process is necessary. Commonly the literature just report the percentage of chitosan and tripolyphosphate mass used [3], and omit parameters such as viscosity of the chitosan solution and the role of the tripolyphosphate pH in the CTPP-bead´s roundness. In this wok we report the optimal ranges of the process variable to obtain spherical and stable CTPP-beads as shown in figure 1.

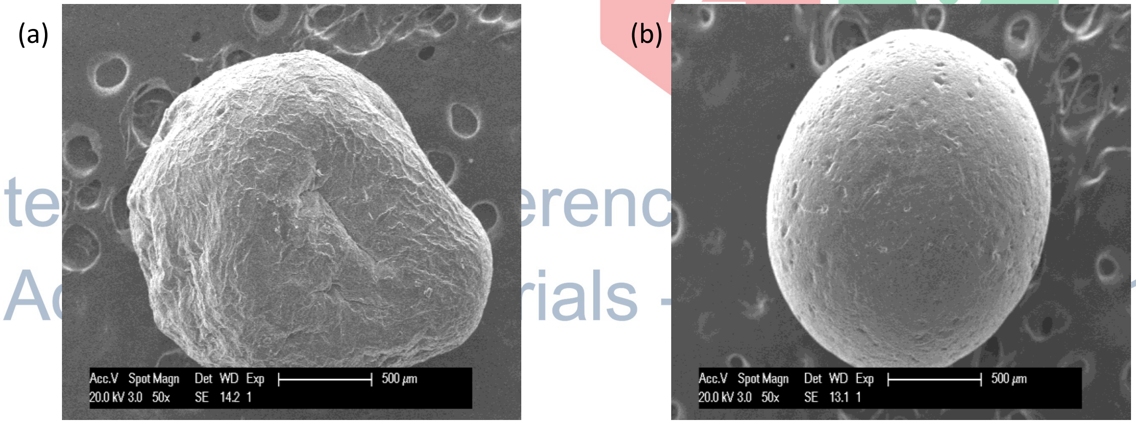

Figure 1. CTPP-beads (a) out and (b) within the optimal parameters of the process.

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SPECTROSCOPY AND MICROSCOPY CHARACTERIZATION OF POROUS POLYMERS SYNTHESIZED USING HITENOL BC 10 AS POLYMERIZABLE SURFACTANT

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Polymerization in bicontinuous microemulsion results in a polymer with an interconnected porous structure [1]. A series of porous poli(butyl acrylate-co-Divinylbencen-co-Hitenol BC 10) were synthesized and it was investigated the effect of the organic fase (OF)/aqueous phase (AF) ratio (1/1; 2/1 y 5/1) using Hitenol BC 10 (Polyoxyethylene alkylphenyl ether ammonium sulfate). Reactants were mixed, stirred mechanically and polymerized at 70°C. The conversion was close to 90% wt and it was proved that all reactants were present in the polymer chains. The presence of butyl acruylate was confirmed with Raman spectroscopy using the 1732 cm^{-1} chemical shift meanwhile the Hitenol BC 10 was confirmed by solid state $C^{+}13$ NMR using the signal close to 70 ppm. Divinylbencene was confirmed by Raman and $C^{+}13$ NMR. Additionally it was possible to identify the opened doble bond resulting from the polymerization and the residual double bond of the divinilbencene. Figure 1 shows that the morphology changes drastically according to the OF/AF ratio with pore zises ranging from micrometer to the nanometer scale. The specific area ranges from 15 to 30 m^2/g.

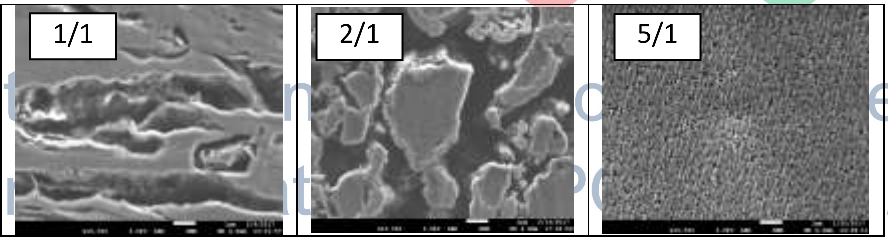

Figure 1. SEM images of the porous copolymers

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Acknowledgements

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Biopolyesters preparation from tomato agroresidual wastes using ionic liquid

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10,16-dihydrohixihexadecanoic acid (10,16-DHPA) is one of the main components of cutins (Heredia, 2003), which forms part of the cuticle of different plants and fruits, This monomer is the most abundant and have great potential for its use in the synthesis of new biopolyesters or biopolymers. New routes of chemical synthesis are being used, using ionic liquids, as solvents and catalysts, replacing the organic solvents.

This work had as main objective the study of the polymerization reaction of the 10,16-DHPA, in ionic liquids to obtain biodegradable polyesters.The polymers obtained at different temperatures of 10,16-DHPA had different physico-chemical characteristics. The polymers obtained at 80 ° C were mainly powders, whereas those obtained at 90 ° C were amorphous solids and those obtained at 100 ° C were mainly of viscous consistency (Fig. 1).

According to the analysis by FTIR and CPMAS ^{13}C NMR, the reaction produces mainly linear polymers. However, at higher times and elevated temperatures, it can produce polymers cross-linked with the hydroxyl of the C-10 position.

Conclusions. The use of choline chloride: 2ZnCl2 for obtaining polymers obtained from long chain aliphatics is an efficient, fast and inexpensive process. The polymers obtained may have a high potential for use in the biomedical industry.

Fig. 1. Polymers derived from 10,16-DHPA, obtained at different temperatures.

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Acknowledgements

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EFFECT OF FeO(OH) NANOPATICLES CONTENT IN THE PROPERTIES OF P3HT/FeO(OH) COMPOSITES AND THEIR APPLICATION IN SOLAR CELLS.

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In this work we report the synthesis and characterization of P3HT-FeO(OH) nanocomposites, as well as their application in solar cells. The P3HT-FeO(OH) nanocomposites were synthesized by in-situ oxidative chemical polymerization at different concentrations of FeO(OH) (weight ratios 3HT/FeO(OH): 1/0.03, 1/0.05 and 1/0.08). Effect of FeO(OH) nanoparticles content in P3HT on its physicochemical properties was studied. The nanocomposites showed higher absorbance, better thermal stability, good regioregularity and greater photoluminescence in relation to P3HT. The following configurations were used for the manufacture of solar cells: ITO/CdS/P3HT-FeO(OH)/CP/Au and ITO/PEDOT:PSS/P3HT-FeO(OH):PC71BM/PFN/FM. The yield of the solar cells depended on the concentration of FeO(OH) and the type of configuration employed. For the case of the hybrid solar cells using the first configuration an efficiency improvement of an order of magnitude was observed when was incorporated the FeO(OH) in P3HT. An efficiency of 0.04% was obtained for the P3HT-FeO(OH) composites compared with 0.005% for P3HT. However, for the case of organic solar cells using the second configuration, a small decrease in efficiency was observed by incorporating FeO(OH), obtaining an efficiency of 1.08% for the composite with a higher concentration of FeO(OH) compared to that of P3HT of 1.12%.

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Obtaining and characterization of the hetero junction of ITO/PEDOT:PSS/PANI/Al for its application on organic solar cells.

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Organic semiconductors are of increasing interest as new materials, owing to their possibilities of low production cost and easy manufacturing process. These properties make them good
candidates for applications in optoelectronic devices such as organic light-emitting diodes (OLED), field-effect transistors (FET), photo-diodes, and solar cells [1]. The organic conjugated materials allow such devices to be fabricated at a low cost with an easy solution process that is compatible with flexible substrate application [2,3]. We investigate the optics, electric and structure properties
of the PEDOT:PSS/PANI mixing about glass, ITO and FTO sustrates, for organics application. Also it is proposed the fabrication of organic solar cells (OSCs) using the next architecture ITO/PEDOT:PSS/PANI/Al indicate in fig. 1 and using as PANI layer active. The technics using for deposition of the PEDOT:PSS transparent layer is spin coating about glass on the initial way. For active layer and catod terminal evaporated for obtain it.

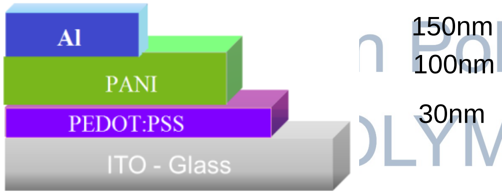

Figure 1. Estructure OSCs

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SEMI-INTERPENETRATING POLYMER NETWORKS OF METHYL CELLULOSE AND POLYACRYLAMIDE PREPARED BY FRONTAL POLYMERIZATION

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In this study, the frontal polymerization (FP) is used as an alternative and convenient technique for the preparation of semi-interpenetrating polymer networks made of methyl cellulose (MC) and cross-linked polyacrylamide (PAAm). Generally, FP reactions occurs in high boiling medium because the front is not stable at low temperature and it is not self-sustaining (mainly because of the heat lost during the evaporation process).[1] In this work, FP was performed in water and glycerol, as largely available, non toxic solvents. Although FP occurred in both media, differences were found by comparing the samples made in the two solvents. In particular, those prepared in water are characterized by larger inhomogeneity and less reproducibility, thus accounting for the boiling effects that influence propagating polymerization fronts when water was used. The effects of the ratio among MC and PAAm, the amount of cross-linker and solvent medium were studied in terms of influence on temperature and velocity of FP fronts, glass transition temperature (dried samples), swelling behavior, dynamic-mechanical properties (gels swollen in both water or glycerol), and tensile behavior. The obtained results indicate that PAAm–MC gels are excellent candidates for several applications, such as matrices for cell transplantation, controlled release (agrochemicals and drugs), tissue repair and regeneration as changing the amounts of monomer, crosslinker and initiator makes it possible to modulate the characteristics of hydrogels.

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Biopolymers obtained from tomato residual wastes

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Introduction. The synthesis of polymers having reactive functional groups plays an important role in the development of various materials for the pharmaceutical and food industry, such as drug or nutraceutical compounds. In addition to these developments, there is a need for such chemical processes to be based on the use of renewable and biodegradable sources. There are appreciable amounts of polyesters in nature, mainly in the higher plants, for example the cuticle. The monomers of the tomato peel have been isolated and characterized and can be considered as a potential raw material for obtaining functionalized biopolymers.
Lipase catalyzed polymerization, especially the immobilized lipase of *Candida antarctica* B (Novozyme 435), allows the synthesis of long chain aliphatic polyesters, which are difficult to obtain by conventional polymerization methods. In the present work we report the co-polymerization of 7-oxo-hexadecanedioic acid with 1,8-octanediol catalyzed with CAL-B using toluene as the reaction solvent, analyzing different amounts of enzyme at two different temperatures. The polyesters were analyzed by NMR and MALDI-TOF, reporting chains of up to 14 diacid-diol units, in a range of Mw of 1700.69 to 2362.18.

Methodology. Preparation of 10,16-dihydroxyhexadecanoic acid (1) and 7-oxo-hexadecanedioic acid (2): 10,16-dihydroxyhexadecanoic acid (1) was obtained from the cutin of agroindustrial tomato waste by means of protocols already reported [1] and oxidized to 7-oxo-hexadecanedioic acid (2) by means of periodic acid and PCC in acetonitrile, as previously reported [2]. For the co-polymerization 20 mg of 7-oxo-hexadecanedioic acid and 10 mg of 1,8-octanediol were dissolved in 1 mL of toluene and heated at 110 ^{o}C for 10 min. The reaction was then brought to 60 or 70 ^{o}C and CAL-B lipase was added. Reactions were maintained with orbital shaking for 48 or 72 h.

Results. 7-oxo-hexadecanedioic acid was efficiently obtained from 10,16-dihydroxyhexadecanoic acid. Both compounds were characterized by NMR and mass spectrometry. The co-polymerization reaction was studied using toluene as solvent. 10-50% of the total weight of the monomers of the enzyme were added and carried out at two temperatures (60 and 70 ^{o}C) for two different times (48 and 72 h). The ^{1}H NMR analysis of the polyesters obtained shows that there is more ester formation using 30% enzyme at 60 ° C in a 48 h time, where the ester forming peak (4.01 ppm) is observed with greater intensity. These data were corroborated by MALDI-TOF, using DHB as a matrix.

Conclusions. The optimum co-polymerization reaction conditions, where the highest Mn and Mw were obtained, were using 30% CAL-B at 60 oC for 48 h using toluene as solvent. The co-polymers obtained have a molecular weight distribution of Mn 1700.69 and Mw 2300.43.

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PREPARATION AND OPTICAL PROPERTIES OF PYRENE-LABELED RUTHENIUM(II) TRISBIPYRIDINE COMPLEX CORED DENDRIMERS

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Dendritic macromolecules are presenting unique physical and chemical properties. One of them is the faculty of transferring energy from a donor moiety introduced at the periphery to an acceptor moiety at the core, mimicking the antenna effect of the process of photosynthesis. The mechanism of energy transfer is based on the Förster resonance energy exchange and requires some overlap between the emission spectrum of the donor and the absorption spectrum of the acceptor. Since it requires a coupling of transition dipole but no overlap of the physical wavefunctions, the energy transfer by Förster mechanism can occur over quite long distances from 1 to a maximum of 10 nm. However, the efficiency of the transfer depends strongly on distance. The Förster radius is the distance at which 50% of the donor's emission is deactivated by FRET.

In this work, we synthesized and characterized a novel series of dendrimers bearing pyrene moieties at the periphery and a Ru (II) complex at the core. The optical and photophysical properties of these compounds were studied by absorption and fluorescence spectroscopy. Pyrene is a well-studied chromophore that have the particularity to present monomer as well as excimer fluorescence emission. The coordination compounds of Ru (II) are red emitters with low quantum yield and long excited lifetime. We observed an efficient singulet to singulet energy transfer in such constructs. Moreover, it is known that the energy of the MLCT emitting state of Ru (II) can be tuned to become almost isoenegetic with respect to the triplet state of pyrene, leading to an extended phosphorescence lifetime. Using dendrimers bearing pyrene moieties as ligands for Ru (II), we could combine the antenna effect of dendrimers as well as its protection effect to the quenching by dioxygen with lifetime increase due to triplet-triplet equilibrium.

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Dendritic molecules, Pyrene, Energy transfer.

Tapered optical fiber coated with P3HT for concentrations measurement in liquids

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In this work, the evaluation of the optical response of a thinned optical fiber coated with P3HT as a sensor of concentrations in liquids is reported. The sensing mechanism is based on the interaction of the evanescent field with the chemically sensitive material deposited on the fiber. The fabrication technique of tapered optical fibers consists of stretching a section of fiber with an oscillating gas burner. Such a process allows controllable fabrication taper fibers with a uniform waist diameter [1]. P3HT was deposited on taper fibers by an immersion coating method. P3HT is a conjugated polymer with a high carrier mobility and optical absorption coefficient in the visible spectrum [2]. Therefore, the optical response of the fiber optic sensing structures immersed in different concentrations of liquids was measured and analyzed at room temperature. Finally, the sensitivity and dynamic range of optical sensor was evaluated.

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SYNTHESIS AND CHARACTERIZATION OF A NEW OLEIC ACID-DERIVED POLYAMIDE BEARING FLUORINATED MOIETIES

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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 a polycondensation reaction at high temperature with the diamine 4,4'-(hexafluoroisopropylidene)bis(p-phenyleneoxy) dianiline (**HFDA**). Triphenylphosphite (TPP) was used as catalyst, 1-methyl-2-pyrrolidone (NMP) in addition to pyridine were used as solvents (**Figure 1**). From the synthesized polyamide dense film membranes were prepared by the solution-evaporation method using *N*,*N*-dimethylformamide (DMF) as solvent. The chemical structure of the new material was confirmed by FT-IR, ^{1}H-NMR, ^{13}C-NMR and ^{19}F-NMR which showed the presence of amide groups. The new polymer was fully characterized by thermomechanical analysis (TMA), thermogravimetric analysis (TGA) and X-ray diffraction measurements (XRD), among others.

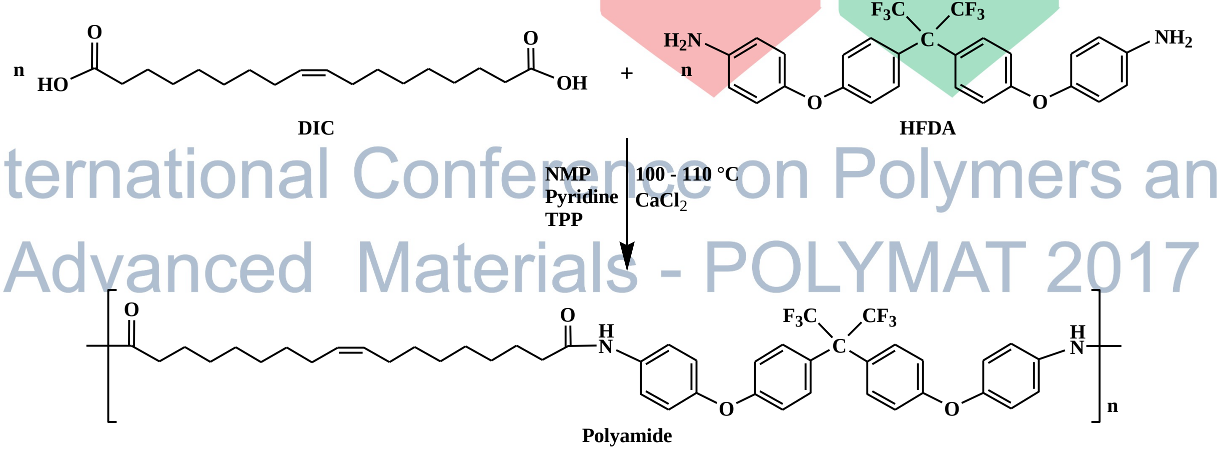

Figure 1. Synthesis route of the new oleic acid-derived polyamide.

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Modification of polyethylene terephthalate to obtain surfaces containing primary amines

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The development of this material capable of having cellular adhesion response to function as a scaffold, polymer scaffolds have been synthesized by other methods[1]. Using gamma radiation is wanted that the properties of the matrix do not change too much but if they improve with the graft to make them more viable and biocompatible with the cells to cultivate[2].

Surface modification of polyethylene terephthalate films (PET) is obtained by grafting acryloyl chloride (AC) using γ-irradiation [3], under different conditions as absorbed dose, monomer concentration, reaction temperature and reaction time. To perform the grafting, the kinetic study of polymerization was carried out by the method of oxidative pre-irradiation. PET films were weighed and placed into glass ampoules and exposed to Co^{60} γ-source in the presence of air and enviromental temperatura at different doses (2 – 20 kGy) in order to promote the formation of peroxides and hidroperoxides groups. Then in the ampoules a solution of AC in toluene is introduced at different concentrations (15 – 50 % vol. 8 mL). It is then degassed by the freeze-thaw process to remove the present air and are sealed. They are placed in a temperature bath (50 – 80 °C) at different reaction times (3 – 21 h). The films are washed in dichloromethane to remove homopolymer residues for 24 h, then reacted in a solution of diethylamine in dichloromethane (0.2 M) for 48 h, and were dried under vacuum and temperature of 40 ° C for 5 h. From the results of this study we can know the ideal conditions to carry out the grafting. The techniques used to characterize these films and to know the physical and chemical changes before and after the grafting are infrared spectroscopy (FTIR-ATR), contact angle, scanning electron microscopy (SEM), x-ray photoelectron spectroscopy (XPS), as well as thermal analysis (TGA and DSC).

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Nanohybrid films of recycled polystyrene for environment UV protection

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Solar energy UV Protection has been a major factor to be considered by specialists because in current years the high intensity of environment UV has affected to people in many forms and it has converted in a problem of public health in many countries [1]. On the other hand, the design and characterization of new materials with UV protection characteristics is necessary to cover these problems either protectors of excessive UV exposure of single people or they can endure the adverse environmental conditions on building infrastructure, including solar UV radiation [2].

Recycled Polystyrene has become an environmental problem for the large amount of waste, which increases over the years [3, 4]. Much of the science and technology of recycled polystyrene have been interested in the synthesis, characterization and applying of polystyrene and others polymers when this are expose to UV sources; from to investigate photo–sensitivity of materials as recycled polystyrene when it is degraded by UV source in laboratory [5]

In this work, hybrid films of SiO_2 nanoparticles embedded in recycled polystyrene (PSR) matrix were prepared as an alternative to reuse wasted containers of polystyrene. Silica nanoparticles were produced from alkoxide precursors in the presence of recycled polystyrene. Spectroscopic analysis of the films was used to give information on the structural changes consequent upon exposure to UVA irradiation (FT-IR and Raman). All the samples, used for coatings glass, were evaluated by hydrophobicity, which was determined by contact angle measurement, also the UV-Vis analysis indicates that exist UV protection.

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Single ion polymer electrolyte for lithium ion batteries, based on blends derived from boron SP3 and Si, Ti, and Zr atoms

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In the last few decades there were many problems associated with the safety of the energy storage devices during operation, due to the use of conventional liquid electrolytes that have risks of leakage and explosion, that is why it was proposed the use of polymer electrolytes for security reasons. Poly(ethylene glycol) (PEG) was widely used in polymer electrolytes, due to their repeating units of ether help with the ionic dissociation due to the polar oxygen units, Several strategies have been developed, such as organically modified ceramics (ORMOCER), that improve the mechanical properties. However, the improvement in the mechanical properties due to the sites sources ceramic-polymer interactions, are accompanied by a decrease in the ionic conductivity [1].

In this work, the electrochemical characterization of the single ion lithium Polymer electrolyte (SILPE), doped with Si, Ti and Zr. Synthesized from Lithium tetra methoxy borate LiTMB lithium, poly (ethylene glycol) PEG400 and the Alkoxides ($Si(OCH_2CH_3)_4$, $Zr(OCH_2CH_3)_4$, $Ti[OCH(CH_3)_2]_4$) as a source Si , Ti and Zr atoms respectively, by polycondensation in a single step. The effect of doping atoms and the content of these in the SILPE's is studied, as a function of the temperature.

In general, the ionic conductivities 10-5 Scm-1 to 30°C of these electrolytes makes them good candidates to be assembled in lithium ion batteries. In addition, it is shown that the increase in the concentration of dopants in the SILPE's can increase the conductivity of lithium ion to concentrations of 10%w, where functionality is lost with the concentration and species dopant, without modifying the preferential driving mechanism between polymer chains.

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Preparation and characterization of polymer poloxamer P-407 functionalized with esters derived from citric acid (1-propanol and 1-heptanol)

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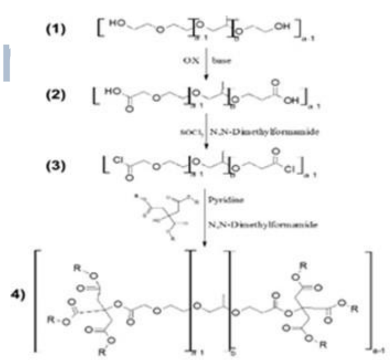
Poloxamer is a copolymer composed of three nonionic block, formed by a central hydrophobic chain, flanked by two hydrophilic chains. Poloxamer P-407 is widely used as a vehicle or drug matrix due to their physicochemical properties to generate a modified release [1]. In addition, citric acid has been incorporated in pharmaceutical applications as precursor of new materials [2]. The objective of this work was functionalizing the poloxamer polymer P-407 with esters derived from citric acid, which will generate a new material with potential application in confinement and release of drugs. Experimental Part. Compound (2) it was obtained by oxidation of compound (1) with $KMnO_4$. Compound (3) it was synthesized by chlorinating the compound (2) with $SOCl_2$. Compound (4) was obtained from the compound (3) and the ester derivatives of citric acid in dimethylformamide as a solvent and pyridine as catalyst. The ester derivatives of citric acid were synthesized using citric acid, together with the corresponding alcohol (1-propanol and 1-heptanol). The characterization of the compounds obtained were determined using FTIR instruments (Brucker Tensor 27) and NMR (FT-NMR (60 MHz) ANASAZI). Results and Discussions. Scheme 1 shows the sequence of the compounds obtained. Compound (2) had a yield of 80%, and was as a white solid. Compound (3) it was obtained as a light yellow solid with 30% yield. Compounds (4a) had a white semisolid, for the case of compound (4b) with the ester derivative with 1-propanol yield was 30%, while the product of the ester derivative of 1-heptanol was 30%. The results of the characterization of the compounds shown in Table 1. Two new materials (4a and 4b) according to the spectroscopic characterization, which may be a potential for the containment system and modified drug release was obtained.



Scheme 1. Synthesis of compound (4). R=1-propanol; 1-heptanol.

Compound	FTIR (cm^{-1})	RMN ^1H (ppm)	RMN ^{13}C (ppm)
(2)	3420,1677, 1609, 1468	1.16,1.24, 4.16, 4.79, 4.88, 4.95	17.64,75.90,80.23,173.08, 173.37
(3)	3499,2972, 2884,1736, 1468,664	1.04,1.12, 4.75, 4.83, 4.93	17.23,39.28,77.39, 79.35, 164.74
(4a) R= 1-Propanol	2968,1735,1670,1092	0.75,0.91,1.52,2.81,3.46,3.86	10.62,17.27,42.86,171.66,167.39
(4b) R= 1-Heptanol	2929,1738, 1680,1118	0.69,0.76,1.11,2.78,3.45,3.88,4.00	14.66,17.92,23.18,26.44, 43.87,80.26,170.44, 174.04

Table 1. Signals characteristic of the compounds obtained.

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MULTIFUNCTIONAL MACROMOLECULES BASED NANOSTRUCTURES FOR DRUG DELIVERY

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Cancer, congestive heart failure and diabetes are the leading causes of morbidity and mortality in industrialized nations. The ever-increasing complexity of these diseases, and managing them with highly potent pharmaceutical agents, lead to serious reduction in an individual's quality of life. This may largely be attributed to our inability to deliver drugs in sufficient quantities at the diseased site. Polymer therapeutics has evolved as an advantageous platform to address these issues.[1] Despite significant progress, key challenges related to simplifying their synthetic schemes, enabling them to cross biological barriers, and understanding nano-bio interactions, still remain. This has provoked the design of tailor-made macromolecules based nanocarriers that can perform multiple desired tasks with high efficiency.[2] An important parameter for constructing these scaffolds is to develop synthetic tools that can provide desired spatial distribution of different units in these nanostructures. The synthetic methodologies need to be simple, highly versatile and adaptable to the needs of biology. We shall describe how chemical innovation has given access to a variety of branched and hyperbranched macromolecules and combinations thereof.[3-4] Functional nanostructures from these macromolecules can be used for monotherapy through physical encapsulation or drug conjugation, or combination therapy using multiple drugs.[5-6] Their desired structural integrity makes them ideally suited to perform multiple tasks including targeting and visualizing drug delivery.

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POLY(METHYL 6-ACRYLOYL-β-D-GLUCOSAMINOSIDE) AS A CATIONIC GLYCOMIMETIC OF CHITOSAN

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Chitosan, a cationic polysaccharide derived from one of the most abundant natural polymers, chitin, has been investigated extensively for its antimicrobial properties. However, it suffers from the inherent drawbacks of natural products such as batch-to-batch variability, limited supply, contamination, and potential adverse reaction. Additionally, its solubility depends on the degree of deacetylation and pH, as it is only soluble under acidic conditions. As an alternative to chitosan, we synthesized the protected cationic glycomimetic monomer methyl *N*-Fmoc-6-acryloyl-β-D-glucosaminoside from glucosamine. This monomer retains structural features critical to recapitulating the properties of the chitosan repeat unit, namely the pKa of the protonated amine. We optimized the free radical polymerization of methyl *N*-Fmoc-6-acryloyl-β-D-glucosaminoside and fractionated the resultant poly(methyl 6-acryloyl-β-D-glucosaminoside) to obtain a range of molecular weights. Following Fmoc deprotection, the cationic glycopolymers retained 95% of their expected amine content by mass and exhibited a pKa of 6.61. Poly(methyl 6-acryloyl-β-D-glucosaminoside) mimicked the molecular weight-dependent bacterial inhibitory property of chitosan in acidic solutions. Importantly, poly(methyl 6-acryloyl-β-D-glucosaminoside) remained soluble at elevated pH (conditions under which chitosan is insoluble) and maintained its antibacterial activity. Mammalian cell viability in the presence of poly(methyl 6-acryloyl-β-D-glucosaminoside) at acidic pH is good, although somewhat lower than viability in the presence of chitosan. No cytotoxic effect was observed at neutral pH. These results demonstrate that poly(methyl 6-acryloyl-β-D-glucosaminoside) is not only a suitable biomimetic for chitosan, but that it can be utilized as an antibacterial agent in a broader range of biologically relevant pHs.

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GUIDING LIGHT WITH CHEMISTRY: INTERACTIONS BETWEEN OPTICALLY SELF-TRAPPED BEAMS IN POLYMERS

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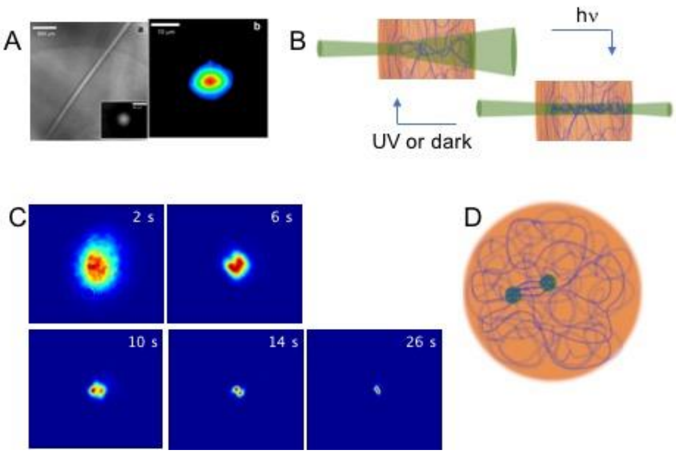
Self-trapped beams are self-reinforcing waves that travel long distances (>>Rayleigh length) without suffering changes to their profile [1]. We find that self-trapped beams can be elicited through a variety of photochemical reactions with varying degrees of reversibility: from the photopolymerization of polymer systems that create permanent structures [2] (A) to the photo-reversible contraction of a spiropyran-functionalized hydrogel that reverts to its original state in the dark (B). Although originating from richly diverse molecular mechanisms, these systems all undergo a positive change in refractive index and in this way, satisfy the macroscopic prerequisite for self-trapping [3].

These channels of high refractive index are able to interact with one another as they form, providing a means for all-optical manipulation of light beams [4]. The interactions between self-trapped beams that rely on photochemical changes in refractive index has yielded interactions of attraction, interweaving and even spiralling (C), depending on the initial conditions. Long-range interactions have been found in the spiropyran-functionalized hydrogel, including in the absense of overlap between their respective optical fields (D). These findings provide new insight into the interaction dynamics of self-trapped beams and could ultimately open routes to photonic systems involving light-guiding-light technologies. The mechanisms of action will be highlighted, along with insight from the associated beam interactions.



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PREPARATION, CHARACTERIZATION AND RELEASE PROFILE OF (-) EPICATECHIN FROM CELLULOSE ACETATE AND POLYVINILPYRROLIDONE ELECTROSPUN SYSTEMS.

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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[1]. 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[2].

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 electrosprayed 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.

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SYNTHESIS OF AMPHIPHILIC NANOPARTICLES BY STEP-WISE CROSSLINKING OF BLOCK COPOLYMERS CONTAINING 1-FUNCTIONALIZED BENZOCYCLOBUTENE UNITS

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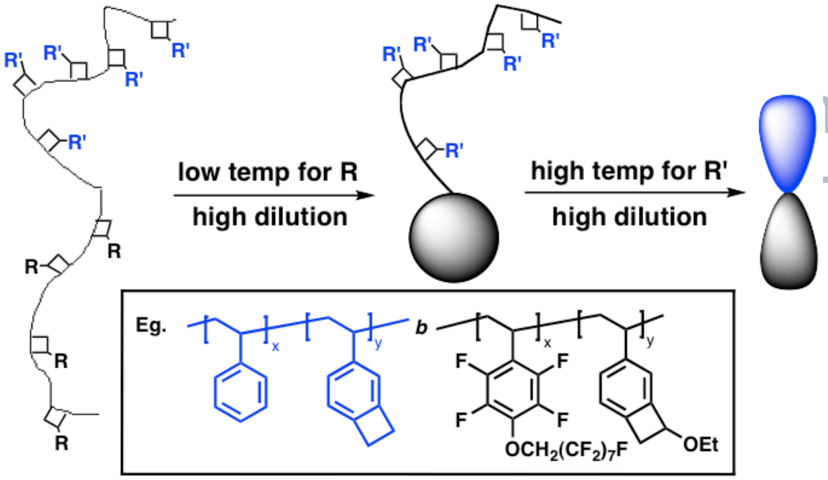
Nanoparticles must be ordered into complex arrays with the control and reproducibility of biological systems for both nano- and biotechnology applications. Although asymmetrically functionalized nanoparticles are expected to self-assemble directly into complex structures without the need for template assistance, most nanoparticles are spherical in shape with isotropic surfaces. This paper will present a route to create amphiphilic nanoparticles from block copolymers of styrene and pentafluorostyrene. The different parts of the nanoparticle were created stepwise using 1-functionalized benzocyclobutene units that react at different temperatures for the two different lobes. Since the nanoparticles contains, a fluorinated component and a hydrocarbon component, the hydrocarbon lobe interacts with a film of polystyrene, leaving the fluorinated lobe exposed.



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ENHANCED PERFORMANCE OF ELECTRODES IN ETHANOL OXIDATION USING CTAB:PTFE POLYMER BLEND.

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Nowadays there are some polymer backbones, cation linkers, and cationic headgroups with possible applications as support, conductive polymers or ion exchange membranes [1]. They can be applied in ionic conductive support for catalytic materials, based on organic compounds like sodium dodecyl sulfate as organic ionic holder, It shows the alternative materials with stability and capacity to increase the catalyst activity [2]. In this work Polytetrafluoroethylene (PTFE) emulsion was used as electrode binder for catalyst to carry out the ethanol oxidation reaction, and it was functionalized with cetyl trimethyl ammonium bromide (CTAB). Catalytic ink was prepared using 10 µl solution 60%wt PTFE and 2mg of Pt 10% on carbon Vulcan XC72. The ink was dispersed in 990 µl isopropyl alcohol for 30 minutes by using an ultrasonic bath at 60 kHz. 10 µl ink was deposited onto a Ø = 3mm glassy carbon electrode and then 2 µl of CTAB:isopropyl alcohol solution 1 mg/ml. Cyclic voltammetry (CV) measurements in 0.1M KOH solution for activation of the electrodes at 10 mV/s, in cycle 10 ethanol was added to obtain a 1M for oxidation process.

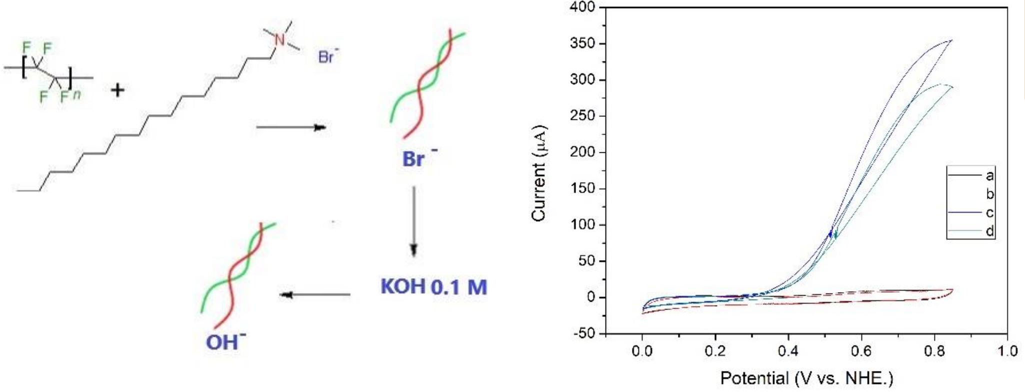

Figure 1. (left) Ionic polymer composite (right) cyclic voltammetry; (a,b) activation cycles and (c,d) ethanol oxidation for CTAB;PTFE blend and PTFE.

Figure 1 shows that the activation cycles in alkaline media allows the functionalization of the obtained polymer from the mixture. CV measurements show a change in current intensity for polymer blend and the ethanol oxidation reaction for polymer blend (figure 1c) has a higher current intensity at 0.8 V and faster activation curve at 0.4 V than the presented for PTFE (figure 1d). The activation process for nonconductive polymers is an alternative to use it in electrodes and fuel cell membranes.

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Synthesis of Unsaturated Linear Polyester Poly(ω-Hexadecenlactone) via Ring-Opening Metathesis Polymerization

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Plastics have presence in almost every area of our modern culture, having a cheap price and diverse tailored properties; because of these the polyolefins (**PO**) annual production is estimated to be 180 million of tons. In the last two decades there has been an interest in the use of biodegradable polymers as alternative to **PO**, this concern has been driven by the increase of pollution derived from their resistance to environmental degradation **[1]**. Biodegradable polymers can be originated from renewable and petrochemical sources; the most widely studied biodegradable polymers are polysaccharides and aliphatic polyester because they can achieve similar properties as the traditional **PO** **[2]**. In order to find an efficient method of synthesis of those polyester materials, the ring opening metathesis polymerization (**ROMP**) foreground from others due the control of physical and chemical properties. In this synthetic route a ruthenium complex polymerizes a strained cyclic olefin. Nowadays, the **ROMP** challenge is the polymerization of non-strained macrocyclic monomers and those that possess functional groups able to deactivate the catalyst, for example the oxygen containing groups **[3]**. The aim of this study is the synthesis and characterization of unsaturated polyester via **ROMP** of ω-6-hexadecenlactone (**HDL**) using ruthenium-alkylidene {[Ru(Cl$_2$)(=CHPh)(1,3-*bis*(2,4,6-trimethylphenyl)-2-imidazolidinylidene) (PCy$_3$)] (**I**), [Ru(Cl$_2$)(=CH(*o*-isopropoxyphenylmethylene))(1,3-*bis*(2,4,6-trimethylphenyl)-2-imidazolidinylidene)] (**II**) and [Ru(Cl)$_2$(=CHPh)(PCy$_3$)$_2$] (**III**)} and ruthenium-vinylidene [RuCl$_2$(=C=CH(*p*-C$_6$H$_4$CF$_3$))(PCy$_3$)$_2$] (**IV**) catalysts. The polyhexadecenlactone (**PHDL**) obtained via **ROMP** in the presence of catalysts **I** and **II** shown high molecular weights between M_n = 114,800 – 155,400 g/mol, with yields > 96 %. In addition, conversion of **HDL** to **PHDL** using catalysts **III** and **IV** was around 46-52 %, with molecular weights of M_n = 71,600 – 85,000 g/mol. The catalysts **I** and **II** with the *N*-heterocyclic carbene ligand (NHC) showed superior activity and stability upon catalyst **I** and **IV** bearing PCy$_3$. The product **PHDL** showed 31 % cristallynity and a melting temperature 47.60 °C.

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POLY (VINYL PIRROLIDONE)/PROPANOLOL NANOFIBERS AS A POTENTIAL TREATMENT OF CHILD HEMANGIOMA

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Infantile hemangiomas are the most frequent benign vascular tumors of childhood, sickness arise from an uncontrolled reproduction of endothelial cells followed by a slow involution stage, between 10% and 15% tend to complicate during their proliferative phase, in which can cause a permanent aesthetic deformation, and in more serious cases they will affect vital functions [1]. The objective of this work was to synthesize and characterize poly (vinyl pyrrolidone) nanofibers loaded with propanolol for their potential use in the treatment of childhood hemangioma. Different formulations of the polymer solution were prepared and different ratios of the drug were loaded for the preparation of fibers through the electrospinning technique. The produced nanofibers were characterized by the Fourier Transform Infrared Spectroscopy (FTIR) technique to search for drug-polymer interaction sites. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were used to evaluate the behavior of nanofibers with respect to temperature, and to characterize the average fiber diameter and percentage of porosity, the scanning electron microscopy (SEM) was used. To evaluate biocompatibility a cytotoxicity assay was done using HFF1 human fibroblast cells. In the case of TGA, the total weight of the sample was lost for 10% propranolol nanofibers at 692.64 °C, 20% at 494.54 °C, 30% at 495.05 °C, 40% at 487.36 °C and 50% at 492.93 ° C. In the case of DSC, dehydration was also found between 57.87 ° C and 64.59 °C for the various samples. Polymeric nanofibers loaded with drug showed homogeneous fibers and FTIR demonstrated evidence of drug incorporation. Finally, nanofibers with 10% and 30% demostrated excelent biocompatible characteristics. Studies of drug release and degradation assays has to be done to determine the efectivity of the drug delivery system.

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ENCAPSULATION AND RELEASE STUDIES OF RHODAMINE USING AMPHIPHILIC CROSSLINKING POLYESTERS CONTAINING SILICON FATTY COMPOUNDS

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In the present work, we report the encapsulation and release studies of rhodamine using crosslinking polyesters containing silicon fatty compounds. Crosslinked polyesters (PE) are formed by a polycondensation reaction between a hydrophilic segment (polyethilenglicols with different molecular weights, Mn: 400, 1500, 3000 and 6000 g/mol), and a hydrophobic block (tetra siloxane cyclic compound) as reported previously [1]. We obtained four PE (PE400, PE1500, PE3000 and PE6000) and they were used for encapsulation studies and subsequent release of the Rhodamine dye.

Rhodamine was effectively encapsulated in these crosslinked polyesters, and the experimental encapsulation capacity for the serie correlated with the molecular weight as follow: PE400< PE1500< PE3000< PE6000. This denotes the importance of the crosslinking grade of the PE. As the degree of crosslinking increased, the capacity to encapsulate decreased. For the encapsulation experiments using Rhodamine, the following experimental protocol was used: 100 mg of each PE was added into 1,2 ml of a Rhodamine solution with known concentration and incubated at 25°C for 24 hr with constant stirred at 130 rpm. The release of Rhodamine from PE was carried out using dialysis tubing retaining Mw 12,000 or greater. The dialysis solution was PBS buffer pH 7.4 and the release was followed for 100 hr, measuring the absorbance every hour using an extinction coefficient of $10.1x10^4$ (M^{-1}cm$^{-1)}$ [2,3] The release during the first 10 hr (Figure 1) was used to compare the releasing capabilities for the different PE.

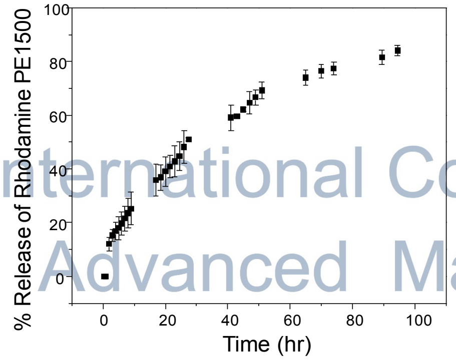

Figure 1. Release of Rhodamine (PE1500)

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Functionalized Graphene Oxide with Organic Groups and Their Effect on the Mechanical Properties of Electrospun Nylon6

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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 functionalized GO (FGO) have not been adressed. On the other hand, the development of new methodologies to functionalize GO are highly demanded.
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 modifiying an improved Hummer´s method[1]. APTS was investigated to introduce free amine groups to GO. The reduction of GO and the presence of chemical bonds C-N, C-O-Si and NH_2 (C1s, O1s and N1s, respectively), from ATPS 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. The graft density effects on the tensile strength and Young's modulus of the electrospun FGO/Nylon-6 fibers are performed by the tensile tests. It is found that the tensile strength, strain and modulus change with increasing graft density. Brittle and ductile fibers were obtained, respect to Nylon-6 fibers, changing only the graft density.

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THE CARBON VALUE, ENRICHMENT BEYOND RICHNESS:
CHEMICAL *VS* MATERIAL FUNCTIONALITIES OF *CARBO*-BENZENES

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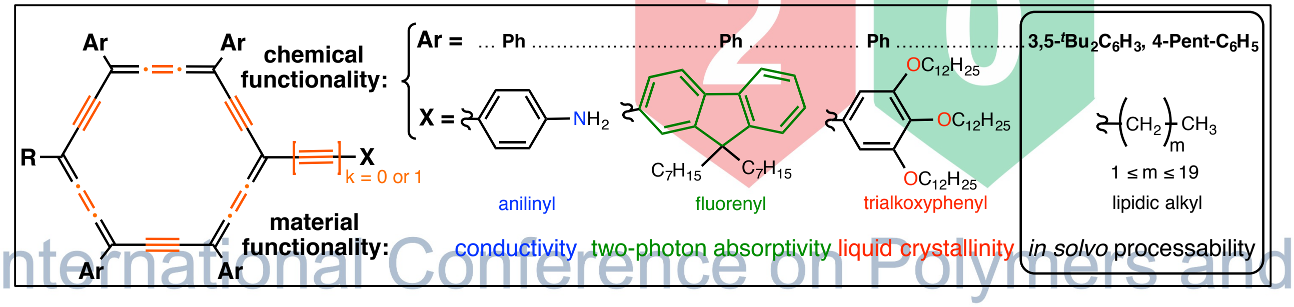
More than generic carbon-*rich* compounds, *carbo*-benzenes are carbon-*enriched* molecules based on a C_{18} functional core exhibiting a unique combination of features: 30-π-electron richness, extended π-conjugation, flatness, flexibility, D_{6h} symmetry, ambivalent aromaticity [1]. Peripheral *chemical* functionalities have been shown to ensure specific *material* functionalities, such as electrical conductivity (106 nS conductance over 2 nm) [2], two-photon absorptivity (656 GM cross-section at 800 nm) [3], liquid crystallinity (rectangular columnar mesophase at 115°C) [4], and *in solvo* processability [5]. In the latter case, dispersive association of lipidic alkyl substituents in the crystal also induces direct interaction between C_{18} rings, with π-π-stacking distances close to the DFT-calculated one between layers of α-graphyne (*ca* 3.23 Å) [6]. The existence of the latter, the putative *carbo*-mer of graphene, is suggested by a recent synthesis of a *carbo*-naphthalene [7].



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TUNING PORE MORPHOLOGY AND FUNCTIONALITY IN FUNCTIONAL ORGANIC MATERIALS

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Over the last decade, the generation of organic porous (nano)materials with tunable pore sizes and desired functionalities has been the subject of increasing attention in materials science. Interest in such porous frameworks originates from the large variety of applications in which they are involved, *e.g.* size/shape-selective nanoreactors, monoliths for advanced chromatographic techniques, nanofiltration membranes, high specific area catalytic supports, as well as 3-D scaffolds for tissue engineering.

This lecture examines the scope and limitations of three different approaches to porous polymers with controlled porosity and functionality at different length scales. The first approach relies on the synthesis of polystyrene-*block*-poly(D,L-lactide) diblock copolymers with functional groups at the junction between both blocks, followed by their macroscopic orientation, and the subsequent selective removal of the polyester block to afford ordered nanoporous materials with channels lined with chemically accessible functionalities (*e.g.*, COOH, SO_3H, SH, COH) [1-4]. The second strategy entails the preparation of biocompatible doubly porous crosslinked polymer materials through the use two distinct types of porogen templates, namely a macroporogen in combination with a nanoporogen. To generate the macroporosity, either NaCl particles or fused PMMA beads are used, while the second porosity is obtained by using a porogenic solvent [5]. Alternatively, a straightforward and versatile methodology for engineering doubly porous polymers is implemented through a thermally induced phase separation process [6]. Finally, 3-D macroporous scaffolds based on biodegradable polyesters have been engineered by electrospinning to generate nanofibrous biomaterials that mimic the extracellular matrix [7,8]. The potentialities afforded by these approaches will be addressed, and some typical applications of the resulting porous materials will be illustrated.

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"EVALUATION OF COFFEE EXTRACT (COFFE ARABIC) AND TULE (TYPHA DOMINGENSIS) FOR THE SEPARATION OF HEAVY METALS IN INDUSTRIAL RESIDUAL WATER"

Presenting Herón Hernández García[1], Dra. Minerva Ana María Zamudio Aguilar[2], Dra. M. Teresita Oropeza Guzmán[3] , Dr. Eduardo A. López Maldonado[3]

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Water pollution, its irrational use and overexploitation, prepare a predictable deficit, and for the moment still controllable. It is necessary to implement concrete solutions that help to ration use, treatment and disposal, it is necessary to develop new technologies, or optimize existing ones, immediately.

To evaluate the extract of Coffee and Tule for the separation of heavy metals by coagulation and flocculation in industrial residual water.

This work presents the study for the use of vegetal residues, considered as waste, such as lignin extracted from coffee (Coffea arabica) and Tule (Typha domingensis) figure 1 for the separation of heavy metals by coagulation-flocculation in industrial waste water. Extraction of extracts in model water, Cr, Cd, Pb, Ca, Zn, Ni, Cu, simulating the characteristics of electroplated waste water.

According to the results lignin extracted from coffee residues had a higher percentage of removal compared to lignin extracted from tule residues.

In most of the heavy metals a removal of more than 50% was obtained.

The decreasing order of removal with the coffee lignin is shown below: Cu (99.24%)> Cr (99.40%)> Pb (97.55%)> Zn (88.14%)> Cd (67.01%)> > Ni (66.57%) And for the lignin of tule: Cu (98.91%)> Cr (99.25%)> Pb (97.18%)> Zn (84.03%)> Cd (55.11%)> Ca(49.7860%)> Ni (49.53%).

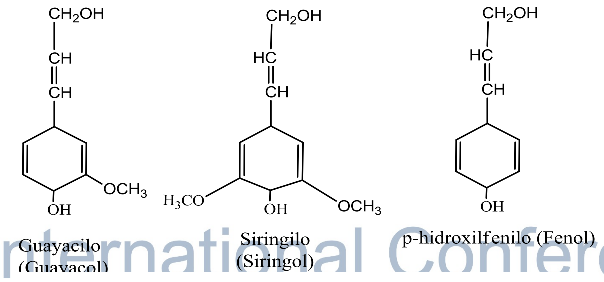

Figure 1. Main functional groups of Lignin

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ORGANIC OPTICAL BISTABLE DEVICE FOR MAZE EXPLORATION BY WAVEFRONT PROPAGATION

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A bistable system with spatial expanse can keep two stable states (e.g. "on" and "off" states) simultaneously at different locations [1]. The interface between "on" and "off" area, here we call it "wavefront", can spatially propagate. Such wavefront propagation can be utilized for natural computing, a novel information processing scheme utilizing dynamics of various natural phenomena. Maze exploration is one of popular topics in natural computing, and so far, Belousov-Zhabotinsky (BZ) oscillatory reaction wave, self-propelling oil droplet, movement of true slime mold, and many other natural phenomena have been reported to solve mazes.[2] Here we introduce a two-dimensional thermo-optical bistable device for maze exploration.

In our device, optical bistability is realized through positive feedback between heat generated by photoabsorption and temperature-dependent optical absorption. Under irradiation of bias light at an intensity in the bistable (hysteresis) region, the whole area can stay at ‘'off'' (low photoabsorption) state without any perturbation. Once the light intensity is increased above the turn-on threshold at one location, the medium is locally triggered to turn on to high photoabsorption ("on") state, and the turn-on wavefront expands two-dimensionally through thermal diffusion. Maze pattern can be easily defined by patterned light irradiation, and exploration can be started by irradiating strong trigger light at the starting point of the maze.

Theoretically, this device can be modeled using a thermal diffusion equation with heat loss at the device boundary and heat source due to photoabsorption.[3,4] Temperature-dependent optical absorbance is realized by optical transmission change due to nematic-isotropic phase transition of a liquid crystal. We have demonstrated maze exploration by numerical simulation using the finite element method (FEM). Moreover, we found that, not only extension of on-state area, but also retreat of that can be realized by reducing light intensity. This "reduction mode" enables retreatment from the dead-end paths in the maze, so that only the connected path (correct solution) finally remains in "on" state. We are also fabricating experimental devices, and have demonstrated exploration of simple maze.

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A COMPARATIVE STUDY OF NITROGEN AND NITROGEN-SULFUR DOPING AGENTS ON GRAPHENE OXIDE BY ANNEALING FOR ELECTROCHEMICAL DEVICES

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Abstract: Over the last decade, graphene has emerged as a highly active research topic owing to its outstanding properties and numerous applications. Recently, doping of graphene with heteroatoms such as nitrogen and sulfur into the carbon lattice has demonstrated to be one the most effective methods to tailor and improve their chemical and electronic properties. Although several approaches have been developed, the electrochemical performance of doped-graphene materials is related not only to the heteroatom content but also to the nature of the formed species. Moreover, the precise configuration control and optimization over the technique employed is still by far a challenge for its future implementation. Herein, we report a comparative study of nitrogen doping of graphene oxide (GO) via annealing with melamine and urea as the N-doping agents. In addition, novel thermal treatment was extended to co-doping of graphene oxide containing both N and S in one step with thiourea as the single doping agent. All samples with different GO/doping agent mass ratio were treated at 800 °C under inert atmosphere. The simultaneous reduction and successful doping of graphene oxide materials were identified by Raman spectroscopy and X-ray diffraction (XRD). Morphological differences of GO upon doping treatments were analyzed by scanning electron microscopy (SEM). The different surface configurations of heteroatoms were evaluated by X-ray photoelectron spectroscopy (XPS). Electrochemical measurements on Li-ion half cells using the synthesized materials as working electrodes were performed by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The results revealed that the incorporation of heteroatoms in GO structures by annealing plays an important role in enhancement of electrochemical properties. The synthetic route represents a useful tool for the design of new graphene materials with potential applications in electrochemical devices.

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SYNTHESIS OF CELLULOSE NANOFIBRILS USING POLYMERIC BIOMASS

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In nature, a large number of plants synthesize extra-cellullar skeletal structures consisting of a matrix reinforced by fibrous biopolymers.[1] The cellullose 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 cristallinity, 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 ellucidate what happen after each treatment step. SEM reveals the surface modification of the nanofibrils with the differents chemical and physical treatments. XRD showed the appearance of crystalline structures related with the nanocellulose structure.[2] Finally, we obtained semi-crystalline Cellulose nanofibrils (CNFs) by facile synthetic approaches.

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SYNTHESIS OF NANOCELLULOSE WHISKERS FROM NOPAL (*Opuntia ficus-indica*)

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Nopal (*Opuntia ficus-indica*) is an indigeneous and endemic cactacea of the desertic and semidesertic áreas from América. [1] 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. [2] In this work is presented a facile and tunable approach to obtain Cellulose nanowhiskers (CNWs)from nopal cladodes, using basically a combination of of chemical and physical treatments. In order to extract the lignin and hemicellulose (who helps to mantain together the cellulose macrofibrils) a variety of chemical treatments were carried out (sosa treatment for soaking the cladodes, soxhlet extraction, etc). The succesfully elimination of lignin was verified by FTIR and Fluorescence. After the chemical extraction, different mechanical treatments using high shear rates (ultraturrax), lyophilization and ultrasonic dismembrator were used. The influence of these diverse methods over the final cristallinity, morphology and size of the CNWs is discussed. SEM analysis showed our evidences.

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PREPARATION OF THIN FILMS BASED ON POLYTHIOPHENES BEARING PYRENE GROUPS THROUGH FLEXIBLE SPACERS: INTERACTION WITH REDUCED GRAPHENE IN SOLUTION

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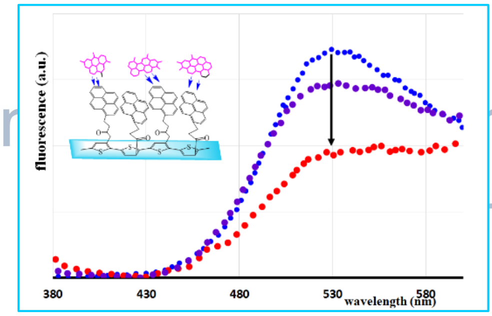
A series of pyrene containing thiophene monomers, TPM1-5, were synthesized and fully characterized by FTIR, MS, 1H- and 13C-NMR spectroscopy; their thermal properties were determined by TGA and DSC. The monomers showed an absorption band at 345 nm due to the S0 - S2 transition of the pyrene group, whereas the fluorescence spectra showed a broad emission band arising from the "monomer" emission at 375–420 nm. They were polymerized following two ways: i) using FeCl3 as oxidizing agent to give the corresponding oligomers TPO1–5 and ii) using electrochemistry to obtain the corresponding TPP1–5 polymer films deposited onto ITO. The oligomers exhibited good thermal stability, with Tg values varying from 36 to 39 °C. They displayed two absorption bands centered at 245 and 355 nm, whereas the corresponding polymers absorb up to 500 nm. The fluorescence spectra of both oligomers and polymers revealed a broad and intense excimer emission band at 570 nm, due to pyrene excimers formation. The polymer composites deposited on ITO resulted in thin, homogeneous and electroactive polythiophene polymers with pendant pyrene units regularly positioned on the surface. We demonstrated that the excimers emission can be quenched by graphene adsorption achieved by simple dipping in aqueous RGO solution. The presence of graphene aggregated onto pyrene rich areas was evidenced by AFM analysis. This highlights the benefit of using such polythiophene/pyrene thin films for the development of new organic fluorescent probes.



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ANALYTICAL ELECTRON MICROSCOPY STUDY IN THE INTERDIFFUSION ZONE USING Fe/Fe-40Cr DIFFUSION COUPLE

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Abstract

An atomic scale analysis in the interdiffusion zone have been studied from compositional variations measured across the Fe/Fe40Cr diffusion couple interface with the combination of High Resolution Transmission Electron Microscopy (HRTEM), Scanning Transmission Electron Microscopy (STEM) and hardness tests. The diffusion couple were solution treated at 1050 ° C for 96 hours and quenched in water, and then aged thermally at 500 ° C for 500 h. HRTEM was used for microstructural observation in the vicinity of pure Fe and Fe-40at.%Cr alloy. The EDS-STEM analysis permitted to obtain the concentration profile that shows the difference of composition between the Fe-rich side and the interdiffusion zone. The hardness measurements of the aged diffusion-couple indicated the age hardening due to the presence of nanometric Cr-rich precipitates in a Fe-rich matrix.

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Design of ferrocenyl amphiphilic dye-like compounds for potential optoelectronic applications

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Nowadays, dye-like and π-conjugated organic compounds represent attractive targets for diverse application in advanced functional materials.[1] Organic π-systems end-capped with an electron donor (D) and an electron acceptor (A) represent a subclass of these kinds of molecules, widely known as push–pull systems. They have predominant applications as chromophores with nonlinear optical (NLO) properties, electro-optic, and piezochromic materials, NLO switches, photochromic, charge-based information storage and solvatochromic probes as well as active layers in DSSCs. In this sense, the research on exploring novel efficient sensitizers, based on the donor–π bridge–acceptor (D–π–A) configuration is mainstream in the design of organic sensitizers due to its convenient modulation of the intramolecular charge-transfer nature.

In this context, we have focused our efforts in the synthesis and study of the molecular absorption, energy levels and voltammetry behavior of a series of novel ferrocenyl amphiphilic push-pull dyes,[2] which have demonstrated promising results that prompt us to explore their incorporation as precursor of active layer in DSSCs.

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SYNTHESIS AND CHARACTERIZATION OF CONDUCTIVE POLYMER FILMS FOR ITS APPLICATION IN SENSOR DEVICES

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Polyaniline is a conductive polymer which has a wide variety of applications in various fields. Sensor devices manufactured with conductive polymers require to be synthesized in film form. To obtain the polyaniline film was used the chemical bath deposition (CBD) technique, it is simple, economical, and it allows us to obtain uniform films, with good adhesion and low optical absorption [1]. In CBD technique, the polyaniline was deposited by the polymerization of aniline with ammonium persulfate in an acid medium. We present the results obtained from the structural, optical, morphological and electrical characterization of polyaniline films. Several studies show that polyaniline doped with metal oxides improves its electrical properties. SnO_2 nanoparticles were synthesized by precipitation using an aqueous solution of $SnCl_2.2H_2O$ then were added a few milliliters of an ammonium hydroxide solution, that solution was kept stirring for 30 minutes, obtaining a white sediment which is filtered and washed with deionized water. The nanoparticles obtained from SnO_2 were dissolved in acid and added during the synthesis of the polyaniline following the same sequence of the films without doping. The structural characterization shows that the SnO_2 nanoparticles are encoded in the film obtained by CBD method.

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GELATIN/COLLAGEN NANOFIBERS AND ITS POTENTIAL USE IN BIOREACTORS

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Currently, there are a large variety of pharmaceutical and industrial products on the market that can be obtained through bioreactors. The objective of this work is biologically characterized Gelatin/Collagen electropun nanofibers for biotechnological applications. Through the electropinning technique, 15% Gelatin nanofibers with different proportions of Collagen (1%, 5% and 10%) were synthesized and evaluated through cell culture in HFF1 human fibroblast cells and in bacterial cell cultures of *Escherichia coli, Staphylococcus aureus, Pseudomona aeruginosa*, and *Proteus mirabillis*. In the case of cell culture in fibroblasts, the cells exposed in the presence of nanofibers for 2 days, presented a 63% average proliferation among all the formulations. Nanofibers that presented the highest growth were Gelatin formulations with the highest Collagen ratio (10%). In the case of bacteria growth in all cases nanofibers were efficient to promote bacteria growth, especially in the case of *Escherichia coli* and *Staphylococcus aureus*. *Pseudomona aeruginosa*, and *Proteus mirabillis* do not showed a statistically significant difference of its growth with and without the presence of the nanofibers. These results demonstrate the efficiency of Gelatin/Gollagen nanofibers as a substrate in the culture of fibroblast cells and bacteria of biological interest. As future work, we intend to incorporate the nanofibres in the walls of a bioreactor and to compare the growth with and without the nanofibers, to evaluate the amount of biomass produced in both conditions.

Acknowledgements

The authors are grateful to the Fondo de Cooperación Internacional en Ciencia y Tecnología (FONCICYT) Movilidad Bilateral Mexico-India of CONACYT for funding through project number CAR 266380.

EFFECT OF PHOTOLUMINISCENCE IN SRO FILMS DUE TO THE TYPE OF SUBSTRATE USED.

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This work describes the behavior of photoluminescent emission in silicon-rich silicon oxide (SRO), deposited by the LPCVD technique (Low pressure vapor phase chemical deposition) In a hot-wall reactor employing silane and nitrous oxide as precursor gases and annealing at 1100 °C in Nitrogen. The chosen SRO deposits were Ro = 10 and Ro = 25 in monolayers and bilayers, with and without a polysilicon layer, on silicon and quartz substrates. The FTIR spectra of the SRO films are shown in Figure 1, Figure 2 shows the Transmittance spectra and Figure 3 shows the photoluminescence. Different behaviors that depend on the Ro of the SRO film are observed. By means of Elipsometry the thicknesses of the SRO films with and without heat treatment were obtained, ranging from 89.7±9.8 to 178.1±13.8 nm and 76.3±5.4 to 169±38.8 nm, respectively.

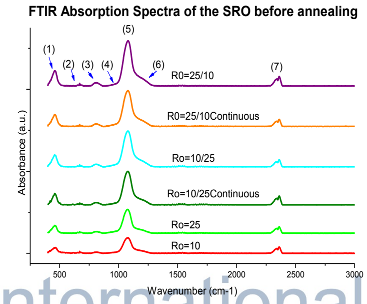
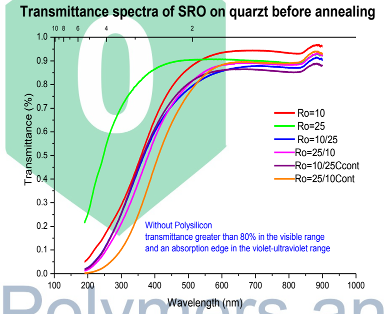


Figure 1. FTIR Absorption Spectra of the SRO films on silicon before annealing.

Figure 2. Transmittance SRO films on quartz without polysilicon, greater than 70% between 600 and 900 nm over a wide spectral range



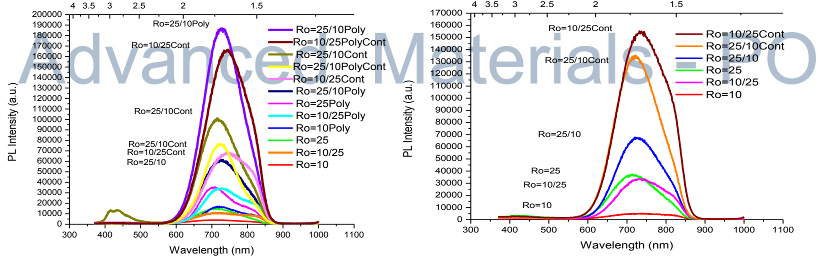


Figure 3. *PL spectra of SRO on quartz and silicon monolayers and bilayers deposited by the PLCVD technique.*

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Synthesis and characterization of nanocomposite coating based on epoxy resin, montmorillonite and (3-glycidyloxypropyl)trimethoxysilane

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In the present work, organic-inorganic nanocomposites based on epoxy resin DER 332 and modified montmorillonite (MMT) were obtained at different proportions 0%, 0.5%, 1%, 3% and 5% wt. MMT [1]. It was used 3 -Glycidoxypropyl Trimethoxysilane as pretreatment film. The nanocomposites were deposited on carbon steel substrates which were cleaned with detergent and abrasive paper, the coatings were cured at 120°C for 1 hours [2]. The characterization of the coating was performed using physical techniques such as Scanning Electron Microscopy (SEM), Optical Microscopy (OM), Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetry Analysis (TGA), X-Ray Diffraction (XRD), adhesion was evaluated using standard ASTM D3359-02 and the corrosion assessment was carried out using Electrochemical Impedance Spectroscopy (EIS) technique, in parallel with visual corrosion tests according to ASTM D610-01 and ASTM D1714-02 [3]. The results of the characterization and the electrochemical evaluation by EIS showed the formulation with the best anticorrosive performance in a solution of NaCl 5% wt.

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Composites of polycaprolactone reinforced by clay Cloisite 20A®

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Introducction

The development of environmental friendly and biodegradable polymeric materials has attracted extensive interest of researchers[1]. Polycaprolactone (PCL) belongs to this class of synthetic biodegradables polymers[2], which properties can be improved by fillers such as clays. The aim of this work is the study of the effect of clay on the morphology and mechanical properties of PCL/clay composites.

Experimental

Composites containing 3, 5 and 10 wt%, of Cloisite 20A were prepared in a double-screw extruder DSM Xplorer 15CC microcompouder at 100ºC, screw rotating speed of 100 rpm and residence time of 5 min. Specimens for mechanical tests were injection molded at 100ºC in a mold kept at 35ºC using 16 bar pressure during 1 min.The composites were characterized by XRD, DSC and Tensil test (ASTM D638).

Results and discussion

The interlayer space of clay in the composites was calculated from XRD measurements using Bragg´s law (Table 1). In general, the interlayer space is higher for the layer in the composites, suggesting a possible polymer intercalation [3]. However, DRX data show that the clay structure is preserved, leading to a conclusion that the shear stress in the extruder was not enough to promote clay exfoliation. This is a possible explanation for the similarity of the mechanical properties of the composites compared with those of neat PCL. A slight increase in the degree of crystallinity was observed when the clay was incorporated to the matrix, regarding increase in the temperature of cooling from DSC.

Table 1.Mechanical properties of the composites and clay interlayer space.

Sample	Modulus [MPa]	Strength [MPa]	Xcr [%]	Interlayer space [nm]
Cloisite 20A	------	------	------	24.8
PCL	243 ± 13	17.8 ± 0.9	47	---------
PCL/Clo3%	235 ± 7	13.9 ± 0.8	49	28.9
PCL/Clo5%	214 ± 9	12.1 ± 1.1	50	30.5
PCL/Clo10%	230 ±18	10 ± 1.9	50	32.0

Conclusion

PCL/Clay composites were prepared by extrusion and injection molding. The Cloisite 20A clay showed compatibility with PCL which led to the composites with a good clay dispersion degree.

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PTB7:$PC_{71}BM$ BULK ORGANIC SOLAR CELL DOPED WITH IRON DISULFIDE NANOPARTICLES

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Among 23 semiconductors, iron sulfide (FeS_2) is the best candidate for development of large-scale solar cells at a lower extraction cost ($<2x10^{-6}$¢/W) [1]. FeS_2 nanostructured present excelent optoelectronic properties; direct band gap (0.93 to 1.38 eV), high optical coefficient ($2x10^5$ cm^{-1}), high mobility (2.12 -80 cm^2/Vs) and large carrier lifetime (200ps) [2-4], making it good alternative for photovoltaic applications. In this work, FeS_2 nanoparticles were obtained at 220 ºC by using octadecylamine as solvent and, sulfur and iron chloride as precursors, the reaction was kept under Ar gas for 1 h. These nanoparticles (20 nm) were added at 0.25 wt.%, 0.5 wt.% and 1 wt.% in the active layer, which was deposited by spin coating on PEDOT:PSS/ITO substrate in order to build the ITO/PEDOT:PSS/PTB7:$C_{71}BM$:FeS_2/PFN/FM devices. The roughness value of the PTB7:$C_{71}BM$ active layer (3.42 nm) drecreased as a function on the concentration of FeS_2 NPs (1.97 nm, 1.95 nm and 2.86 nm at 0.25, 0.5 and 1wt.%, respectively). The solar cells without FeS_2 NPs presented an average efficiency conversion (η) of about 3.87 %. The η decreased to 0.79% and with 0.25 wt.% of FeS_2 NPs, but at 0.5 wt.% it increased at 4.55%. The efficiency conversión of the organic solar cells was improved with the addition of FeS_2 NPs in the active layer, so that these nanoparticles could be function as charges-transporting or surface modifier.

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Hydroxyapatite impregnation with neem oil as a promising bactericidal material

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The synthetic hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$ is used in tissue engineering and regenerative medicine due to its biocompatibility. Furthermore it has a chemical composition and similar structure to the mineral phase of bones. The most widely used application is as absorbable material to help in osteointegration, as drug delivery agent or as gene delivery system [1]. The main limitation to the use of synthetic hydroxyapatite, is a lack of antibacterial activity. For this reason, incorporation of inorganic antibacterial cations such as silver, copper and zinc can prevent microbial infections [2]. Also impregnation with essential oils can enhance its bactericidal activity. Among essential oils, the neem oil extracted by the seeds of the neem tree commonly found in India, Africa and America, is used in a grand variety of medical applications such as antiallergic, antipyretic, antimycotic, pesticide and antimicrobial. The neem oil is constituted by several active principles with great antimicrobial capacity.

In this work, hydroxyapatites containing copper cations were impregnated with neem oil by adsorption methods. The crystallization was carried out by ultrasound. The promising bioactive materials were characterized by X-ray diffraction, scanning electron microscopy, nitrogen physisorption and FTIR spectroscopy. The materials obtained will be tested as antimicrobial.

Keywords

Hydroxyapatite, neem oil, impregnation, antimicrobial activity

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VIEP-BUAP, CUVyTT-BUAP

Manganese complexes with calix[8]arene as potential electrocatalyst for CO_2 reduction

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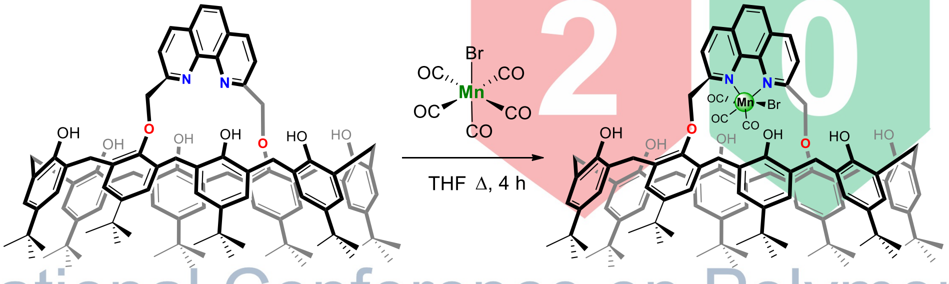
The chemical reduction of CO_2 to fuels offers a way of recycling carbon dioxide and could therefore ameliorate associated climate change and increase the sustainability of oil reserves for other purposes. There are several ways to achieve this including electrocatalytic and photocatalytic processes. Recently, manganese has been used as substitute of more expensive metals like rhenium in electrocatalyst with the general formula $[Mn(L)(CO)_3Br]$ to achieve the transformation of CO_2 to CO [1]. Using the calix[8]arene as scaffold to make a ligand with a chelating phenantroyl moiety inside the hydrophobic cavity has led to the formation of supramolecular complexes [2, 3]. The second coordination sphere provides the characteristics that appear to be essential for CO_2 reduction, such as a sterically restricted environment [4], and -OH groups near the metal center [5]. The behavior of the complex $[Mn(C8fen)(CO)_3Br]$ (C8fen = 1,5-(2,9-dimethyl-1,10-phenantroyl)-*p*-*tert*-butylcalix[8]arene) under reducing conditions via cyclic voltammperometry under CO_2 atmosphere will be reported, with methanol and water as proton donors.



C8fen

$Mn(C8fen)(CO)_3Br$

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INTELLIGENT COATINGS BASED ON VANADIO DIOXIDE (VO_2), FOR ENERGY SAVING APPLICATIONS

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Summary

The increase in energy costs, the growing interest in green technologies and global warming, allow the development of intelligent materials to save energy.

Recent advances in the development of thin films and the transition of some thermochromic materials have caused a high interest among researchers due to the phenomena that these materials present in their structure by the effect of the metal-semiconductor phase transformation [1] [2].

In the present work, thin films of vanadium dioxide (VO_2) were made on silicon substrates. In addition, to obtain a better response in the reduction of the phase temperature (T_c) of the vanadium dioxide (VO_2). Molybdenum (Mo) ions with dopant element were used at different concentration percentages (1, 2, 3, 4 and 5%), to result in a reduction in the phase temperature of vanadium dioxide.

According to the optical measurements of transmittance in the near-infrared region, the vanadium dioxide (VO_2) films exhibited a characteristic optical behavior of thermochromic materials in the phase temperature range between 30 and 50 ° C (Fig. 1). As well, a decrease in the grain size of the nanoscale crystal was clearly observed.

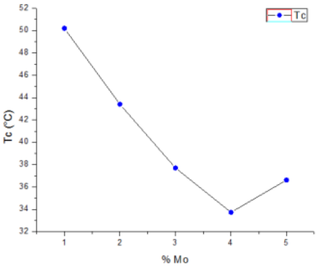

Fig. 1: Phase temperature range (T_c) for each concentration percentage of Molybdenum (Mo)

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Shining Light on Indium Phosphide Quantum Dots: Nucleation, Growth, and Post-Synthetic Transformation

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Indium phosphide quantum dots are an emerging material of interest in a diverse set of applications including displays, solid-state lighting, catalysis and solar energy capture. Our ability to harness the unique properties of these quantum-confined semiconductors relies on our ability to prepare monodisperse samples in high yield and with near unity quantum efficiency. Addressing these challenges requires controlling the solution synthesis of these nanocrystals with atom-level precision. This is particularly challenging for phosphide semiconductors due to both the nature of the reagents used to make the particles and the covalency within the particles themselves. This presentation will outline the progress we have made on understanding the precursor conversion reactions, nucleation and growth mechanisms, and approaches to the post-synthetic transformation of indium phosphide quantum dots.[1] In particular, our recent discovery and characterization of a kinetically persistent magic sized cluster intermediate enables condition-dependent resolution of each of the different steps in the synthesis of indium phosphide nanomaterials from the monomer constituents,[2,3] which has been critically important to our understanding of the mechanism of nanomaterial growth.

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Acknowledgements (10 pt)

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Cadmium removal from solid surfaces by using surfactant molecules: experiments and computer simulations

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Experiments and computer simulations were used to study removal of cadmium particles from solid surfaces with Sodium Dodecyl Sulfate (SDS) as surfactant to promote desorption of ions from graphite. Different experimental techniques, such as scanning electron microscopy and atomic force microscopy, were used to investigated desorption of cadmium sulfate from highly oriented pyrolytic graphite. Desorption of cadmium was also studied with molecular dynamics techniques and comparisons with experiments were conducted to understand from a microscopic level the removal process. Good agreement was found between experiments and computational results in terms of the desorption mechanism.

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Ga(III) COMPLEXES WITH PNC LIGANDS, AS SINGLE SOURCE PRECURSORS FOR MATERIAL SYNTHESIS

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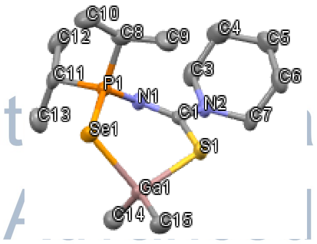
We report the synthesis of single source precursors (SSPs) with the general formula $[Ga(CH_3)_2({}^iPr_2P(X)NHC(Y)NC_5H_{10})]$ (X = S, Se ; Y = O, S); the ligands and complexes were prepared as we report earlier[1,2]. These compounds were used to produce nanocrystalline thin films of Ga_2X_3 by Aerosol-Assisted Chemical Vapor Deposition[3]. The precursors were characterized by multielement NMR, IR, monocrystal X-ray diffraction, mass spectrometry, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC); while the thin films were characterized by X-ray diffraction (GIXRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDXA), Raman and UV-vis spectroscopy. Crystal X-ray molecular structural of Ga compounds showed that they were four-coordinate with tetrahedral geometry (a). Thermogravimetric studies of complexes showed a fast weight lost between 175°C and 350 °C to give metal chalcogenide residue (b). The SEM images of the synthesized material Ga_2S_3 (c) exhibited a spherical morphology.

a



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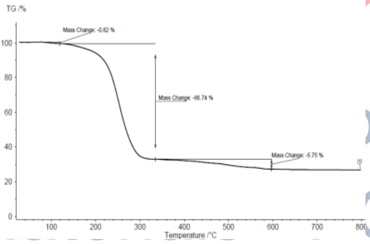

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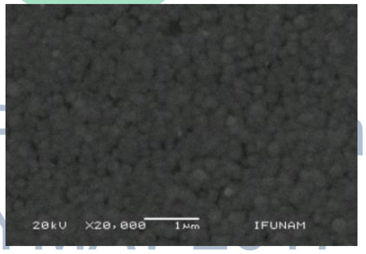

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Dye-sensitized solar cell using extract from Justicia Spicigera modified with TEOS

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Solar energy has always generated great interest for scientists in recent years as a kind of alternative energy, which has led to explore new technologies and methodologies, such as solar cells [1]. Recent research focuses on improving the functioning of cells, so there is a great interest in using natural dyes as sensitizers. Several pigments, including anthocyanins, flavonoids, carotenoids and chlorophyll, are extracted from various parts of plants, such as leaves, flowers, fruits and roots [2, 3]. Justicia spicigera (common name muicle or muitle) is a plant that has been used in Mexico since the pre-Hispanic times as a natural pigment [4].

Flavonoids can be grouped as anthocyanins, flavonols and proanthocyanidins, anthocyanins has been detected in ethanol extracts from J. Spicigera, these compounds are the most abundant in this plant and can absorb light at longest wavelength [5]. It is interesting that J. Spicigera contains anthocyanin compounds, since it has been shown that molecules are attached to the surface of the semiconductor aid in the excitation and transfer of electrons [6].

In this work, solar cells sensitized with natural dye from the extract of the Justicia Spicigera plant modified with Tetraethyl orthosilicate (TEOS) and using substrates of ITO (indium tin oxide) by the technique of Dr. Blade were constructed. They were characterized by current-voltage and power curves [7]. In addition, we study the efficiency of the conversion energy, the effect on darkness and illumination, as well as the life time of the cell.

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ZINC AND CADMIUM COMPLEXES WITH PNC LIGANDS AS SINGLE SOURCE PRECURSORS FOR MATERIAL SYNTHESIS

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Zinc and cadmium complexes of N-(chalcogen)phosphorylated(chalcogen)ureas $[\mathrm{M}\{^{i}\mathrm{Pr}_2\mathrm{P(X)NC(Y)NC}_5\mathrm{H}_{10}\text{-}\kappa^2\text{-X,Y}\}_2]$ (M = Zn, Cd; X = S, Se; Y = O, S) were synthesized[1,2]. The complexes were characterized by elemental analysis, multielement NMR, IR, monocrystal X-ray diffraction, mass spectrometry, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). TGA confirmed that all eight complexes decomposed in a single step to their corresponding metal sulfides and selenides MX. The complexes were used as single source precursors to obtain MX and solid solutions thin films by aerosol assisted chemical vapor deposition (AACVD)[3] at 450 °C, as well as MX quantum dots by thermolysis[4] at 300 °C. The elemental composition of nanomaterials was confirmed by energy dispersive X-ray spectroscopy (EDXA). The morphology and optical properties were investigated using transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (GIXRD (Fig. A) and pXRD), UV-Vis absorption, photoluminescence (PL) and Raman spectroscopy.

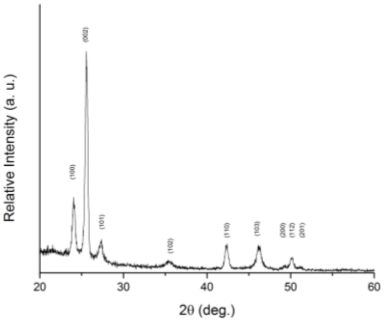

Fig. A. XRD pattern of the solid solution $\mathrm{CdS}_{0.2}\mathrm{Se}_{0.8}$ thin film.

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ZINC AND CADMIUM(II) COMPOUNDS AS SINGLE SOURCE PRECURSORS FOR GROUP 12-16 THIN FILMS AND QUANTUM DOTS

Verónica García-Montalvo[1], Alejandra Aguirre-Bautista[1], Víctor Flores-Romero[1], Oscar L. García-Gúzman[1], Iván D. Rojas-Montoya[1], Miguel-Ángel Muñoz-Hernández[2] and Margarita Rivera[3]

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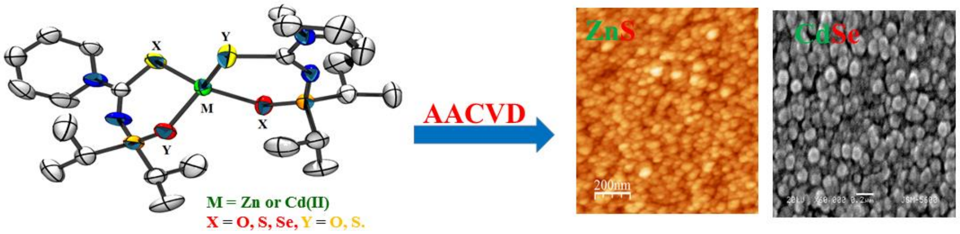
Coordination compounds are useful as single sources precursors for the deposition of metal chalcogenide thin films or the preparation of nanoparticles. Group 12–16 semiconductors have a wide variety of applications [1, 2]. A series of *bis*-chelates of zinc and cadmium with general formula $[M({}^{i}Pr_2P(X)NHC(Y)NC_5H_{10}\text{-}\kappa^2\text{-}X,Y)_2]$, $ML^{X,Y}_2$ (X and Y= O, S, or Se), were synthesized and characterized by common spectroscopic methods. These compounds were crystalline solids and the structures of six complexes and two ligands were determined by X-ray single crystallography. Chelates thermal behavior was investigated by simultaneous thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). They all were used as single-source precursors for metal sulfide (MS) and/or selenide (MSe) thin films)[3], and quantum dots (QDs). The as-obtained materials were characterized by X-ray diffraction (GIXRD and pXRD), Raman and UV-vis spectroscopy. The morphology of the films was studied by scanning electron microscopy (SEM), atomic force microscopy (AFM), and by transmission electron microscopy (TEM) in the case of QDs. The elemental composition was confirmed by energy dispersive X-ray spectroscopy (EDAX). The influence of precursor with different donor atoms on the nature of the obtained materials is discussed.



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SYNTHESIS, MICROSTRUCTURE, AND SENSING PROPERTIES OF $NdCoO_3$ NANOPARTICLES

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$NdCoO_3$ nanoparticles were successfully synthesized by a simple, inexpensive and reproducible solution-method for gas sensing applications. Cobalt nitrate, neodymium nitrate and ethylenediamine were used as precursors and distilled water as solvent. The solvent was evaporated later by means of non-continuous microwave radiation at 290 W. The obtained precursor powders were calcined at 200, 500, 600 and 700 °C in a standard atmosphere. The oxide crystallized in an orthorhombic crystal system with space group *Pnma* (62) and cell parameters a = 5.33 Å, b = 7.52 Å and c = 5.34 Å. The nanoparticles showed a diffusional growth to form a network-like structure and porous adsorption configuration. Pellets prepared from $NdCoO_3$ were tested as gas sensors in atmospheres of carbon monoxide and propane at different temperatures. The oxide nanoparticles were clearly sensitive to changes in gas concentrations (0 – 300 ppm). The sensitivity increased with increasing concentration of the gases and operating temperatures (25, 100, 200 and 300 °C).

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Analysis of the Insitu porosity formation of $Al_{62}Cu_{28}Fe_{10}$ and $Al_{66}Cu_{28}Fe_{12}$ alloy compositions

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The present investigation continued the study of Al-Cu-Fe base metallic foams production via the in-situ process, i.e. without the need of foaming agents or space holders. Two new $Al_{62}Cu_{28}Fe_{10}$ and $Al_{66}Cu_{28}Fe_{12}$ compositions are presented and discussed. The alloys were melted in an induction furnace and then cooled to room temperature. The alloys were heat treated to produce a higher percentage of porosity. The multiphase system consisting mainly of I (Al_6Cu_2Fe), λ ($Al_{13}Fe_4$), ($\theta AlCu_2$) and ω (Al_7Cu_2Fe) phases were characterized by means of SEM, XRD and TEM. The transformation temperatures that were used during the heat treatment were obtained with the DTA. The optimum heat treatment temperature was 750 °C for $Al_{66}Cu_{28}Fe_{12}$ and 850 ° C for the $Al_{62}Cu_{28}Fe_{10}$. The percentage of porosity and pore morphology were characterized using an image analyzer. It was identified that the mechanism that forms the porosity is due to a peritectic reaction. The interaction between liquid and λ($Al_{13}Fe_4$) phase formed a highly dense I (Al_6Cu_2Fe) and ω (Al_7Cu_2Fe) phases leading to the formation of porosity.

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SYNTHESIS OF $LiMn_2O_4$ BY IONIC EXCHANGE

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Depending on the precursors to obtain a compound and the route of synthesis, as well as the treatment applied; different structures can be obtained for the same chemical compound. This is very important, because the properties of materials in general, change depending on the structure they have, and this is why, for this work, we want to study the obtained structure for $LiMn_2O_4$ synthesized from $NaMn_2O_4$ by ionic exchange.

In addition, with the increasing demand for energy, lithium batteries are taking an impressive boom [1, 2]. That is why we are in the research for new materials that increase the energy density in the batteries, as well as the reduction of recharge times. The possible application of the ceramic material $LiMn_2O_4$ to rechargeable lithium batteries has been an important motivation for this work [3].

We prepared $LiMn_2O_4$ by ion exchange of $NaMn_2O_4$ with fused lithium salts (nitrate or chloride) and the results were compared with $LiMn_2O_4$ obtained by solid-state reaction from lithium and manganese carbonates and acetates. Characterization results by x-ray diffraction and scanning electron microscopy will be showed.

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ENERGY SAVING TECNOLOGY FOR WATER FILTRATION USING CARBONATED POROUS CERAMICS.

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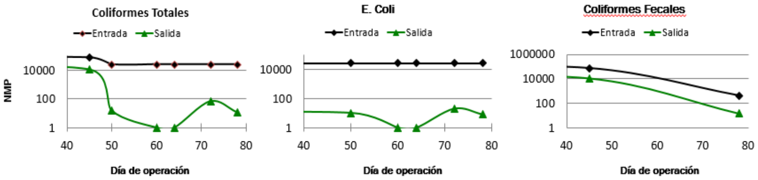
The microbiological quality of drinking water is a determining factor in the transmission of diseases. The contamination of fecal origin found in the water that serve for human consumption is one of the mayor problems that face third world countries [1]. The presence of microorganism's indicators like the total coliforms and the fecal coliforms and E. Coli are of significant help to evaluate water contamination.

It is known that filtration and purification in organic material from suspended solid particles is successfully carried out by porous materials. The advanced porous ceramics are being used, in a broad number of applications with the finality of solving various ambient problems, biologist, and from transportation. This material has many advantages from the other materials like the polymers o metals and qualities like hardness, chemical inertial, thermal shock resistance, corrosion resistance, wear and low density, essentials for many applications. For this reason the ceramics can offer properties for the impurities capture in a filter. The filtration made with porous ceramics like the filter material is known and it has been studied to be use in the elimination of the turbidity and other pathogens agents in the water. The objective of this work is to develop a technology that promotes the synthesis of porous ceramics based on aluminosilicates (clays) and the establishment of regularities in the filtration of water with pathogenic microorganisms, and in case of inadequate cleaning, the introduction of a second water stage using carbonized reed.

The proof consisting in the porous ceramics elaboration, evaluating its effectiveness in a filter medium to be used in the removal of pathological microorganisms. The principal answer variants correspond to the microorganism indicators like the total coliforms, fecal coliforms and E Coli. The volume of the biologic filters was 10L, in which 2L of active carbon was included, and 3L of porous ceramics and 5L of water to be treated.

The results obtain showed that the filter system based on porous ceramics are efficient for the removal of total coliforms (98%), fecal coliforms (97%) and E coli (98%), in bigger concentration to 1x10^5 NMP/100ml.

In conclusion, we can say that there was a good response in the removal efficiency of microorganism's indicators. Furthermore, the physical-chemical characterizations showed inferior levels than the ones showed at LMP marked in the NOM-127-SSA1-1994. And the utilization of porous ceramics like the filtering material can be considered for the removal of microorganism's indicators like total coliforms, fecal coliforms and E. Coli.



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CAPACITIVE PROPERTIES OF CONDUCTING POLYANILINE FILMS.

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Electrochemical capacitors (EC) are novel energy storage devices with high power density; they exhibit excellent pulse charge/discharge property and long lifetime [1]. Polyaniline (Pani) is considered the most promising conducting polymer for supercapacitors due to its high capacitive characteristics, low cost and easy of synthesis [2-4]. In this work we present a comparative study of charge storage in acid and neutral electrolytic systems 1M H_2SO_4 and 1M $NaNO_3$. The electrodes were prepared by electropolymerization of aniline on Indium thin oxide (ITO) substrates. The surface morphology of PANI electrodes was characterized by atomic force microscopy (AFM). The electrochemical properties and the capacitive behavior of the PANI electrodes were systematically studied using cyclic voltammetry (CV) and constant current charge/discharge tests, respectively. Is important to mention that the specific capacitance of PANI electrodes is strongly influenced by the electrolytic system used and it is manifested in the capacitive responses.

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MODIFICATION OF MCM-TYPE MESOPOROUS SILICAS WITH POLY(ALLYLAMINE)

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Supported amine materials have attracted much attention in recent years for CO_2 capture due to their high adsorption capacities [1, 2]. These materials are prepared by incorporating organic amines into porous solids by different methods such as impregnation, grafting, and *in-situ* polymerization of amine-containing materials [3]. MCM-type mesoporous silicas have used as supports due to their order mesostructure, high surface areas (> 1000 m^2/g), high pore volumes, and narrow pore size distributions [4]. On the other hand, poly(allylamine) (PAA) is a interesting material containing primary amines on the side chain of the hydrocarbon backbone which makes it very attractive for many applications such as, gas adsorption, water treatment or drug delivery [1, 5]. Here, we report the modification of MCM-type mesoporous silica with PAA by the "grafting to" method. Firstly, mesoporous MCM-41 and MCM-48 silicas were functionalized with 3-glycidyloxypropyltrimethoxysilane (GPS) in order to obtain materials with epoxy groups onto their surface. Then, the previously obtained MCM-GPS silicas were reacted with PAA through their expoxy groups with the amine groups from PAA to obtain the hybrid materials MCM-PAA. The hybrid materials were characterized by X-ray diffraction, infrared spectroscopy, thermogravimetric analysis and transmission electron microscopy.

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The influence of Ni content over the Sn-Zn eutectic alloy

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The Sn-Zn eutectic alloy has been considered as an interesting candidate to substitute conventional Sn-Pb solder alloys because of its good mechanical properties, low cost and melting temperature similar to Sn-Pb solder alloys. [1]

The poor oxidation resistance of the Sn-Zn eutectic alloys, as result of the oxidation of Zn that is present in primary and eutectic phases, has limited its application. Also, the poor wetting of Sn-Zn eutectic alloy, on Cu substrate, is attributed to the high surface tension and oxidation sensitivity of Zn over it. In this fashion, the oxidation resistance can be increase by the reduction of the Zn content forming intermetallic compounds (IMC's). Some authors have reported that the modification of Sn-Zn eutectic alloy with a third element to control the formation of IMC's can improve the melting temperature, wettability, oxidation resistance, corrosion and mechanical properties.

The objective of the present work were to study the influence of small addition of Ni content on the microstructure and thermal properties of the eutectic Sn-9Zn (wt %) alloys.

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Synthesis and characterization of Zn and Cu nanoparticles

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Nowadays, contamination of water by microbial agents has generated a need to produce new microbicidal agents in order to guarantee the complete elimination of these microorganisms [1]. Metal nanoparticles have emerged as antimicrobial materials able to eliminate the bacterial resistance mechanisms to traditional antibiotics [2]. In this work, nanoparticles of Cu and Zn were synthesized by a bioreduction method using water hyacinth as the reducing agent in metal solutions at pH = 7. It is expected that these nanoparticles may function as microbicidal agents. The synthesized Zn nanoparticles (ZnNPs) showed an independent formation with no presence of agglomerates, their estimated size was between 2 and 5 nm, their observed structure was hexagonal corresponding to the ZnO chemical formula [3]. Cu nanoparticles (CuNPs) did not show the formation of agglomerates and their size ranges between 5 to 10 nm, presented a cubic corresponding to the chemical composition of CuO [3]. The presence of copper was confirmed by an EDS analysis of these nanoparticles (CuNPs). Although the ZnNPs and CuNPs formed different crystal structures the composition of both corresponds to a metal oxide, and the particule size of CuNPs was larger than the ZnNPs.

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Design and study of Ni(II) supramolecular catalysts based on ligands derived from calix[8]arene

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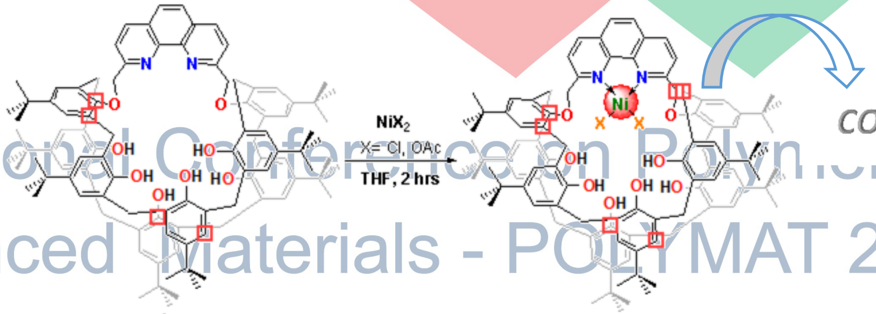
The formation of supramolecular catalytic systems such as nanoreactors, provides the opportunity to obtain properties that are not commonly observed for conventional catalysts with exposed reaction centers, which in some cases leads to higher reaction rates[1]. In our research group, we have worked with a Cu(I) complex based on calix[8]arene functionalized with a phenanthroline group (**L**). This compound demonstrated good catalytic activity towards C-S coupling reactions due to confinement of the substrates within the calixarene cavity, which appears to increase the efficiency of the reaction[2]. In this work, we reporte an extension of the use of **L** to obtain Ni(II) complexes that may be applied for the reduction of CO_2, the main greenhouse gas produced in industrial processes[3]. Thus, the synthesis and characterization of [**L**Ni(II)] complexes will be presented, as well as initial tests to evaluate its electrocatalytic potential for the reduction of CO_2, which should be favored by the presence of the intramolecular phenolic OH groups.



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EXTRACTION AND CHARACTERIZATION OF POROUS BIOGENIC SILICA FOR LIPASE IMMOBILIZATION.

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Plants with high content of silicon are a sustainable alternative for the production of biogenic silica (BS) used in many applications as support for bio-catalyst, drug delivery systems, polymer composites, enzyme immobilization [1] and other applications.

This work reports the process of acidic extraction of BS obtained from the horsetail plant (*Equisetum myriochaetum*) and the enzyme immobilization study for *Candida rugosa* (CR) and *Rhizomucor miehei* (RM). The plant was submitted to a process of dehydration and milling, followed by acid wash (*H_2SO_4/HNO_3*) at 70 °C. The obtained powder was washed with distilled water until pH 7 was reached and then heated to 650 °C for 6 hours to remove water and carbon.

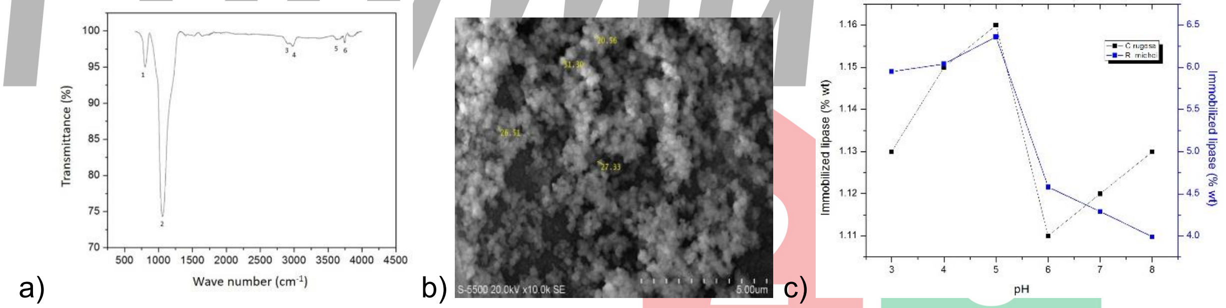

Figure 1. a) FTIR spectrum of BS, b) SEM Micrograph 20 keV, c) pH lipase immobilization isotherm.

The presence of SiO_2 and characteristic functional groups of BS [2] such as C-CH_3, O-SiH_2 and OH was verified by FTIR (Figure 1a), X-ray diffraction and X-ray Energy Dispersive Spectroscopy (EDS) measurements. Scanning electron microscopy (SEM) (Figure 1b) and BJH method for absorption isotherm were used to measure surface properties. Particle size of 2-5 µm was found and an average size pore diameter of 5.8 nm. The immobilization study was performed at different pH (figure 1c), presenting the maximum absorption at pH 5 for both enzymes.

Immobilization of CR and RM (4.8nm diameter) in BS was achieved. This confirms that BS can be used as a lipase support [3] for catalytic esterification reaction applications.

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Graphene oxide membranes as supercapacitor separators

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Although supercapacitors are now produced at an industrial scale, the number of studies devoted to testing various materials, which could possibly be utilized as electrodes of supercapacitors, is rapidly growing. Particularly, carbon nanostructures with high specific surface areas and high conductivity are considered as perspective supercapacitor materials. The new carbon-based material, the graphene oxide, is dielectric and therefore it is natural to explore whether graphene oxide could be used as a supercapacitor separator. The present work reviews the experimental studies involving the possible usage of membranes composed of graphene oxide as supercapacitor separators. This report also describes briefly the properties of graphene oxide and graphene oxide membranes and how they may be produced. Special attention is paid to studies related to the pore distributions in the graphene oxide membranes, the dependence of membrane properties on humidity, and the protonic character of wet membranes composed of graphene oxide. The fabrication of symmetric mini-supercapacitors with acid electrolytes and graphene oxide membranes is described along with their major characteristics [1-4].

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BISMUTHATE COMPLEX AS A NEW PRECURSOR MATERIAL FOR THE PREPARATION of β-Bi_2O_3 OR α-Bi_2O_3 PHASE

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As a type of important functional inorganic material, bismuth oxide (Bi_2O_3) has attracted great interest due to its application in catalysis, solid fuel cell, microelectronics, gas sensors, optical coatings, blue laser recording, and glass manufacturing, etc. [1]. Indeed Bi_2O_3 has proved to be a good photocatalyst with a direct band gap ranging from 2 to 3.9 eV and can be used to decompose dyes in water. The Bi_2O_3 has six polymorphs, among them, the low-temperature α phase and the high temperature δ-phase are thermodynamically stable, while the other phases (β,$\gamma, \omega, \varepsilon$) are metastable. However, β Bi_2O_3 is the most active heterogeneous photocatalyst. Since beta phase represents a metastable high temperature modification and is known to transform to α Bi_2O_3. In this line, different precursor materials like bismuth oxalate [2], bismuth oxide nitrate hydroxide hydrate [4] and $Bi_60_4(NO_3)_5(OH)_5 \bullet 0.5H_2O$ [3], etc. are employer for the preparation of either α-Bi_2O_3 or β-Bi_2O_3. On the other hand, bismuthate complex prepared with diamine molecule has been recently reported as an inorganic-organic material [4], but it has never been tested or used as a precursor material for get Bi_2O_3. In this work bismuthate complex obtained by chemical precipitation method was used as precursor material of the Bi_2O_3 by annealing a different temperature in the ranging from 350 to 600ºC. The influence of the relation HNO_3/ethylenediamine on the crystalline structure and morphology during the bismuthate complex preparation was investigated. Both precursor and Bi_2O_3 were characterized by x-ray diffraction and FT-IR showing that the crystalline structure is completely amorphous with a peak at a low angle suggesting a superstructured materials. FTIR analysis exhibits the presence of ethylenediamine of the possible bismmuthate. The thermal analysis show the temperature at which β-Bi_2O_3 and the α-Bi_2O_3 phases are well transformed. SEM analysis showed that when relation HNO_3/ethylenediamine is 0.1, the precursor material shows particle size of 1-3 micrometer, but after of the calcination, the obtained nanostructures β- Bi_2O_3 showed nanoparticle of 90 nm and microstructures of 1-5 µm for α-Bi_2O_3 caused by sintering process.

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Effect of the addition of Montmorillonite on the anticorrosive properties of a coating hybrid.

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A hybrid epoxy-silica coating reinforced with a clay was synthesized using epoxy resin DER 332 and 4,4-diaminodiphenylmethane as cured agent [1]. The clay was natural montmorillonite modified with methyl-tallow-bis-2-hydroxyethyl quaternary ammonium salt. The hybrid coating with 0, 0.5, 1, 3, and 5 wt% clay loadings, respectively, were prepared and deposited onto carbon steel coupons and cured at temperature of 125°C for 2 hours. The coupons were chemically treated with a 5 wt% NaOH solution. The samples were characterized by X-Ray Diffraction (XRD), Thermogravimetric Analysis (TGA) for to evaluate coating thermal resistance, Scanning Electron Microscopy (SEM) showed that the surface of the coatings were uniform and defects free, and had good adherence to metallic substrate, Fourier Transform Infrared Spectroscopy was used to follow the curing reaction by means of the epoxy group. The coating adhesion was evaluated by ASTM D 3359-02, and the corrosion performance was evaluated using test ASTM D610-01 [2]. Electrochemical tests were performed using electrochemical impedance spectroscopy (EIS) to evaluate the anticorrosive performance of the coatings. The coating with 3% of montmorillonite had the highest impedance of the order of 1x109 ohms, being the coating with better anticorrosive performance [3].

Keywords: Hybrid coating, Montmorillonite, Nanocomposite coating.

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ELECTROCATALYTIC WATER SPLITTING IN ALKALINE MEDIA USING HYDROTALCITE-LIKE MATERIALS

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High activity, durable, and cost effective electrocatalyst for the oxygen evolution reaction (OER) plays an important role in electrochemical science and technology , for example, water- splitting by electrolysis for production of hydrogen. The first-row transition-metal-based OER catalysts, especially iron-, cobalt- and nickel-containing materials, are versatile candidates for replacement of precious catalysts due to their earth abundant nature, low cost, environmentally friendly, multiple valence state and high theoretical activity.[1]
This contribution reports the effect of the iron content and M^{2+}/M^{3+} ratio cation arrangement-distribution on the oxygen evolution reaction (OER) catalyzed by layered double hydroxides. The electrocatalysts, containing variable contents of Ni and Fe, were successfully prepared through a homogeneous precipitation method. The formation of LDH structure was verified by powder X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). Other properties were determined such as specific surface area, electrical conductivity, and surface basicity. First-principles DFT+U calculations complemented and supported the electrochemical results. According to both the electrochemical and simulation results, the increase of the catalytic activity for the OER on the presence of Fe^{3+} is closely related with the configuration and distribution of Fe and Ni cations in the brucite layer structure. The effect of iron is indirect, favoring the electron hopping on the Ni sites for certain local configuration.

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Hybrid Halide Perovskites: New Optical Materials for Energy Conversion Devices

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Organometal halide perovskites have quickly become one of the most interesting semiconductors for photovoltaics, reaching power conversion efficiencies of over 22% [1i 5]. We were among the first to synthesize colloidal $CH_3NH_3PbX_3$ (X = I, Br) nanocrystals with different morphologies (dots, rods, wires, sheets) [4]. At the single particle level, these nanostructures show shapei correlated PL emission across whole particles, with little photobleaching observed and very few off periods [3]. We are particularly interested in mixedi halide perovskites such as $CH_3NH_3PbX_{3i\ a}X'_a$ (X, X' = I, Br, Cl) because of their enhanced moisture stability, and band gap tunability. Using a combination of optical absorption spectroscopy, powder Xi ray diffraction (XRD) and, for the first time, ^{207}Pb solid state nuclear magnetic resonance (ssNMR), we have probed the extent of alloying and phase segregation in these materials [2]. ^{207}Pb ssNMR reveals that nonstoichiometric dopants and semicrystalline phases are prevalent in samples made by solution phase synthesis. We have shown that these nanodomains are persistent after thermal annealing up to 200 °C. Our observations are consistent with the presence of miscibility gaps and spontaneous spinodal decomposition at room temperature, and underscore how strongly different synthetic procedures impact the nanostructuring and composition of organolead halide perovskites. Better optoelectronic properties and improved device stability and performance will be achieved through careful synthetic manipulation of these materials.

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MATERIALS FOR SOLAR CELLS ON BASE OF ORGANIC−INORGANIC HYBRID PEROVSKITE OBTAINED BY CO2 LASER CRYSTALLIZATION

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Organic−inorganic halide perovskites have emerged as promising materials for optoelectronics, particularly photovoltaics. Materials based on perovskites attract research interest for next generation of solar energy cells. Crystal structures containing organic and inorganic components allow the creation of perovskite films for solar cells. A continuous process of crystallization of perovskites on flexible substrates of a large area is of great importance for the production of solar batteries. In this paper we present the results of laser crystallization of hybrid perovskite cells using infrared (IR) CO_2 laser radiation (λ=10,6 μm). Laser crystallization allows to achieve improved characteristics of perovskite films in comparison with the traditional thermal annealing. Direct irradiation of the laser beam on to a perovskite precursor layer formed an instantaneous phase transformation into uniform polycrystalline films with large grain sizes ranging from 150 to 600 nm. Laser scan rate is another significant parameter for grain growth. A low scan rate delivers a high energy at the same power density resulting in a large crystalline grain size. As-deposited film lacks well-defined grain structure, whereas laser crystallization induces clear distinction of perovskite grains throughout the entire film thickness. An insufficient power density yields small grains with many grain boundaries both in horizontal and vertical directions to the substrate. By contrast, sufficient high power density (typically 60 W cm^{-2}) induces large grains with much less boundaries. A further increase in the power density over 60 W cm^{-2} causes nonuniform film morphology. Our analysis on surface temperature clarifies the underlying mechanism of phase transformation induced by CO_2 laser irradiation. Laser photothermal crystallization has been successfully implemented for organic−inorganic hybrid perovskite solar cells. Reliable controllability of perovskite crystalline structure and morphology with low energy CO_2 laser beam realizes high performance solar cells on flexible polymer as well as hard glass substrates.

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Process of marking by an inorganic material in a ferrous metal base, using the irradiation of a CO_2 laser

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This work developed a brand with the assistance of CO_2 laser equipment. Using the marking technique by sintering and crystallization of glassy powders forming a ceramic-vitreous matrix in a ferrous metal base.

The ceramic-vitreous matrix adheres to the substrate forming a layer with mechanical properties: such as corrosion resistance, wear resistance, fracture strength as well as toughness and aesthetic functions. The ceramic-vitreous matrix will be obtained by a mixture of various inorganic raw materials conformed by silicate, metallic oxides of cobalt, zinc, alumina, frits, and feldspars.

The application was made by enameling, in this process depends on two important factors: the nature of the surface of the substrate and the type of glass-ceramic used. For enameling, two processes are used: 1) Porcelain enamel moist. 2) Dry-silicon porcelain enamel. During the synthesis process to create the glass-ceramic matrix CO_2 laser radiation will be used, reaching a temperature at approximately 870 ° C.

This marking process using the radiation density of the CO_2 laser is made up of four main regions which can be identified: a) the pure metal region. B) The region where the constituent metals are dominant compared to the vitreous ceramic components. C) The region where the vitreous ceramic constituents are dominant compared to those of metal, d) the compound for the ceramic-vitreous material. Each region of the composite structure has a specific adjective in the process: the ferrous metal base functions primarily as a structure for the support of the ceramic-vitreous matrix.

Due to the different vitreous-ceramic compounds and the thermal properties of the metal substrate, residual stresses are generated affecting the adhesion of both. As a result a vitreous-ceramic will be developed capable of generating the smallest residual stresses to ensure the development of a line layers to identify as a brand.

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SYNTHESIS, CHARACTERIZATION AND CATALYTIC BENEFITS OF MULTINUCLEAR 1,2,3-TRIAZOL-5-YLIDENE COMPLEXES

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In the last decade, N-heterocyclic carbenes (NHCs) were the carbene center is not flanked by heteroatoms in both sides of their structures, have attracted great attention as they show stronger σ-donation towards the metal center compared to classical analogues.[1] These ligands, often referred as abnormal carbenes (aNHCs) or more recently entitled mesoionic carbenes (MICs), owe this description due to the fact that their structures can only be represented as zwitter ions and not in the neutral canonical form.[2] In particular, a subclass of MICs namely 1,2,3-triazol-5-ylidenes, have emerged as a useful alternative for the coordination of transition metals and main group elements, due to their easy synthetic design via click chemistry.[3]

Despite the easy access to ligand platforms with various levels of modification, most of the chemistry of 1,2,3-triazol-5-ylidenes is dominated by monometallic complexes. Only recently, few ligand platforms allowing the generation of di-[4] and tri-nuclear[5] metal complexes based in MICs have been reported in the literature.

The current development of multinuclear catalysts have attracted the interest of both academia and industry as it has shown its superiority in terms of selectivity and reactivity compared to mononuclear partners. On the basis of these previous findings and targeting the introduction of new frameworks able to coordinate several metal centers, we will present the preparation of a series of multicationic-triazolium salts and their one-pot metallation to generate multinuclear triazol-5-ylidene metal complexes. The catalytic application of these multinuclear complexes in C-C and C-N bond forming processes will be discussed.

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A C1-conversion puzzle with a bio-inspired organometallic approach

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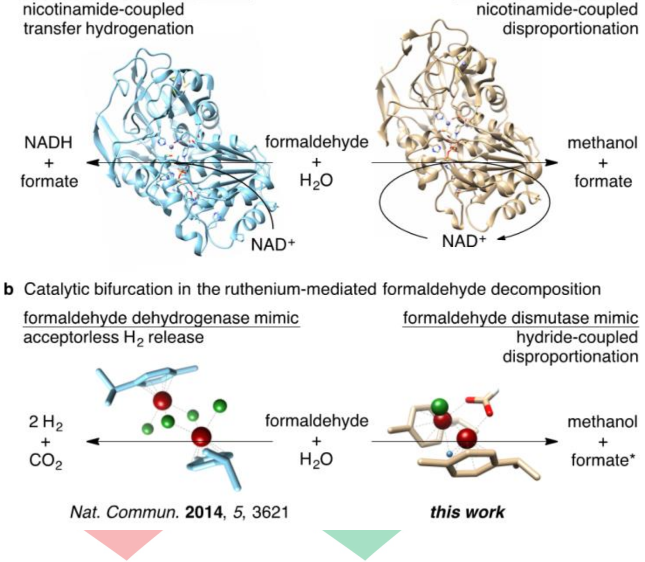

Our current studies include coupled conversion of *in situ* generated H_2 and CO_2 towards an extended (de)hydrogenation cycle of the C_1-interconversion between MeOH, FAH, formic acid, CO_2 in water.[1-2] Inspired by nature, where many organisms use C_1-molecules as hydride sources for the energy conversion, we develop organometallic biomimetic catalysts exhibiting oxidoreductase-like reactivity applicable under ambient conditions for not well, respectively not yet, investigated C_1-interconversions (Scheme).[3] Our studies are of fundamental nature for tailoring artificial methylotrophic pathways and open new windows of opportunities towards an extended cycle of the not yet fully resolved C_1-conversion network which requires to add important missing pieces to this C_1- puzzle.[4] Additionally to the bio-inspired approaches using organometallic dismutase and dehydrogenase mimics.[3] We are further developing our tool-box also with nanoscale hybride catalysts which are active for hydrogenation reactions in general,[5-6] and therefore interesting for CO and CO_2 hydrogenation as well.[7]

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REACTIVE AND REDOX-ACTIVE LIGANDS - NEW AVENUES FOR ORGANOMETALLIC CHEMISTRY, SELECTIVE BOND ACTIVATION AND HOMOGENEOUS CATALYSIS

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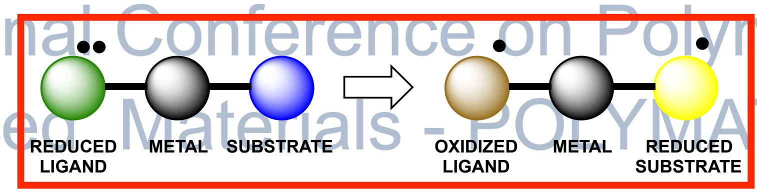
Redox-active ligands can induce noble metal reactivity upon base metals by acting as an electron reservoir [1]. However, establishing 'base metal-like' odd-electron reactivity with closed-shell noble metals using redox-active ligands is very rare. We introduced novel redox-active tridentate ligand designs that form paramagnetic palladium complexes (S = ½) that undergo reversible ligand-based redox-chemistry. Interestingly, the unpaired electron can be transferred to a bound organic substrate, effectively generating a single-electron reduced substrate in the coordination sphere of Pd^{II}. This activated intermediate can subsequently react in an intramolecular fashion following an odd-electron pathway. This exciting feature has been exploited to convert alkyl azides into pyrrolidines for the first time using Pd^{II} [2]. Following the same protocol, homolytic bond scission of disulfides gives rise to unique ligand mixed-valent dinuclear species [3]. The magnetic properties of related mono-ligated bridged complexes have also been investigated [4][5]. This presentation will discuss the concepts and potential of this chemistry, including results on base metal catalyzed C-H amination and Ru-mediated azide activation will also be presented, as well as ongoing work on redox-active supramolecular cages.



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Photosensitized Cobalt Nanocrystals

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Organometallic chemistry plays an increasing role in the synthesis of nanoparticles, as it provides a reliable access to metal and metal oxide nanoparticles with efficient control over their morphology, organization and surface chemistry.[1] In case of magnetic nanoparticles, the synthetic tools provided by organometallic chemistry allow access to nanomaterials of very small size and controlled magnetization. These objects are thus good candidates to study interface phenomena such as electron transfer. We will show that it is possible to photomodulated the magnetization of Co nanocrystals by grafting an organic dye at their surface[2] and that efficient catalysts for water oxidation can be synthesized.[3]

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“Crown ether Na/K PCP complexes for the ROP of *rac*-lactide”

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Na/K complexes are of the most promising catalytic systems for the obtention of polymers, specially for those with medical applications, due the low toxicity and costs of the alkaline elements. Recently, crown ether-Na/K complexes with monophenoxides, naphtalenolates and sulphonamides have been evaluated as initiators for the ROP of *rac*-lactide. Polymers with IPD values ~ 1.16 and P_m~ 0.8 have been obtained by using these complexes in addition to a co-catalyst [1]. In this research work, two new crown ether K (**1**) and Na (**2**) iminophosphoranyl complexes were used as catalysts in the polimerization of *rac*-lactide (Figure 1). Both complexes were characterized by m.p., ^{1}H, ^{31}P-NMR and IR spectroscopy, mass spectrometry and X-ray cristallography.

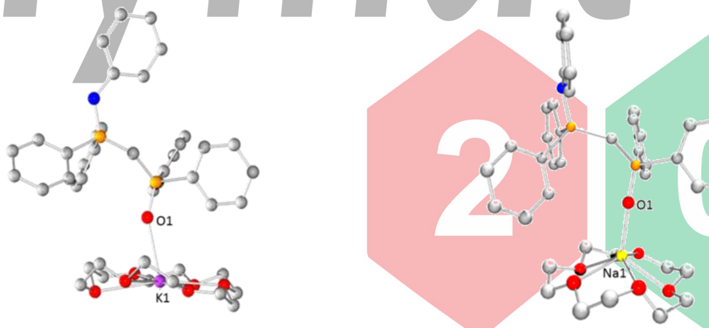

Figure 1. Asymmetric unit of **1**(left) and **2**(right). Color code: Grey (C), Orange (P), Blue (N), Red (O), Purple (K), Yellow (Na). H atoms were ommited by clarity.

Polymerization experiments were conducted in the standard conditions at room temperature, using BnOH as co-catalyst and toluene as a solvent [2]. For both complexes, polymer conversions are >99% in 3 minutes and the obtained polymers have P_m values ~ 0.7.

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Acknowledgements

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SYNTHESIS AND REACTIVITY OF SILYL RHODIUM AND IRIDIUM COMPLEXES WITH BENZYLSILYL PHOSPHINE LIGANDS

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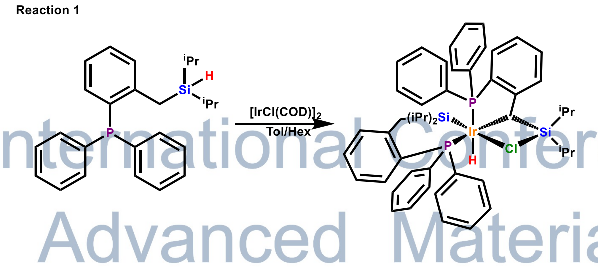
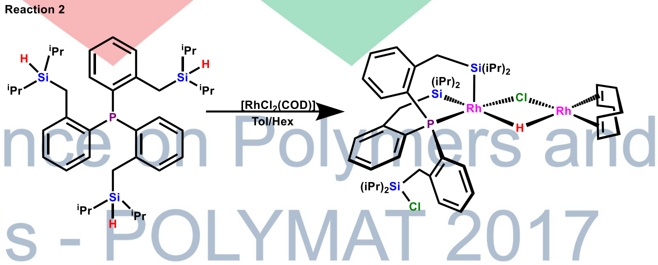
Transition metal complexes bearing Si-H bonds have attracted the attention of diverse many research groups for a variety of reasons including their use as a catalyst in reactions of industrial interest [1]. The design of new catalysts for important transformations such as hydrosilation and dehydrogenative silylation compels deep knowledge of the fundamental reaction steps often invoked including Si-H bond activation and M-Si and Si-C bond formation [2,3].

This contribution will present the results related to the coordination to Rh or Ir of new multidentate ligands that incorporate phosphorus and one, two, or three atoms of silicon in their structure.

Amongst other examples which will be presented, we show that in Reaction 1, the formation of a monomeric compound generated from $[IrClCOD]_2$ and a bidentate silylphosphine involves an intramolecular C-H activation of a benzylic fragment. On the other hand, in Reaction 2, the reaction of $[RhClCOD]_2$ and a potentially tetradentate silylphosphine, generates a dimeric compound of mixed valence (I and III). The silyl ligands show strong σ-donating character and display a stronger *trans* influence than many other common ligands in TM chemistry [4]. The influence of the substituents on the Si and P atoms will also be discussed. All new compounds have been extensively characterized by spectroscopic means and in some cases by single crystal X-ray diffraction analyses.





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Synthesis and characterization of the first organotin complexes with seven-member cyclic dithiocarbamate ligands.

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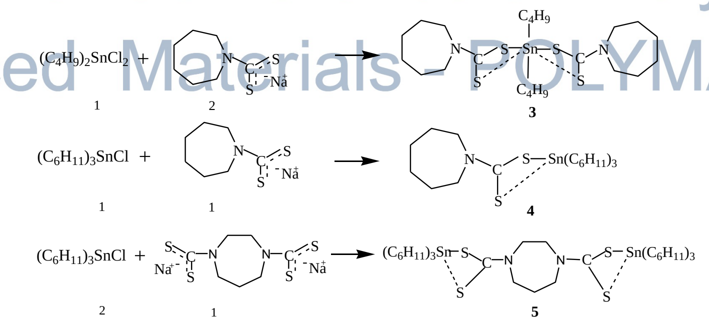
In this work, us report the synthesis and spectroscopic characterization of the first organotin(IV) complexes with cyclic seven-member dithiocarbamate ligands: azepane-1-carbodithioate-, and homopiperazine-1,4-bis-carbodithioate, with two different organotin entities di-*n*-butyltin and tricyclohexyltin, $[(C_4H_9)_2Sn\{S_2CN(CH_2)_6\}_2]$, **3**, $[(C_6H_{11})_3Sn\{S_2CN(CH_2)_6\}]$, **4** and $[\{(C_6H_{11})_3Sn\}_2$ (μ-$S_2CN(C_5H_{10})NCS_2)]$, **5**. The obtained compounds have been characterized by elemental analyses, IR, FAB$^+$MS, and multinuclear NMR (^{1}H, ^{13}C, and ^{119}Sn) spectroscopy. Their molecular structures were established by single-crystal X-ray diffraction studies. The geometrical arrangement around the tin atom can be described as distorted octahedral for **3** and trigonal bipyramid for **4** and **5**, these highly distorted of the regular geometry. The coordination mode for both ligands is considered as anisobidentate. The complex **3** presents intermolecular interactions between the tin and a sulfur atom in the reciprocally neighboring molecule, giving rise to a zig zag polymer.



Scheme 1. Preparation of tin dithiocarbamates **3–5**.

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The spectroscopic analyzes (EI-MS and multinuclear NMR ^{1}H, ^{13}C and ^{119}Sn) were performed at the Centro de Investigaciones Químicas, UAEM and single-crystal X ray diffraction at the Instituto de Química de la UNAM. The authors are grateful to the staff for this service.

Lanthanides coordination compounds with luminescent properties in the Visible-NIR

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Abstract

The lanthanides(III) ions show intraconfigurational *4f-4f* electronic transitions, when they are irradiated with UV-Vis radiation to give rise to ligth emission. To achieve an efficient emission of the lanthanides, chromophores were used as luminescence sensitizers. The latter must be able to absorb light and transfer this energy to the lanthanide ion. These compounds obtained between sensitizers and lanthanides are of great interest due to their luminescent properties since they can be used for luminescent materials, such as OLED´s.

In this work the optimal conditions for the syntheses of the coordination compounds with the ions: La^{3+} to Lu^{3+} (except Pm^{3+}) using the ligand 2,6-bis(benzoimidazol-2-yl)pyridine are discussed. The coordination compounds and the ligand were characterized in solid state and in ethanolic solution using analytical and spectroscopic techniques.

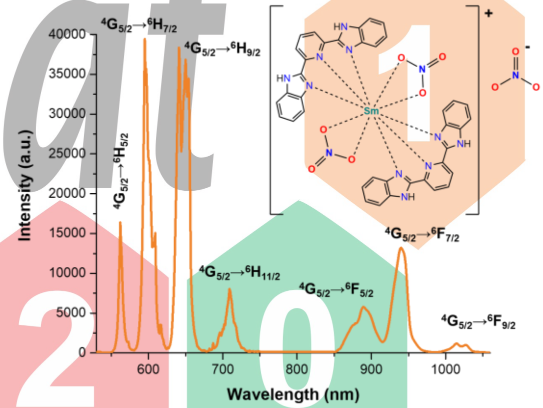

Figure 1. Solid state emission spectrum of the Sm compound, λexc= 370 nm T=298 K.

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Iridium-NHC complexes derived from theophylline with fluorinated substituents

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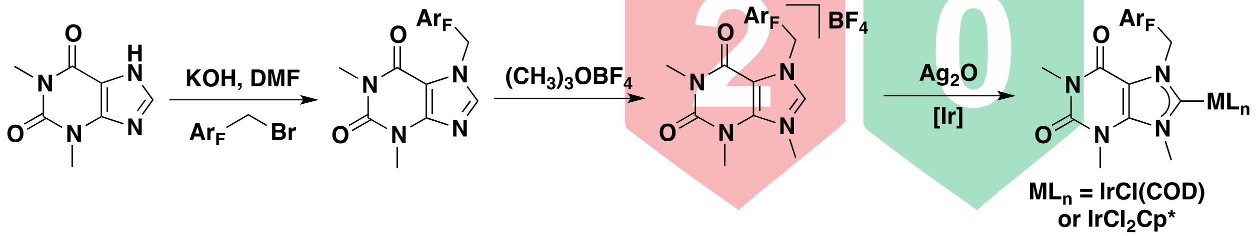
Caffeine, theophylline and theobromine are commonly known as Xanthines. They are natural compounds that can be obtained from cacao, coffee and tea. Furthermore, their pharmaceutical properties have been widely studied and established. The combination of natural products with biological active transition metals has provided suitable compounds for their potential use as antitumor and antibacterial agents.[1-3] Recently, xanthine compounds have been employed as platforms for the design of N-heterocyclic carbene (NHC) ligands with potential pharmaceutical properties. Willans and Phillips have described a series of Ag complexes with xanthine NHC ligands and their evaluation as anticancer compounds.[1] The complexes were active against malignant melanoma, glioblastoma and pancreatic carcinoma.

Based on the aforementioned, we envisioned that by combining the biological activity of theophylline, fluorinated substituents and the antitumor potential of Ir complexes we could enhance the activity of their related drugs. As shown in **Scheme 1**, the complexes were synthetized in three steps. The first one allowed us the incorporation of fluorinated benzyl fragments in the backbone of the theophylline. The reaction of these precursors with trimethyloxonium tetrafluoroborate produced the corresponding azolium salts. Finally, the coordination to Ir was performed through a transmetallation reaction. The antitumor tests are currently under process in our laboratory.



Scheme 1

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Sodium and Potassium complexes with ketiminate ligands for the ROP of *rac*-LA

Garcia-de Jesús, Omar J.[1], López-Cruz, Nazario[1], Montiel-Palma, Virginia[1], Reyes-Ortega, Yasmi[2] and Muñoz-Hernández, Miguel A.[1]

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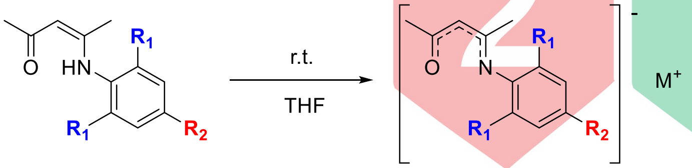
New sodium and potassium complexes were evaluated as catalysts in Ring Opening Polymerization (ROP) of *rac*-Lactide (*rac*-LA). The bidentate ligands ***O, N*** utilized include: 4-[(2,6-dimethylphenyl)amino]-3-Penten-2-one, 4-[(2,6-diisopropylphenyl)amino]-3-Penten-2-one, 4-[(4-tert-butylphenyl)amino]-3-Penten-2-one, The polymerization studies were performed under mild conditions. [1], The present complexes may be less toxic than tin octanoate (II), which is the most common catalyst utilized in the industrial production of PLA [2]. Our catalysts showed good performance, with 95% conversion to PLA in just 3 min at room temperature. The polymers were analyzed by GPC and ^{1}H NMR, and presented some isotactic selectivity in the 60% to 70% range and weighted up to 9.1×10^3 Da.

Complementary, the synthesis of new Na and K complexes which incorporate crown-ethers is under investigation [3].



L$_1$) R$_1$=Me R$_2$=H
L$_2$) R$_1$=^{i}Pr R$_2$=H
L$_3$) R$_1$=H R$_2$=^{t}Bu

1) M=Na R$_1$=Me R$_2$=H
2) M=Na R$_1$=^{i}Pr R$_2$=H
3) M=Na R$_1$=H R$_2$=^{t}Bu

4) M=K R$_1$=Me R$_2$=H
5) M=K R$_1$=^{i}Pr R$_2$=H
6) M=K R$_1$=H R$_2$=^{t}Bu

Figure 1. Synthesis of sodium and potassium complexes

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Synthesis and characterization of Ni^{2+}, Cu^{2+}, and Zn^{2+} complex supported by tridentate Schiff base ligands for the electrocatalytic reduction of carbon dioxide

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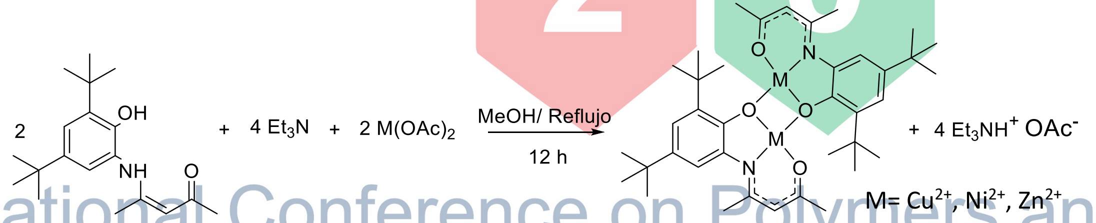
One of the main issues right now is global warming, which is caused mainly by the increase of greenhouse gases such as CO_2, so it is now very important to reduce the concentration of this molecule in the environment.[1] Small molecules complexes can act as photocatalysts or electrocatalysts in the activation of CO_2. In recent years, CO_2 conversion using molecular electrochemical catalysts has attracted great attention due to the folowing: (1) the electrocatalysts activity can be tuned by ligand modification; (2) the electricity used to drive the process can be obtained from renewable sources, thus avoiding the generation of additional CO_2; and (4) the electrochemical reaction systems are compact, modular,on-demand, and easy for scale-up applications. [2]

In this work , we will discuss the synthesis of three dimeric Ni^{2+}, Cu^{2+}, and Zn^{2+} complexes supported by tridentate Schiff base ligands (ONO),(Scheme 1) these complex were caracterized by IR, UV-VIS spectroscopy, Mass espectrometry, termogravimetric analysis, and the case of Zn^{2+} by 1H NMR spectroscopy. The potential to reduce CO2 is very negative (-1.9 vs NHE)[3], it is expected that these complexes will be able to capture CO_2 and reduce it at a more positive potential and would be able to obtain value-added products such as formate, oxalate or metanol by adding a proton source.[4]



Scheme 1. Synthesis of dimeric Ni^{2+}, Cu^{2+}, and Zn^{2+} complexes

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Expanding Ta Bis(Imido) Chemistry: Synthesis of Lithium Free Unsymmetrical CCC-NHC Bis Imido Complexes and Their Reactivity with Hydrazine Derivatives

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The previously reported methodology to synthesize CCC-NHC Ta bis(imido) complexes has been extended to unsymmetrical pincer complexes. Specifically, synthetic results from the preparation of a benzimidazole/imidazole CCC-NHC Ta(V) pincer complex will be reported. The coordination sphere was further manipulated to synthesize a benzimidazole/imidazole CCC-NHC Ta (V) bis(imido). Unexpectedly, the incorporation of the single benzimidazole NHC in to the pincer architecture resulted in a product that did not contain a bridging lithium atom unlike the symmetrical imidazole/imidazole CCC-NHC Ta bis(imido) analogue. The reactions of the CCC-NHC Ta bis(imido) complexes with hydrazine derivatives, towards the study of a tantalum analogue of the Schrock cycle, will be included. The latest computational results supporting all new CCC-NHC Ta complexes will also be reported.

Acknowledgements

We greatfully acknowledge We gratefully acknowledge partial support from the Mississippi State University Office of Research and Economic Development and the National Science Foundation (CHE-0809732, -0955723; OIA-1539035).

NHC Pincer Complex Donor Ability? PtEP (Platinum (Pt) Electronic Parameter): A Donicity Scale Incorporating Strictly Meridional, Tridentate Ligands.

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Parameters and scales that provide understanding of steric and electronic effects are essential to predicting properties, and, therefore, to systematically designing new ligands. One ligand class, namely, tridentate, rigidly-meridional pincer ligands, are neither conveniently nor accurately described by existing options. A scale has been developed based on the ^{195}Pt NMR chemical shift that is reflective of the total donor ability of a multi-dentate ligand in a square planar complex and that does not suffer from cis/trans stereochemical issues. An inexpensive, readily-accessible computational model for predicting the chemical shifts correlates well with the experimental data and provides a basis for predictions. This scale, Platinum Electronic Parameter (PtEP, pronounced P-tep), revealed significant deviations of CCC-NHC ligand donor abilities from predicted extrapolations using existing TEP parameters. This initial data set demonstrates the applicability and broad potential of the PtEP scale.

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Ruthenium complexes with NHC-fluorinated ligands for alcohol oxidation and antitumor properties

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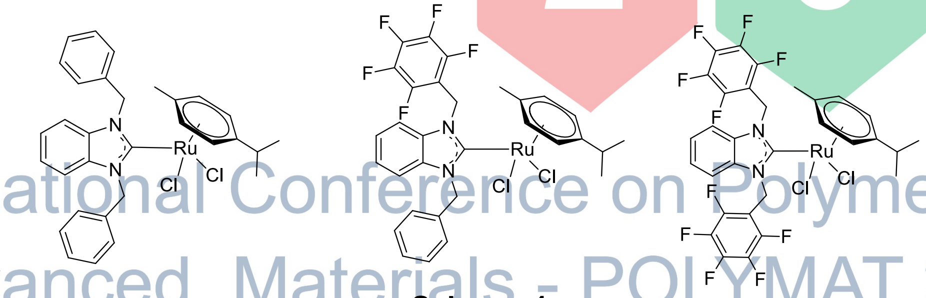
The conversion of alcohols to ketones, aldehydes or carboxylic acids represents a very important organic transformation that nowadays can be performed under catalytic conditions. In this sense, the promoterless acceptorless alcohol dehydrogenation (PAAD) with the release of H_2 constitutes the most valuable procedure from the point of view of atom economy and hydrogen storage. In recent years, several experimental and theoretical studies have been published. Some of the most known catalysts were described by the groups of Milstein, Szymczak, Fujita and Yamaguchi and are based principally on ruthenium and iridium.[1,2]

Furthermore, ruthenium complexes have showed very good cytotoxic activity against cancer cells. Today there are two ruthenium species in clinical trials and there is a great effort in the study of the mechanism and interaction of these species with DNA. Thus, Ru has emerged as a good alternative to Pt since Ru is cheaper and exhibits slow ligand exchange rate.

Motivated by the wide range of applicability of Ru complexes, we prepared a series of Ru complexes with NHC-fluorinated (**Scheme 1**). We envisioned that the incorporation of fluorinated groups into the NHC ligands could enhance their catalytic activity as well as their antitumor activity, since aromatic group favored π-π interactions.[3,4]

In general the complexes have showed very high antitumor activity against (glia of CNS, prostate, leukemia and colon). In a preliminary catalytic evaluation, the complex that contains the fluorinated substituents showed the best catalytic activity in the oxidation of benzylalcohol. Further catalytic studies are currently under development in our laboratory.



Scheme 1

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Hidrocarburos 2015-2016 for a postdoctoral scholarship (Oficio: COIC/ CSGC/1244/16) and Programa de Becas Posdoctorales-DGAPA-UNAM for a postdoctoral scholarship (Oficio: CJIC/ CTIC/1060/2017).

CYCLOMETALATED COMPLEXES FOR ANTICANCER STUDIES

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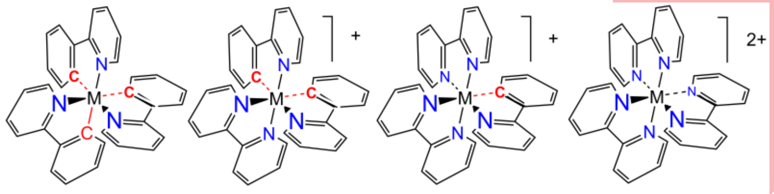
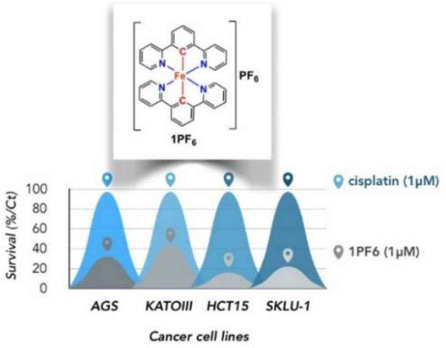
Series of structurally similar cyclometalated ruthenium and osmium complexes of the general formula $[M(C\sim N)_x(N\sim N)_{3-x}]^{m+}$ have been prepared and have displayed a very high *in vitro* and *in vivo* anticancer activity [1]. The redox potentials, charges, lipophilicities, as well as their antitumour activity, change drastically as nitrogen atoms are successively replaced by σ-bound sp^2 carbon atoms. On the other hand, series of bis-cyclometalated iron derivatives have also been synthesized and their biological activity evaluated [2]. As oxidoreductases have been closely associated with the development of diferent cancers, the route of action could be linked to the interaction with such enzymes. In order to shed light on how the complexes can interact with redox proteins, the regulation by the complexes of the *in vitro* activity of oxidoreductases has been evaluated [3]. Studies have also been performed with different markers to characterize the cell death induced by the cyclometalated complexes and the results showed a markedly different pathway than for cisplatin and other metal-based drugs.



1b **2a,b** **3a,b** **4a,b**

M = Ru (a), Os (b)



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A new green method for the synthesis of *L*-proline dithiocarbamates of organotin(IV)

Elia Marcela López-Cardoso[1], **María Elena Rosas Valdéz**[1], **Gabriela Vargas-Pineda**[1], **Perla Román-Bravo**[1], **Raymundo Cea-Olivares**[2].

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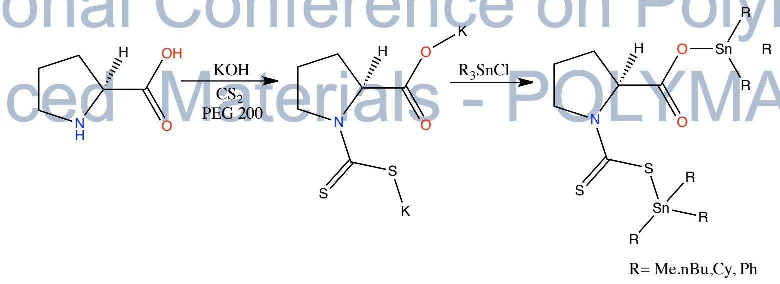
Green chemistry consists of the reduction and/or elimination of the use of pernicious material from a chemical process. This includes, solvents, reagents, feedstock, products, and byproducts [1]. The replacement of organic solvents is one of the major challenges in the green chemistry and water, ionic liquids or supercritical fluids had been used as alternative solvents. PEGs has been used as an alternative reaction medium, has been called an eco-friendly solvent due to their capability to substitute organic, volatile or halogenated solvents [2,3].
The α-amino acids are utilized as building blocks for peptides and proteins synthesis by living cells, and are thus fundamental to all life forms [4], L-proline belongs to this essential group of amino acids.

Synthesis of complexes from amino acids are common in mostly of organic solvents, however here we present an alternative method for the synthesis of complexes proline dithiocarbamate with organotin entities, without organic solvents. The complexes $R_3Sn(L)$ L= *L*-ProlineDTC with R= *n*-Bu, Ph, Cy and Me, scheme **1**, were synthetized in PEG 200 as an eco-friendly solvent. The obtained complexes have been characterized by elemental analyses, IR, FAB$^+$-MS, and multinuclear NMR (^{1}H, ^{13}C, and ^{31}P) spectroscopy and it was possible to obtain three molecular structures by single-crystal X-ray diffraction analysis.



Scheme **1:** Synthesis of organotin complexes.

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“Ring opening polymerization of *rac*-lactide by tetranuclear Al, Ga, and Zn complexes supported on polynucleating ligands”

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Due to their enviromental impact, there is a need for replacing fossil-based materials with renewable and biodegradable polymers. Particularly, Al(salen) complexes have shown to be very effective catalysts for the polymerization of *rac*-lactide leading to highly isotactic biodegradable polymers in good yields [1]. This study describes the synthesis of multinuclear Al, Ga, and Zn complexes using the dendrimeric salen-type ligand named **D4-H_4**. Metallation of **D4-H_4** with $AlMe_3$, $GaMe_3$, and $ZnEt_2$ lead to coordination complexes **1**-**3**, respectively (Figure 1). Complexes **1** and **2** have a composition of **$(MMe_2)_4$D4**, with tetracoordinated metal centers. Complex **3** has composition of **$(ZnMe(CH_3CN)_{0.5})_4$D4**, with the metal centers in a tetrahedral coordination enviroment, as evidenced by Single Crystal X-ray Diffraction studies. All complexes have been characterized by ^1H,^{13}C-NMR, IR, mass spectrometry, and elemental analysis.

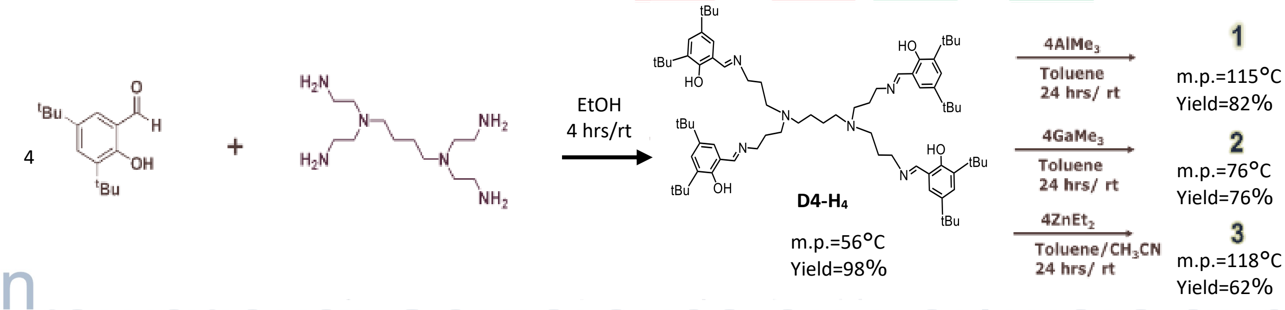

Figure 1. Synthesis of **D4-H_4** and **1**-**3**.

Polymerization of *rac*-lactide was performed using conventional conditions with toluene as solvent, at 70 °C with BnOH as co-catalyst [2]. Polymer conversions were >95% after three days when **1** or **2** were used as catalyst, while **3** turned out to be inactive. The polymer obtained with **1** has IPD = 1.16, P_m = 0.62 and M_n = 3698, which agrees well with the calculated Mn_C = 3600.

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RUTHENIUM NITROSYL COMPLEXES: CANDIDATES FOR PHOTOISOMERISATION OR NITRIC OXIDE DELIVERY

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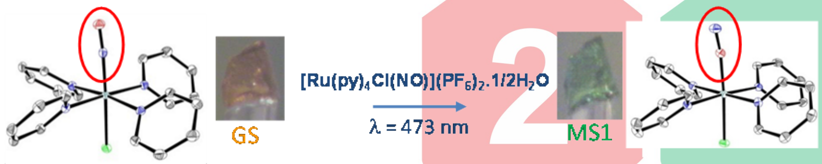
Photoactive nitrosyl ruthenium complexes deriving from $[Ru^{II}Cl(NO)(py)_4]^{2+}$ have recently witnessed an increasing interest in relation to their capability for providing solid state photo-switches with high yields or their ability to release the biologically active $NO^{\bullet}$ radical [1, 2].

Insight on our recent work in the two domains will be presented:

►**Ru-NO / Ru-ON photoisomerisation**

$$[Ru^{II} - NO] \overset{h\nu}{\rightarrow} [Ru^{II} - ON]$$

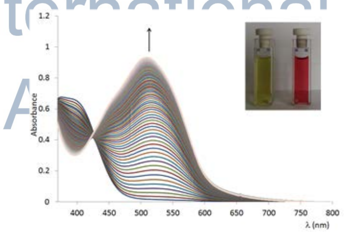


►**NO photorelease**

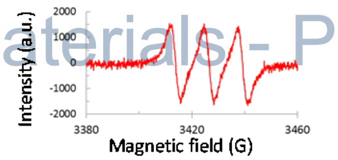
$$[Ru - NO] \overset{h\nu}{\rightarrow} [Ru - solvent] + \boldsymbol{NO^{\bullet}}$$

FT: Fluorene-terpyridine

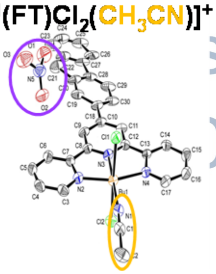
trans/*cis*-(Cl,Cl)- $\mathbf{[Ru^{II}(FT)Cl_2(NO)]^+ + CH_3CN}$ → *trans*-(Cl,Cl)- $\mathbf{[Ru^{III}(FT)Cl_2(CH_3CN)]^+ + NO^{\bullet}}$



Griess test at 405 nm



NO signature by EPR at 810 nm



Photoproduct

References

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The versatility of silylphosphines in transition metal complexation

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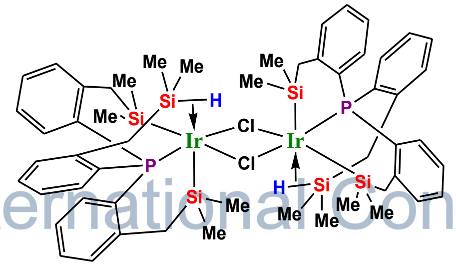
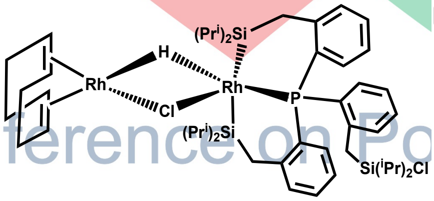
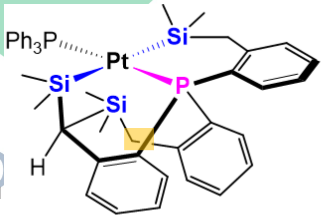
Even the most superficial glance at the inorganic chemistry literature evidences an outburst in the number of studies related to silicon-substituted mixed functionalities as ligands for transition metals **[1]**. This upsurge in silicon chemistry, particularly in the silylphosphine domain, has led to a number of important discoveries in fundamental reaction steps but also to advances on their employment as catalysts and use in material science **[2]**.

Several workers have proved that incorporation of a Si–H function into a semi-rigid polydentate phosphine template leads to very pronounced stereoelectronic control over substrate entry, binding and release on a coordinatively unsaturated transition-metal centre **[3]**.

Herein, the coordination chemistry of a family of new silylphosphine ligands including one phosphorous and either a varying number of Si atoms (1, 2 or 3) or a Si-Si motif in their structure towards late transition metal precursors with emphasis on Ru, Rh, Ir and Pt will be discussed. We observe compounds in which the ligands coordinate in an “intact” fashion but also intramolecular C-H activations preceded by non-classical sigma coordination or even systematic variations on anagostic interactions on the modified ligands.







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“Synthesis, characterization and polymerization activity of K, Na and Cs complexes supported by PCC”

[2]Muñiz-Garcia, Arbeli; Anzaldo-Hernández, [1]Samuel; Lopez, [2]Nazario; Ordonez-Palacios, [2]Mario and [2]Muñoz-Hernández, Miguel A.*

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Synthetic materials derived from oil-based polymers are currently very popular for packing a wide variety of products, but represent serious represent a serious environmental problem because of their slow degradation.

The synthesis of alternative biodegradable polymers for human use involves molecular catalysts which incorporate innocuous metal centers in the catalyst, usually based on Al, Zn, Na K, Ln, In, Mg. [1]

In order to create catalysts with non-toxic and harmless metals, numerous initiators including aluminum, zinc, sodium, potassium, lanthanides, indium and magnesium complexes, have been synthesized and exhibit good selectivities.

Specifically, sodium (Na) and potassium (K) ions are biocompatible, cheap, harmless, and abundant in the earth crust, thus complexes involving such ions are the preferred catalysts for polymerization of lactide for medical applications. [2]

In this work, we explore the use of M-PCC complexes (PCC = chalcogencarbamoylchalcogenphosphine, M=Na, K and Cs) as catalysts for polymerization of rc-lactide and ε-caprolactone. We expect to have stereoregulars polymers with a well-controlled molecular weight and low polydispersity values for medical applications

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Isomeric and hybrid ferrocenyl/cyrhetrenyl aldimines. A new Family of multifunctional compounds.

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Heterobimetallic compounds have attracted great interest in recent years.[1-2] The presence of two proximal metals with different environments, oxidation numbers and spin states can influence their mutual cooperation, their reactivity, electrochemical behaviour, photo-optical properties and also their catalytic or biological activities.[3-4]

In this work, we report the synthesis, characterization and biological evaluation of a pair of new aldimines R^1-CH=N-R^2, with R^1= ferrocenyl and R^2= cyrhetrenyl (**1**) or viceversa (**2**) as the first examples of small molecules containing both organometallic fragments connected by the imine functionality. **(fig. 1)**

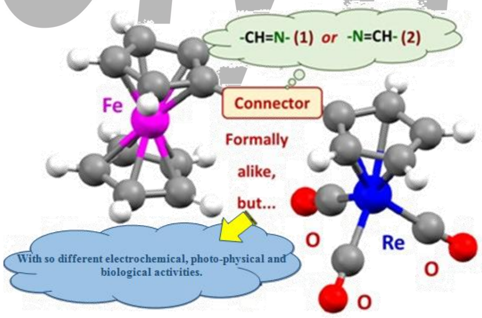

Fig 1. Chemical formulae of the novel hybrid ferrocenyl/cyrhetrenyl-aldimines prepared.

Experimental work and computational studies on both compounds provide conclusive and relevant evidence of the effect produced by the interchange of the two organometallic arrays on their structures, stabilities, electrochemical and photo-physical properties, the electronic delocalization and, also on their effect on: a) two breast cancer cell lines [MCF7 and the triple negative MDA-MB231, b) the colon and the cisplatin resistant HCT116 cell line, and c) the non-tumoral human skin fibroblast BJ cell line.

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SYNTHESIS AND CHARACTERIZATION OF DISILYLBENZYLPHOSPHINE METAL COMPLEXES.

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Disilanes, alongside with hydrosilanes, represent excellent starting materials for the synthesis of organosilicon compounds mediated by metal complexes **[1,2]**. However, little attention had received the research of the reactivity of non-polar disilanes toward transition metals except for Group 10 (Ni, Pd, Pt). Disilanes are notably reactive when the Si-Si bond is incorporated in a strained ring or have electro-withdrawing groups such as halogens attached to the silicon atoms. However, because of the low-energy σ-antibonding molecular orbital of the Si-Si bond, oxidative addition is achieved toward electron-rich metal centers such as Pd(0), Ir(I) or Au(I) precursors **[3,4,5]**. Herein, the reactivity of new di-phosphine ligands which incorporate the Si-Si motif in their structure toward Ir(I) and Rh(I) precursors, is presented. Disilylbencylphosphines compounds **L1** and **L2** were synthesized according to the procedure reported by our research group for similar ligands **[6]**. The variation of the R group around the phosphorus atom (R = Ph, Cy) provides different basicity to the ligands. When equimolar quantities of ligand and metal precursors are placed in solution, the formation of unexpectedly bridged metal complexes for both Ir and Rh are obtained in high selectivity according to the NMR and X-Ray diffraction studies **(Figure 1)**. In these reactions, the coordination of both ligands is exclusively through the phosphorus atom, with the Si-Si motif intact.

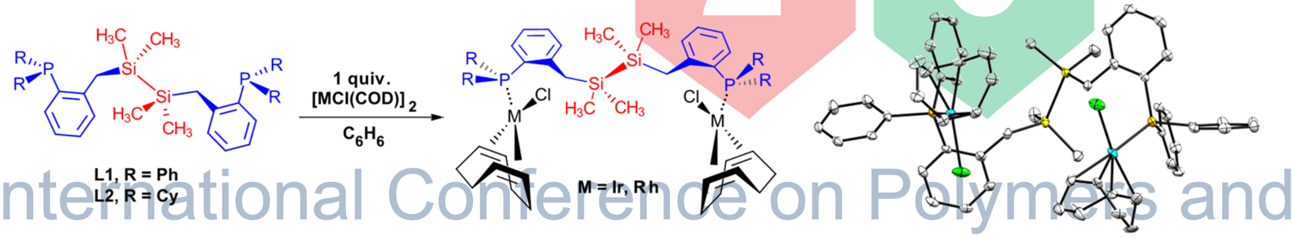

Figure 1 – Synthesis of bridged iridium/rhodium disilylbencylphosphine complexes.

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Palladium(II) complexes with fluorinated thiophenol and phosphinite ligands

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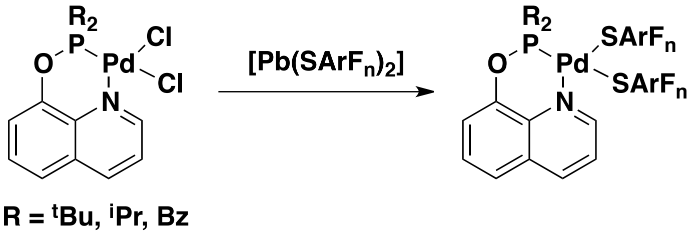
Organometallic complexes have been widely used in the area of catalysis. Their great development has allowed their application in several industrial reactions, favoring greener processes. Among them, C-C cross-coupling reactions have emerged as very useful tools for organic synthesis, being most of them catalyzed by Pd complexes. The design of the ligands is very important since it may provide a suitable environment around the metal. Recently ligands have incorporated other functionalities, for example, they have been functionalized with redox or photoresponse groups.

Considering the growing interest in organopalladium compounds for the past two decades, we decided to prepared a series of palladium complexes with fluorinated thiophenols and hidroxiquinoline ligands (**Scheme 1**). The presence of two fragments capable of forming π-π interaction may promote the better interaction between catalyst and substrate.[1,2]



Scheme 1

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POLY(PYRAZOLYL)ALUMINATES AS METALOLIGANDS

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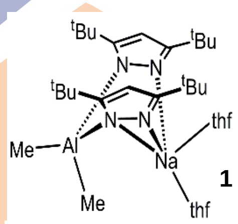
There are few ligands in organometallic chemistry that have proved to be as versatile and useful to stabilize metal centers as the poly(pyrazolyl)borates introduced by Trofimenko [1]. The research of analogs of this ligand system, the polypirazolylaluminates, has been increasing in the last two decades [2,3]. The use of poly(pyrazolyl)aluminates as metaloligands is very attractive for the preparation of new heterobimetallic complexes of transition metals due to the different steric and electronic effects that can be achieved by varying the nature, number and position of the substituents on the pyrazole ring, with the final purpose of modifying the reactivity in the metal center. To our interests they play an important rol in growing areas such as materials science and bioinorganic chemistry [4].



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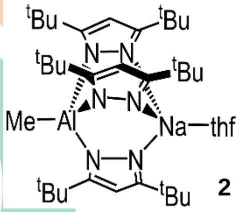

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In this work we are reporting a poly(pyrazolyl)aluminate ligand system achieved by using alkyl groups on the aluminum center and an electron rich organotransition metal center which had given stable and reactive complexes. Herein, we are proposing a novel, easy and efficient synthesis route of the poly(pyrazolyl)aluminate complexes of Zn(II), Rh(I) and Ag(I). We report the preparation and characterization of the new bis and tris(pyrazolyl)aluminates of sodium, $[\{Na(THF)_2\}\{Al({}^tBu_2pz)_2Me_2\}]$ (**1**) and $[\{Na(THF)\}\{Al({}^tBu_2pz)_3Me\}]$ (**2**) and the transference of the aluminate **2** to an electron rich metal center (M= Ag(I), Rh(I) and Zn(I)) by simple metathesis. The successful synthesis of the bimetallic complexes opens the possibility to start a chemical family with potential use in homogenous catalysis to explore possible cooperative effects that may improve the performance of the so far well-studied monometallic complexes.

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Abstract preparation

Synthesis, Structural Analysis and Biological Testing of Metal Complexes Containing As (III) and Sb (III) Metaloheterocycles and a Dithiophosphonate Ligand.

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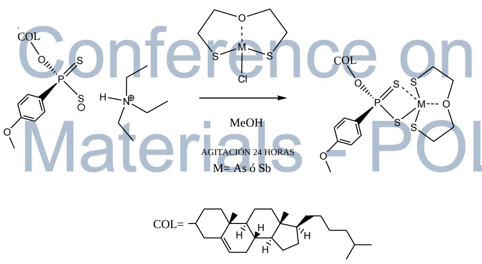
Dithio-organophosphorus compounds are interesting because of their extensive use in basic research as well as in industrial areas[1-3].Cholesterol is a stiff little steroid with a 5-ring skeleton used in the sex hormones of mammals.It is a structural component of all cell membranes modulating its fluidity and especially its tissue, is a precursor of bile acid, steroidal hormones and vitamin D [4]. In this work, a dithiophosphonate ligand was synthesized using cholesterol as a raw material and six new compounds were synthesized with metaloheterocycles of As(III) y Sb(III). The new complexes were characterized by elemental analyses, IR, FAB$^+$-MS, and multinuclear NMR (^{1}H, ^{13}C, and ^{31}P) spectroscopy and it was possible to obtain two molecular structures by single-crystal X-ray diffraction analysis.



Scheme **1:** Synthesis of complexes with metaloheterocyclesAs(III) and Sb(III).

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Ni-POCOP pincer complexes supported in polymers

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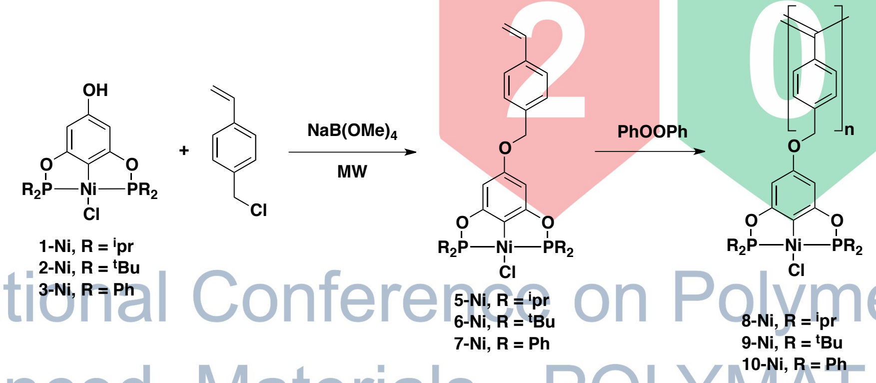
Pincer complexes have emerged as useful tools in several areas. Their very well known robustness has allowed their use in the area of catalysis and material science. In particular, pincer complexes have been used for cross-coupling, (de)hydrogenation, among other catalytic reactions. Recently, our group has reported very attractive catalysts based on CNS, SCS NCN, POCOP pincer ligands. We have centered our efforts in designing functionalized pincer complexes that offer the possibility of a posterior anchor or functionalization. Following our interests we described an easy method for the synthesis of *para*-hydroxy functionalized POCOP complexes.[1] Furthermore, these compounds have been used as bifunctional molecular sensors for inorganic anions and acetate.[2]
Based on the aforementioned, we decided to prepare a series of polymers derived from Ni-POCOP pincer complexes. As **Scheme 1** shows the synthesis of the materials performed in two steps from the POCOP complex. The first one consists in the functionalization of the corresponding *para*-hydroxy POCOP complex with a vinylbenzene fragment. This reaction was promoted by microwave irradiation. Finally, the polymer was prepared by reacting the olefin derivative with benzoyl peroxide. The catalytic evaluation of the polymers is currently developed in our laboratory.



Scheme 1

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EFFECT OF COPPER ADDITIONS ON THE PRECIPITATION OF INTERMETALLIC IN Fe-Ni-Al-ALLOYS

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The effect of copper additions in Fe-Ni-Al alloys on precipitation of the intermetallic β (NiAl) phase in a ferritic matrix was analyzed in two alloys with different copper contents. Samples were treated at 1100 ° C for 24 and subsequently aged at 900°C for 5, 25, 50 and 100h. Scanning electron microscopy (SEM) and Vickers Hardness were conducted to analyze the precipitates. During the initial 25 h the precipitates in the both alloys grow, but the microstructural evolution were different on them and to the 100 h the precipitates of the Cu-low alloy have plate shape while the Cu-high alloy exhibit noodles shape. This microstructural change is reflected in the hardness values with an increase from 460 and 489 HV at 5h to 482 and 505 at 100h to low and high Cu content respectively. The results shown that the precipitation hardening response is better in the 5% at. Cu containing alloy and these were discussed in terms of the copper solubility into the precipitates and the matrix.

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Portfolio of technology transfer at Cinvestav: an approach to the business case of a system of nanoparticles applied for gene delivering

América Padilla-Viveros, Daniel Martínez-Fong and Armando de Jesús Espadas-Álvarez

In the current international economic context the Center of Research and Advanced Studies of the National Polytechnic Institute (Cinvestav), the leader center in research and postgraduate formation in Mexico, has been developing affordable methods for managing and fostering towards industrial sectors its portfolio of knowledge transfer as a result of scientific research and technological development.

In the field of materials (nanoparticles) for gene therapy, Cinvestav has the intellectual property rights of a system of nanoparticles for gene delivering with application in Parkinson Disease (PD).

This paper presents the strategy that have been developed to achieve the entrance of this system of nanoparticles to the market (business case), through the analysis of the competitive environment, based on the study of technological intelligence using scientific and patent documents, feasibility and financial risk analysis to define the value of technology, the design of the strategy to identify potential licensees and the establishment of the bases of negotiation.

All these tools were developed through the Agency for Knowledge Transfer and Commercialization (Agency 3C), that is a Office of Transfer of Knowledge recertified in the framework of the national call to foment to the transference and commercialization of technology encouraged by the National Council of Science and Technology (Conacyt) and the Ministry of Economy in Mexico.

Synthesis and properties of new unsaturated polyurethanes

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Polyurethanes (PUs) are one of the most used polymers in the industry, as: elastomers, foams, adhesives, packaging, automobile components, etc. However, after their useful life, those not receive an a recicle treatment, even tought the degradation in natural conditions is very slow. In Mexico there are no official statistics, but it is estimated that 7% or more of the waste generated corresponds to plastics, among them Pus [1,2].

The commun sinthesys obtention of PUs is a polycondensation reaction between diisocyanate and saturated diols, those lead to a group of stable materials (thermoset), wich makes the natural deagradation a difficult process [2,3].

This work show two new routes to obtain unsaturated PUs, based on butenediol, natural rubber and diisociantate. The first route is the polycondensation reaction between a diisocyanate (TDI) and *cis*-2-butene-1,4-diol in a molar ratio 1:1.2, using dibutyltin dilaurate as catalyst, the reaction is carried out in inert atmosphere at 60 °C for 24 h.

The second route is based in the cross-methatesis of natural rubber (NR) and *cis*-2-butene-1,4-diol (BD) at several molar ratios ([NR]:[BD] =1:1, 2:1, 50:1, etc) then, the route 1 is carried out. The synthesis of unsaturated PUs was verified by the techniques of NMR and FT-IR spectroscopy, MALDI-TOF and GPC, as well as their thermal and mechanical properties.

The employed unsatured diols could facilitate the degradation by natural or chemical methods due to the energy and reactivity of the double bonds present in the PUs. In addition, this type of PUs could be used in metathesis reactions with elastomers [4] to obtain PUs with new properties.

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MOLECULARLY IMPRINTED POLYMERS NANOPARTICLES AS “PLASTIC ANTIBODIES”

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Currently, the nanoscience has been developing new materials able to compete with the specificity of antibodies. These are molecularly imprinted polymers nanoparticles (nanoMIPs), also known as “plastic antibodies” [1], which have high selectivity towards the template or analyte. The use of nanoMIPs offer many advantages in comparison with the antibodies, such as stability, low cost and easy production [2]. All these characteristics make of these nanoparticles a promising alternative for their use in diagnostic, nanotecnology applications, as sensors, among others.
The nanoMIPs synthesis is carried out *via* solid-phase (figure 1), in which immobilized templates reduce of degrees of freedom and the orientation for the polymerization of template can be controlled.
In the present work, nanoMIPs with high selectivity towards biotin and microcystin-LR (MC-LR) were obtained. The size was determinate by dynamic light scattering using a Zetasizer Nano (Nano-S) from Malvern Instruments Ltd (Malvern, UK), the sizes were 148 nm for biotin and 210 nm for MC-LR, with low polydispersity (<0.5) in both cases. Finally, nanoMIPs were tested as “plastic antibodies” in competitive ELISA assay and good results in both cases were obtained.

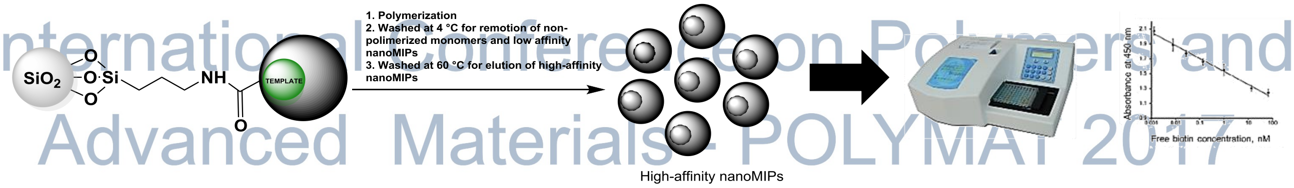

Figure 1. Solid-phase synthesis of nanoMIPs and their posterior use in ELISA assay.

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INNOVAR PARA MEJORAR EL MUNDO Y SER FELIZ HACIENDOLO

ANDRÉS GÓMEZ RENAUD

VIRETEC GESTIÓN Y DESARROLLO S.A. DE C.V., agomez@viretec.mx

Los programas de estímulos económicos directos destinados al sector industrial recomendados por la OCDE e implementados por el gobierno de México en el 2009 a través del CONACYT y la Secretaria de Economía, han estimulado el ecosistema de innovación en nuestro país y han sido acompañádos por políticas, en su mayoría acertadas, que incentivan la vinculación y a la investigación aplicada.

Nuestra empresa es en buena medida, un resultado de este programa. Durante más de 9 años, nos hemos dedicado a innovar para mejorar el mundo y durante todo este tiempo hemos recogido experiencias valiosas y detectado oportunidades de mejora que apuntan a facilitar las vinculaciones y promover la investigacion aplicada, tanto en la academia como en la industria.

Este trabajo, pretende compartir de manera resumida nuestra experiencia y aprendizaje a través de ejemplos reales, con el único interés de resaltar lo bueno e inclinar la balanza hacia las posibles mejoras en el ecosistema de innovación mexicano.

Revisaremos algunos conceptos probados de nuetro modelo de gestión de innovación, enfocados a la vinculación, hablaremos de la responsabilidad que tenemos desde la innovación con las mejoras que requiere el planeta y presentaremos algnos conceptos humanos que nos han ayudado a tener éxito dentro de nuestra compañía.

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EVALUATION OF ANTIMICROBIAL FILMS TO IMPROVE THE SHELF LIFE OF CHERRY TOMATOES (*LYCOPERSICUM SCULENTUM MIL.*)

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In the present paper, seven plastic films were prepared and evaluated for packaging, owned by the company A. Schulman de México S.A. de C.V., to improve or prolong the shelf life of cherry tomatoes (*lycopersicum sculentum mil.*). The films were prepared with polyethylene and polypropylene resin using the extrusion technique at a temperature between 170-190 °C and using different additives (AG/ZnO, AG/TiO_2 and AG-SiO_2 nanoparticles). To evaluate the performance of the films, several quality parameters were measured in the fruit: visual evaluation using photographs taken at different times after packing, analysis by infrared spectroscopy (FTIR), analysis of total dissolved solids (° Brix) and pH measurement. The results showed that all the films improved the shelf life of the tomato packed in it, compared with a witness film, this through a visual analysis of the samples. Tomatoes packed in PAZ2 films, TANCS 2 and Nova 53.2, which contain 200 ppm of AG/ZnO (in Matrix of LDPE), AG/TiO_2 (on matrix of LDPE) and AG/TiO_2 (on matrix of PP) respectively, were the ones that looked best at the end of the test, Figure 1. The pH of the samples tends to increase with the time, which is mainly due to the breakdown of the organic acids of the tomato (malic, tartaric, citric and ascorbic acids), and in general to the degradation of the tomato.

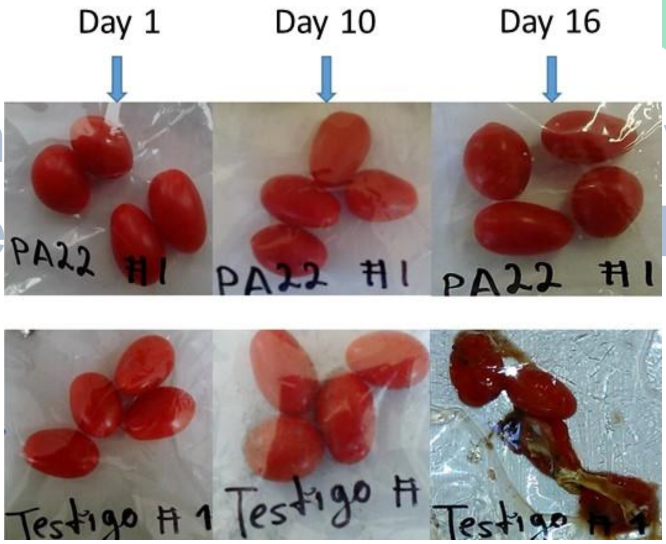

Figure 1. Photographs of tomatoes packed in the film PAZZ and witness, taken at different times

Study on the effect of adhesive configuration on metallic and combined joints

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Over the past few years the use of adhesives has increased rapidly. Mainly the automotive and aerospace industries have shown great interest in their applications.

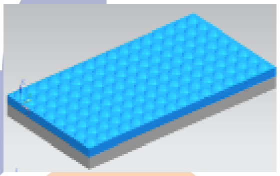
Illustration 1 Continuos Layer Schematic

The main attributes offered by this method are: low material cost, ease of application and high strength-to-weight ratio. In addition to making possible joints between materials that was previously not possible, without having high risk factors in the joints.


Illustration 2 Specimen Preparation

The main objective of this research is to characterize the application configuration of the adhesive and to study its effect on the failure mechanisms. The research will be based on the evaluation of microstructural, mechanical properties and the study of the interface through microscopy techniques.

The systems studied are: steel-steel, aluminum-aluminum, aluminum-steel and metal-composite bonding. The configurations designed were repetitive dot patterns, continuous pattern and uniform film.

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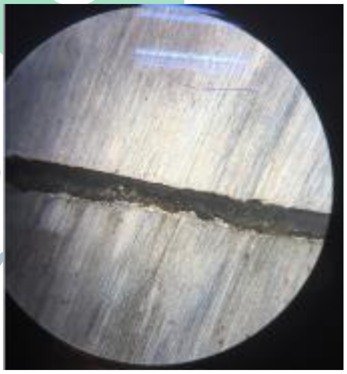
Illustration 3 Al-Al Microscopic View

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PREPARATION, CHARACTERIZATION AND DEGRADATION OF TERNARY EXTRUDED FILMS OF TRADITIONAL POLYMERS AND BIOPOLYMERS

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In recent times, synthetic polymers like polyethylene (PE) and polypropylene (PP) are employed in many diverse applications due to their dielectric properties, high durability, low cost, easy processability and chemical resistance [1]. However, the widespread of polymers has brought an environmental problem; the main issue is the time that residues persist in the environment after their life cycle has ended. Therefore, it is utterly necessary to find materials that comply not only with technical objectives and specifications but also with shorter times of degradation in the environment. A possible solution is to combine the materials mentioned earlier, with others that are easily degraded in the environment, so is the case of biopolymers like chitosan, or recently discovered biodegradable polymers that are in partial or total commercial development like polylactic acid (PLA) [2].

It is then that a methodology has been designed to study the effect of accelerated aging on the physicochemical properties of a set of polymeric blends. Extruded films are prepared with different proportions of synthetic (PE and PP) and biopolymers (chitosan and PLA) with and without compatibilizer. The films are subsequently subject to various times of accelerated aging, going from 12 to 200 h of degradation. Significant impacts on the properties of the polymeric blends are recorded with the use of thermogravimetry, resistencia a la tensión, infrared spectroscopy and scanning electron microscopy [3].

Results show that the combination of biopolymers and synthetic polymers significantly reduces the amount of time required to degrade the polymeric blends without fully compromising the mechanical and thermal properties of the materials; this implies that blends of natural and synthetic polymers may be a suitable eco-friendly alternative to traditional synthetic polymers.

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Comparative Analysis of Biomacromolecules Used for Restoring Blood Plasma Volume

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A Comparative analysis of the behavior of hydroxyethyl starch macromolecule (HES) with respect to commercial adversary Heamaccel® for medical use were performed. HES is a non-ionic starch derivative formed by two natural glucose polysaccharides, amylopectin and amylose [1-3] by chemical modification with hydroxyethylations at the hydroxyl groups of the carbons at positions 1 and 6; Heamacel® is a colloidal solution of polygellin composed mainly of 3.5% degraded gelatin polypeptides (bovine bone). Both macromolecules are used as volume expanders and artificial colloidal blood plasma in human and veterinary medicine, restoring the total volume of blood.

In this work tests are performed to find differences in physical and chemical properties between both colloids. They are characterized using Laser Light Scattering (LLS) for determine of density and particle size distribution, according to the European Pharmacopoeia 8.0; also the structures, were analyzed by FTIR-ATR, NMR, and chemical composition by XPS.

The results of molecular weight (M_w) show standard and raw material of HES in two different buffers: first (acetic acid/NaOH) and the second (acetic acid/sodium acetate) were analyzed, obtaining the best range (120K – 150K) of M_w in the last buffer [4], according to the norm.

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Citrus Oils as Chain Transfer Agents in the Cross-Metathesis Degradation of Natural Rubber Using Ru-Vinilydene Catalysts

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Terpenes are a class of natural products that typically contain carbon atom units built from isoprene molecules. In plants, terpenes are found as a main component of essential oils, which are used in medicines, spices and perfumes. Commercial polymers of monoterpenes usually prepared through Lewis acid catalyzed polymerization, are used for many industrial applications; for example, as pressure-sensitive adhesives, hot-melt coatings, packaging gum and additives. The transformation of terpene-based molecules using efficient catalysts is of great interest in the development of new applications for these biomass-derived compounds. In this perspective, the metathesis transformations are becoming the most attractive choice, as the availability and efficiency of the catalysts increases. **[1, 2]**

This research reports the cross-metathesis degradation of natural rubber using essential oils as chain transfer agents and as green solvents, in the presence of ruthenium-vinylidene catalysts $RuCl_2(=C=HR)(PCy_3)_2]$ (R= -*p*-$C_6H_4CF_3$ (**I**), -*p*-C_6H_4F (**II**) and -C_6H_9 (**III**)). **[3]** Oligomers (isolated products) with molecular weights around M_n x 10^4 g/mol were obtained when the reactions were carried out at 50°C. An enhancement of the catalytic activity was achieved at 80°C, and it was reflected in a decrease in molecular weight of products; with values around M_n x 10^3 g/mol. Experiments also demonstrated that the copolymer styrene-*co*-butadiene depolymerized in the presence of essential oils using vinylidene catalysts, to give the butadiene oligomers with molecular weight values around M_n = 295-698 g/mol. According to GS/MS (EI) analysis, the main products of degradation of SB with *d*-limonene were limonene-terminated butadiene oligomers with m = 1-3. **[4]**

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Keratin Fibres Recovered from Tannery Industry Wastes as Fire Retardant Agent on PLA composites

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As it is well known, tannery leather process is a high pollutant emissor. During beamhouse stage, the wastes have a strong negative environmental impact because of the effluents and solids have a high content of organic matter. Hair skin derived from this stage, which is thrown in sanitary fills without any usual treatment. However, wasted hair is considered an important keratin fibre source with interesting applications in polymer materials [1]. In this work keratin fibres (KFs) were recovered from tannery industry wastes. A specific treatment was applied to KFs in order to obtain polymer composites base on PLA, KFs and aluminium tri-hydroxide (ATH) by extrusion process. The effect of KF content and the joint action of KFs in combination with ATH as fire retardant for poly(lactic acid) -PLA- was studied by thermogravimetric analyses, UL94 classification, dynamical-mechanical, mechanical and rheological analysis. According to the collected results, the fire retardant potential of keratin fibres recovered from tannery industry wastes on PLA composites have been demonstrated. PLA composites were classified as V2 with only KFs (3, 5 and 10 phr). However, when KFs were added to 30 phr ATH, the composites reached V0 rating, the same classification obtained using 50 phr ATH. Therefore, by using low KF content (3 phr), it is possible to replace 20 phr ATH. In addition, KF-based composites exhibited higher mechanical properties than that containing only ATH. Flow behaviour under continuous simple and small amplitude oscillatory shear flows demonstrated that KFs decrease the viscosity of the PLA composites in a remarkable way improving the processability of PLA composites. Materials containing both KFs and ATH exhibited a higher elastic behaviour than those loaded with only KFs. The latter result represents an important advantage from an economical and environmental point of view in flame retarded materials [2].

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SPUTTERED BISMUTH OXIDE THIN FILMS AS A POTENTIAL PHOTOCATALYTIC MATERIAL

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The photocatalytic properties of Bismuth oxide (Bi_2O_3) thin films deposited by magnetron sputtering were evaluated using the photodiscoloration of dye solutions as a preliminar test. The films were deposited on glass substrates using different conditions of power (radio frequency) and substrate temperature. The film structural characterization was done using X-ray diffraction, where it was demonstrated that films presented different crystalline phases were obtained; cubic delta-Bi_2O_3 and a mixture of alfa- and beta-Bi_2O_3 in different proportions. Pure phases were also obtained by annealing the delta-phase films. The photocatalytic activity of all the films was evaluated by measuring the percentage of photodiscoloration of dye solutions using UV and white light. The results indicated that the films were only active under acidic pH and that the cubic delta phase was the most efficient. The explanation of such difference was obtained through the analysis of the photoluminescence spectra done by Marel as a tool to study the radiative recombination [1]. The delta-Bi_2O_3 phase has been further investigated since it shows a extremely rapid discoloration in comparison to other semiconductor films, including TiO_2.

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SYNTHESIS OF CUBIC III-N COMPOUND SEMICONDUCTORS BY MOLECULAR BEAM EPITAXY FOR SOLAR CELLS APPLICATIONS

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III-N semiconductors have a great potential for electronic and optoelectronic applications [1]. In particular $In_xGa_{1-x}N$ alloys are very interesting for photovoltaics [2], because their direct band gap can be changed from infrared to ultraviolet by varying the In content (x). III-N semiconductors with cubic (c) phase have a narrower band gap (about 200 meV) compared to those with hexagonal phase; therefore the visible spectral range can be covered with less Indium content employing cubic $In_xGa_{1-x}N$. In this work, first we demonstrate a solar cell based on cubic-GaN/GaAs heterostructure grown by rf-plasma-assisted molecular beam epitaxy (RF-MBE). The characterization of the devices was carried out by high-resolution x-ray diffraction (HRXRD), transmission electron microscopy (TEM), current-voltage (I-V), external quantum efficiency (EQE), reflectance, photoluminescence (PL), and secondary ion mass spectrometry (SIMS). In order to increase the performance of the device, c-$In_xGa_{1-x}N$/GaN quantum wells (QWs) were grown as the top material in a tandem solar cell structure. The In content (x) in the c-$In_xGa_{1-x}N$ QWs was controlled by the substrate temperature. SIMS depth profiles allowed us to identify the formation of c-$In_xGa_{1-x}N$ QWs, and the corresponding incorporation of In. By decreasing the substrate temperature the incorporation of Indium in the QWs increased due to the increase in the In sticking coefficient. Employing this process we achieved a concentration of Indium in the QWs as high as 27%. These QWs have a PL peak emission centered at 2.2 eV, which shows that these structures are very suitable as absorbing layers for the most intense region of the solar spectrum.

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ELECTRONIC PROPERTIES OF Bi-Cs-Ru SYSTEMS INTERACTING WITH CARBON- NATOTUBES

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Ruthenium nanoparticles supported on carbon-nanotubes have been reported as the systems with the highest rate of hydrogen production via ammonia decomposition. The ruthenium activity is enhanced by the presence of promoters that apparently are electron donors. The best promoter reported to date is cesium, which reduces dramatically the activation energy. The model that explains this effect considers a charge transfer from Cs to Ru. This process weakens the Ru-NH_3 bond, facilitating the decomposition of ammonia. In spite of all the investigation reported until now, there is not a clear explanation about the role of the promoters in the catalysis of the reaction. It was reported before the effect of intruders on potential reactivity of fullerene-like (C_{60}-xBi_x (with x = 0-10) and bismullene-like Bi_{60}-yC_y (with y = 0-10) systems. Bi and C are intruders for fullerene-like and bismullene-like systems, respectively. The most stable structures of bismullene-like systems have cage geometries. The most stable fullerene-like geometries resemble a cup with bismuth atoms at the edge of the bowl. The presence of bismuth increases the electron donor power. HOMO-LUMO gaps indicate that bismullene-like clusters represent better candidates for building solar cells than fullerene-like clusters. Since the presence of bismuth increases the electron donor capacity, it is a good idea to analyze bismuth as a promoter of the ruthenium-based catalysis. To this end, in this investigation carbon-nanotubes with Ru, Bi and Cs (atoms and clusters) are analyzed and the interaction with ammonia is investigated.

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Incomplete capsid formation: coarse-grained and elastic modeling

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The successful assembly of a closed protein shell or capsid is a key step in the replication of viruses and in the production of artificial viral cages for bio/nanotechnological applications. We study the formation of stable incomplete capsids self-assembled from capsomers in solution by means of coarse-grained simulations and an elastic model. We show that during self-assembly, the favorable capsomer-capsomer binding energy competes with the energetic cost of the rim and the elastic stresses generated due to the spontaneous curvature of the capsid. As a result of that competition, incomplete or ribbon-shaped capsids may emerge , thus preventing the successful replication of the virus. We analyze the conditions required for these processes to occur and their significance for virus self-assembly.

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Deposition of Tin Sulfide doped with Copper (SnS: Cu) by Ultrasonic Spray Pyrolysis technique

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Thin films of Tin Sulfide doped with Copper (SnS: Cu) will be prepared on glass substrates by ultrasonic spray pyrolysis technique at different Cu ratios, Tin(II) chloride dihydrate ($SnCl_2 \cdot 2H_20$), N,N´-Dimethylthiourea ($C_3H_8N_2S$) and Copper(II) chloride dihydrate ($CuCl_2 \cdot 2H_20$) were used as precursor materials. Before doping, deposition temperature was varied from 300 - 450 ° C to obtain polycrystalline SnS. After founding the ideal deposition temperature, the mixed solution will be doped with 2, 5 and 10 % with a copper solution. The obtained films will be characterized by XRD, Profilometry, SEM, EDS, Effect Hall-Van Der Pauw to study their optical, structural and electric properties, then, the material will be analyzed to use it in photovoltaic applications.

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DESIGN AND CHARACTERIZATION OF BIODEGRADABLE HOLLOW POLYMERIC NANOPARTICLES AS A NOVEL ULTRASOUND CONTRAST AGENT

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Cancer is one of the most devastating diseases, and its incidence has increased in the last years [1]. Ultrasound technology in combination with echogenic particles is currently having a considerable effect on the diagnostic for many diseases, including cancer. The existing ultrasound contrast agents can not extravasate through tumoral vasculature due to their large particle size, so that the development of nanometric ultrasound contrast agents is necessary [2]. The main aim of this work was to prepare biodegradable hollow polymeric nanoparticles by the emulsification-diffusion method [3], intended to be used as novel ultrasound contrast agents. Box-Benhken experimental design was implemented to assess the efect of porogen amount, stabilizer concentration and homogenization rate, in the physicochemical properties and echogenicity of nanoparticles. It was found that increasing of stabilizer concentration and homogenization rate resulted in particle size and polydispersity index decrease. In contrast, a low homogenization rate caused zeta potential decrease. It was observed an enhancement in the ultrasound images contrast when porogen amount increased. Particle size, polydispersity index, and zeta potential of optimal nanoparticle formulations were 300 nm, 0.05, and -24 mV, respectively. *In vitro* echogenicity was improved using hollow nanoparticles (26%), compared to solid nanoparticles which exhibited an echogenicity of only 15%. Differential scanning calorimetry analysis and density measurement demonstrated the formation of hollow nanoparticles. Scanning electron microscopy images showed the spherical shape of nanoparticles. Finally, hollow polymeric nanoparticles developed in this work are promising contrast agents for their use in cancer ultrasound diagnostics.

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N-heterocyclic carbene complexes derived from thalidomide.

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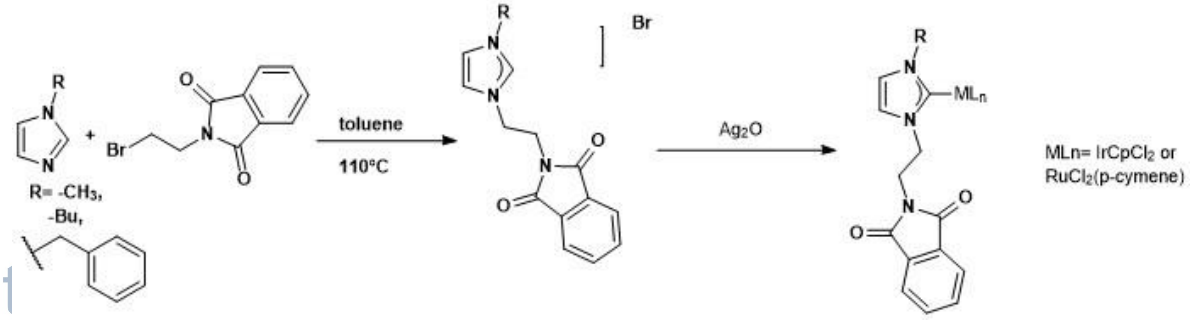
Ruthenium-based pharmaceuticals have brought some importants insights in the chemotherapy of cáncer. The knoledge acquired about the chemistry and biological interactions of these inorganic chemicals has allowed us to undersantd the limits of targeting DNA to achieve selective and innovative drugs. After a number of attempts to copy platinum drugs with a system claimed to be selective because of tranferrin transpotation and activation to cytotoxic species in tumor cells by a reduction mechanism, new innovative ideas are emerging such as those of using Ruthenium to structure organic ligands to enzyme or receptor targets responsable for tumor cell pathways associated to cell survival.

It's know that Angiogenesis is important in embryogenesis, wound healing, diabetic retinopathy, and tumor progression [1]. Since the drug thalidomide can inhibit angiogenesis and induce apoptosis of established neovasculature in experimental models, [2] we used it to check its use for treating cancers combined with the power of N-Heterocyclic complex of Ru and Ir.

As shown in **Scheme 1**, the complex were synthetized in two steps.The first one allowed us the incorporation of the azolium salts in the thalidomide derivate. Finally the coordination to Ir and Ru was implemented through a transmetallation reaction. The biological tests are currently developing in our laboratory as well as catalytic tests for the transfer of hydrogen and the oxidation of alcohols.



Scheme 1

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INTEGRAL BENEFITS OF LINKAGE TO INDUSTRY IN MANUFACTURING PROCESS AND MATERIALS RESEARCH PROJECTS

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[2] *3G Herramientas, S.A. de C.V.*

Since 1967 Mechanical and Electrical Engineering Faculty (FIME) of Universidad Autonoma de Nuevo Leon, has been closely linked with industry of Nuevo Leon, Mexico. When the Programa of Estimulo a la Innovación founds arrived in 2009, FIME was prepared for this new sinergy. In this work present a special projects with 3G Herramientas, S.A. de C.V. company around composite and special nanomaterials.

Acknowledgements

This work was supported by the Mexican National Council for Science and Technology (CONACYT) Mexico with the program "Programa de Estímulo a la Innovación (PEI)"

Semi-Fluorinated Aromatic Ether Polymers via Step-Growth and Modular Mechanistic Polymerization of Fluoroalkenes

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Dennis W. Smith, Jr.[1], Scott Iacono[2], Babloo Sharma[3]

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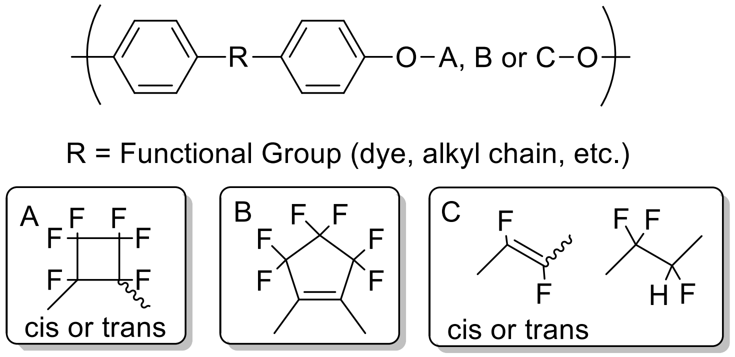
Perfluorocyclobutyl (PFCB) aryl ether polymers are prepared via step-growth [2+2] thermal dimerization of aryl trifluorovinyl ethers (TFVE) and have been demonstrated as processable fluoropolymers for high performance passive optics, electro-optics, polymer light-emitting diodes (PLEDs), space survivability, polymeric fuel cell membranes (PEMs), high use temperature fluorosilcones, POSS composites, and liquid crystalline polymers.[1] More recently, fluorinated aryl vinylene ether (FAVE) polymers were prepared from the condensation of functionalized bisphenols with TFVEs.[2] These fluoropolymers are solution processable, exhibit excellent thermal stability, and possess the ability to undergo thermal crosslinking without the use of post-curatives. In addition, we have introduced a new class of semi-fluorinated polymers from perfluorocycloalkenes (Scheme 1) affording reactive cyclopolymers from commercial monomers.[3] We have successfully synthesized poly(perfluorocyclopentenyl aryl ether) homopolymers and copolymers and others in one step *via* nucleophilic substitution with bisphenols and octafluorocyclopentene. This lecture will overview the projects in our laboratory including three fluoropolymer platforms; and other highlights including; carbon from polymer precursors, renewable resource materials, and car tire rubber composites.



Scheme 1. Semi-fluorinated poly aryl ether platforms with variable fluoro-enchainment.

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Synthesis and characterization of nanocomposite coating based on epoxy resin, montmorillonite and (3-glycidyloxypropyl)trimethoxysilane

Juana Deisy Santamaría Juárez[1], *Jenaro Leocadio Varela Caselis*[2], **Manuel Sánchez Cantú**[1], *José Alberto Galicia Aguilar*[1]. *José Eduardo Tobon Sosa*[1].

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In the present work, organic-inorganic nanocomposites based on epoxy resin DER 332 and modified montmorillonite (MMT) were obtained at different proportions 0%, 0.5%, 1%, 3% and 5% wt. MMT [1]. It was used 3 -Glycidoxypropyl Trimethoxysilane as pretreatment film. The nanocomposites were deposited on carbon steel substrates which were cleaned with detergent and abrasive paper, the coatings were cured at 120°C for 1 hours [2]. The characterization of the coating was performed using physical techniques such as Scanning Electron Microscopy (SEM), Optical Microscopy (OM), Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetry Analysis (TGA), X-Ray Diffraction (XRD), adhesion was evaluated using standard ASTM D3359-02 and the corrosion assessment was carried out using Electrochemical Impedance Spectroscopy (EIS) technique, in parallel with visual corrosion tests according to ASTM D610-01 and ASTM D1714-02 [3]. The results of the characterization and the electrochemical evaluation by EIS showed the formulation with the best anticorrosive performance in a solution of NaCl 5% wt.

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

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STUDY OF AUTOACCELERATION IN FREE RADICAL POLYMERIZATION OF METHACRYLATE ISOMERS

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Free radical polymerizations (FRP) of n-butyl methacrylate (BMA), iso-butyl methacrylate (i-BMA) and ter-butyl methacrylate (t-BMA) were performed by differential scanning calorimeter (DSC). Using a mathematical model[1] an explanation their behavior is proposed in terms of chemical and diffusive control. The analysis of this data show that the FRP reactions are controlled by the chemical step at low conversions until a transition of chemical to diffusive control occurs and the autoacceleration begins to appear (see Figure 1-2). This results show that the transition from chemical to diffusive control is manifested by the apparition of a minimum in the rate of polymerization (R_p) and it was found that the monomer conversion at which the minimum (x_{min}) is observed follows the order BMA>i-BMA>t-BMA and that for monomer conversions smaller than x_{min}, the termination rate coefficient (k_t) shows a plateau.

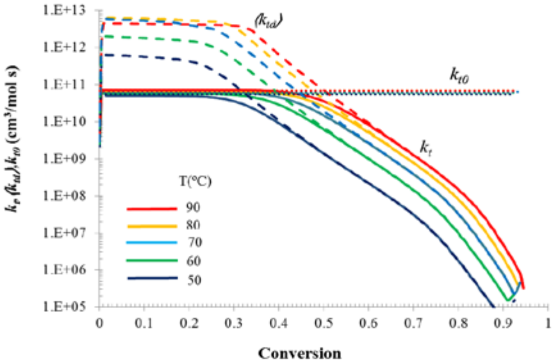

Figure 1. Termination coefficient evolution for BMA polymerizations.

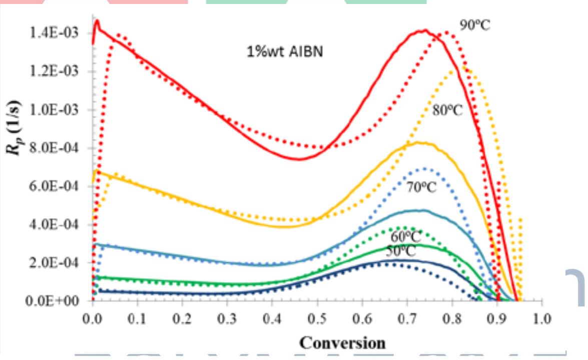

Figure 2. Rp evolution for BMA polymerizations. dotted line: experimental data, model: continuous line.

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Organic Solar Cells based on Perovskite by Spin Coating Method

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In latest decades organic solar cells have become a very promising option for photovoltaic technology. Solar cell research has led to the production of Perovskite-based solar cells whose power conversion efficiency (PCE) has increased exponentially in recent years reaching values above 12% in 2016. In this work, was elaborated Perovskite ($CH_3NH_3PbI_3$) tandem type with the following conformation: ITO/PEDOT:PSS/ Perovskite/PC71BM/FM. The effect of different parameters on the morphology, uniformity and crystallinity of the films was studied. In addition, the relation between the photovoltaic behavior of the cells and the morphology of the active layer (perovskite) was analyzed. The perovskite-1 (deposited with open spin-coating) and perovskite-2 films (deposited with closed spin-coating) deposited in a controlled atmosphere (N_2) followed by a chlorobenzene bath, it was observed that a crystallization of granular type was formed in both cases and also during the manufacturing process a change of color in the films. In the perovskite-1 film a more defined and uniform grain type is observed through the film obtaining better crystallization and homogeneity compared to perovskite-2. The thickness of both films allowed light absorption with good performance of a photovoltaic device, obtaining efficiency of 1.94% with an open circuit voltage of 0.51V and a fill factor of 0.24.

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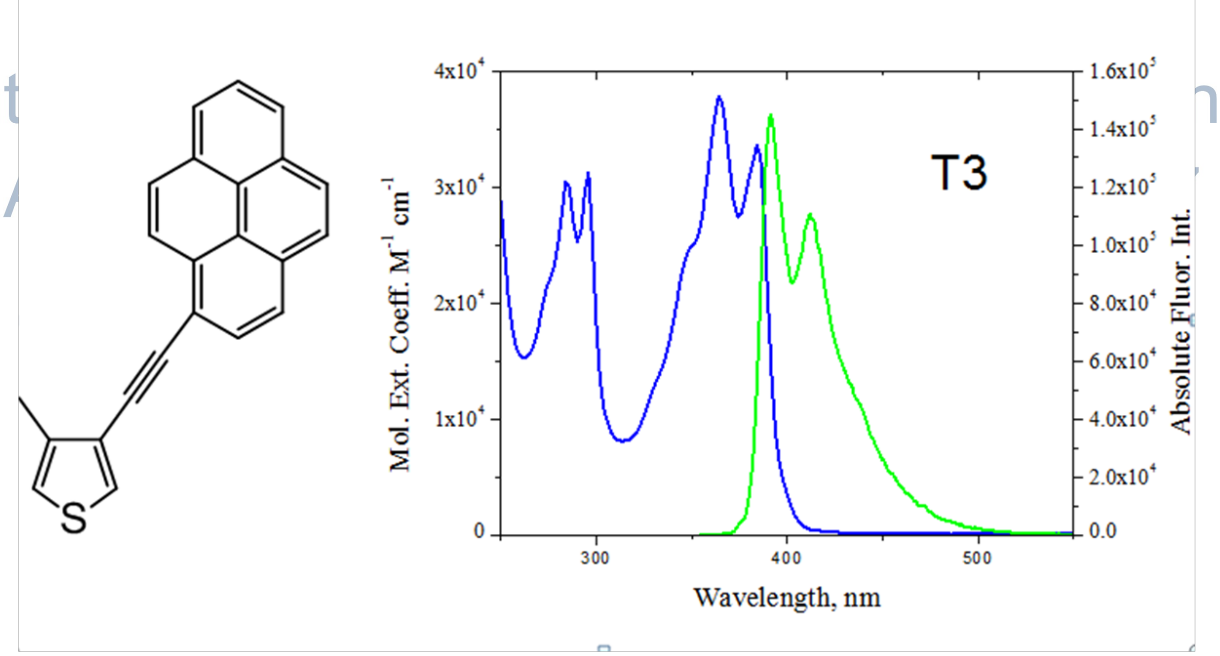
Optical properties of novel thiophene monomers containing pyrene units linked via rigid and flexible spacers

Authors: Eric G. Morales-Espinoza, Ernesto Rivera

Abstract:

In this work, we report the synthesis of three novel thiophene monomers containing pyrene groups linked via rigid and flexible spacers (**T1**, **T2** and **T3**). These monomers can be further copolymerized with 3-alkylthiophenes in order to obtain soluble luminescent polymers with pyrene moieties. These compounds were fully characterized by NMR spectroscopy and mass spectrometry. Monomer **T2** exhibited the typical absorption band of pyrene at 344 nm and a strong "monomer" emission at 375 nm. On the other hand, **T1** and **T3** showed a red shifted absorption bands at 352 and 384 nm, respectively, due to their higher conjugation degree. These monomers exhibited a broad "monomer" emission band between 360-450 nm and no excimer emission was observed.



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SYNTHESIS OF PRIMARY AMINE-RICH POLYMER SURFACES BY GAMMA RADIATION, FOR ADHESION CELULAR

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The present work focuses on the synthesis of different amine-containing surfaces on the polymers poly(tetrafluoroethylene) (PTFE), polyethylenterephtalate (PET), polypropylene (PP) and polyethylene (PE), to be used for adhesion cellular. They were obtained in two steps: grafting of acryloylchloride (AC) in different polymers by direct gamma radiation method, followed by reaction between the grafted AC and ethylenediamine. Modification of PE and PP by allylamine was also synthesized in one step, by gamma radiation. The effects of the monomer concentration, absorbed dose and reaction time were studied. Characterization of different systems was determined by XPS, FTIR, TGA, SEM, AFM and contact angle.

Cell Attachment on surfaces and cell adhesion are critical for biomedical and biotechnological applications such as the development of biomaterials for tissue engineering. Primary amine grafting polymers can be useful surfaces for cell colonization, they are usually prepared by plasma polymerization of alkyl amine monomers or using feed gas mixtures of N_2 and C_2H_4 [1]. During plasma polymerization, the monomer suffers breakage and the recombination of bonds; the amines groups are partially transformed into imine, amide or nitrile functional groups [2, 3]. The plasma process is difficult to control and relative inefficient, for getting just primary amine groups.

In this work, different grafting percentages was obtained in each system, depending on the polymer, required solvent and the radiation effect on the studied polymers; but only a surface modification of primary amines of about 4.5 at% is usually necessary for adhesion cellular. Grafting in bulk was obtained in all cases.

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Acknowledgements

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

"Solar cell transitions; Towards thin-film silicon-based photovoltaic technol

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Session 6.- Memorial Symposium
to Dr. Betsabee Marel Monroy Peláez

Abstract:

Solar photovoltaic systems (PVS) are becoming one of the important clean and alternative-energy technology in several countries. The PVS are safe, reliable with a low-maintenance cost without any on-site pollutant emissions. Nowadays, the utility grid-connected PVS are increasing rapidly in the world and the estimated global PV market grew to over 75 GW during 2016, and about 300 GW cumulatively installed capacity at the end of same year [1]. The underlying deployment scenario assumes 3,150 GW of cumulative installed PV capacity by 2050 [2].

First of all, an explanation about the general photovoltaic development and situation in the world will be given in this presentation. Also, considerations as bulk and thin-film based technologies will be discussed and the possible scheme for solar cell energy conversion improvement by using silicon-based materials and technology are reviewed.

Some of the obtained silicon-based thin-films are analyzed through its light interaction, mostly for the visible range and for down conversion approaches. Some of the sample properties as amorphous and microcrystalline-based materials as SiO_X, SiC_X and SiO_XC_Y thin films fabricated by using Plasma- and catalytic chemical vapor deposition methods (Plasma- and Cat-CVD) are discussed.

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PYRENE CONTAINING DENDRONS AS POTENTIAL SENSORS FOR NITRO COMPOUNDS AND AMINES.

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Abstract: Dendrimers are highly branched, spherical, three-dimensional polymeric macromolecules having a large number of terminal groups that control the size, solubility and reactivity of the molecule. The synthesis of dendrimers as new functional materials for photovoltaic devices and energy conversion technologies are of great interest nowadays.

The aim of this research project is to synthesize different dendrons having pyrene groups in the core (PyNK0, PyNK1 and PyNK2) with tert-butyl and carboxylic periphery groups. Pyrene is a powerful fluorescent probe with peculiar photophysical properties such as long fluorescent lifetime, high fluorescence quantum yields and ability to form excimers. For this reason, it is an excellent candidate for the synthesis of dendritic compounds with applications in materials science, sensors[1], light emitting diodes and photovoltaic devices.

The complex architectures of the synthesized dendritic molecules allow us to study luminescent phenomena, in particular its application as pollutant sensors. The synthesis of pyrene dendrons was achieved via amidation reactions with an easy purification procedure. Structural characterization was achieved using spectroscopic techniques (UV-vis, 1H and 13C NMR and Mass Spectrometry). Because of their tunable solubility, the obtained compounds are promising candidates for the future preparation of sensors.

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Synthesis of L-Lysine dendrimers Using “Click Chemistry” for applications in nanomedicine

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In this work, supramolecular dendrimers based on L-lysine (LL) and polyethyleneglycol (PEG) were designed for the elaboration of novel drug delivery systems, since peptide based dendrimers play an important role in various areas of nanomedicine because they have useful properties similar to proteins, they are biodegradable and soluble in water [1]. Firstly, the synthesis and characterization of LL dendrimers is proposed. L-lysine was incorporated into an aromatic nucleus using "Click Chemistry" followed by C-N (L-lysine-COOH-NH-L-lysine) coupling reactions using a new generation of coupling agents which are considered environmentally friendly [2]. Then, through "Click chemistry" the dendrimer will be linked to the periphery with PEG (**Figure 1**). Finally, through supramolecular interactions a model molecule and a drug will be incoprorated in the arms of the dendrimer and we will carry out the studies of the drug release, and analyze the presence and absence of PEG in the release of the molecules and in the toxicity of the dendrimers [3].

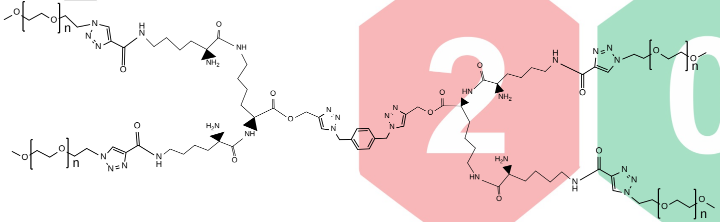

Figure 1. L-Lysine dendrimer conjugated with PEG

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CHEMICAL MODIFICATION OF DIACETYLENE-CONTAINING POLYMERS BY SUBSTITUTED AROMATIC AMINES

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Chemical modification of polymers is employed to improve properties and change structure of conventional polymeric materials. In the present work the modification of diacetylene-containing polymer with isatin by aromatic amines with electron-withdrawing substituents is reported. Diacetylene-containing polymer was synthesized by condensation of isatin with diacetylenic monomer in a superacid medium. The chemical modification of the diacetylene-containing polymer was carried out by the addition of aromatic amines on the triple bond in presence of copper chloride (I), under nitrogen atmosphere to get substituted pyrrole units. Ten new polymers were obtained; each compound was characterized by IR and ^{1}H and ^{13}C NMR spectroscopy, as well as GPC and Thermal Analysis. The obtained polymers share the property of owning electron withdrawing groups link to the enclosed aromatic ring, it seems this characteristic largely explains the improvement in the semiconductor behavior of this sort of materials.

Keywords: diacetylene-containing polymer, pyrrole units, chemical modification

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PREPARATION AND OPTICAL PROPERTIES OF PYRENE-LABELED RUTHENIUM(II) TRISBIPYRIDINE COMPLEX CORED DENDRIMERS

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Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México.

Dendritic macromolecules are presenting unique physical and chemical properties. One of them is the faculty of transferring energy from a donor moiety introduced at the periphery to an acceptor moiety at the core, mimicking the antenna effect of the process of photosynthesis. The mechanism of energy transfer is based on the Förster resonance energy exchange and requires some overlap between the emission spectrum of the donor and the absorption spectrum of the acceptor. Since it requires a coupling of transition dipole but no overlap of the physical wavefunctions, the energy transfer by Förster mechanism can occur over quite long distances from 1 to a maximum of 10 nm. However, the efficiency of the transfer depends strongly on distance. The Förster radius is the distance at which 50% of the donor's emission is deactivated by FRET.

In this work, we synthesized and characterized a novel series of dendrimers bearing pyrene moieties at the periphery and a Ru (II) complex at the core. The optical and photophysical properties of these compounds were studied by absorption and fluorescence spectroscopy. Pyrene is a well-studied chromophore that have the particularity to present monomer as well as excimer fluorescence emission. The coordination compounds of Ru (II) are red emitters with low quantum yield and long excited lifetime. We observed an efficient singulet to singulet energy transfer in such constructs. Moreover, it is known that the energy of the MLCT emitting state of Ru (II) can be tuned to become almost isoenegetic with respect to the triplet state of pyrene, leading to an extended phosphorescence lifetime. Using dendrimers bearing pyrene moieties as ligands for Ru (II), we could combine the antenna effect of dendrimers as well as its protection effect to the quenching by dioxygen with lifetime increase due to triplet-triplet equilibrium.

Photocontroles of Acoustic Alignments of Supramolecular Nanofibers

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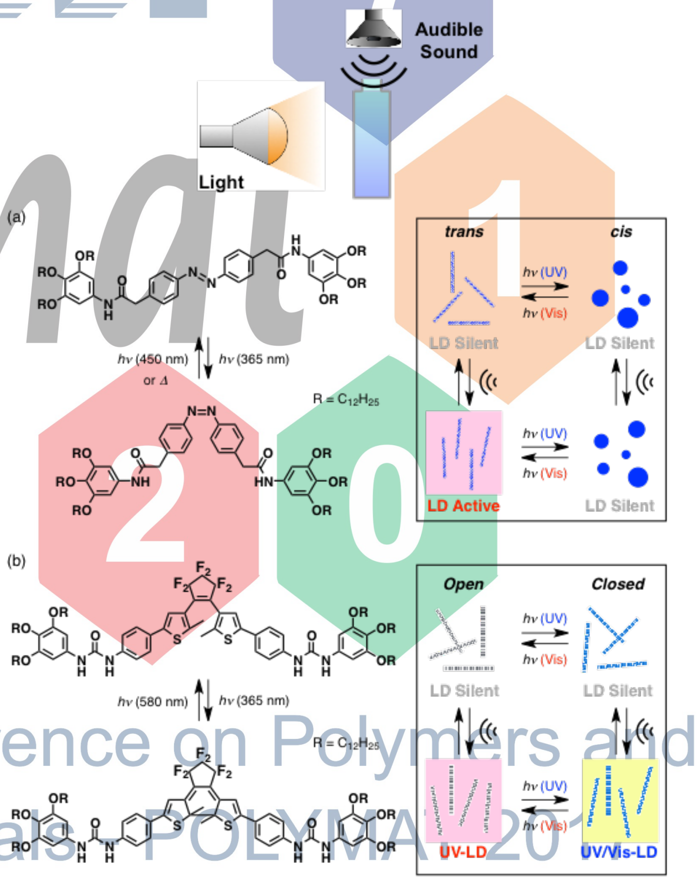
Functional materials composed of macroscopic molecular assemblies that bring about reversible changes of their shape and/or physical properties upon external physical stimuli have attracted much attention in material sciences.

We found that photoisomerizations of an azobenzene derivative reversibly change its self-assembly in a solution to form twisted supramolecular nanofibers and amorphous aggregates, respectively. When irradiating the sample solution with audible sound, the former assembly exhibits a linear dichroism (LD) response due to its hydrodynamic orientation, but the latter one is LD silent, in the sound-induced fluid flows.



To evolve such nanoarchitectures, we subsequently designed an audible sound-responsive photochromic nanofiber capable of switching reversibly the wavelength of the sound-induced LD with UV and visible light. A photochromic supramolecular nanofiber, composed of a diarylethene derivative, exhibits hydrodynamic alignment under exposure to the audible sound. The aligned nanofiber outputs LD, whose wavelength region can be switched reversibly with UV and visible light.

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Anisotropic Exchange Coupling in Nanostructured Oxides

R. Valenzuela[1], G. Vázquez-Victorio[1], N. Flores-Martínez[1], G. Franceschin[2],
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In 1956, Meiklejohn and Bean [1] synthesized ferromagnetic (FM) cobalt nanoparticles (NPs). After a few weeks, a significant shift in the hysteresis loops was observed. A thin layer of antiferromagnetic (AFM) cobalt oxide was formed on the surface of NPs, leading to an exchange coupling between the FM and the AFM phases. They thus accidentally discovered the anisotropic exchange coupling known as "exchange bias". The exchange coupling between phases with different magnetic ordering has always arose scientific and technological interest, but it is presently very strong, as it allows, among many other applications, the preparation of rare-earth-free permanent magnets. Rare earth (RE) materials effectively constitute the strongest permanent magnets, but they have become a strategic material as 97% of RE deposits are found in a single country (China).

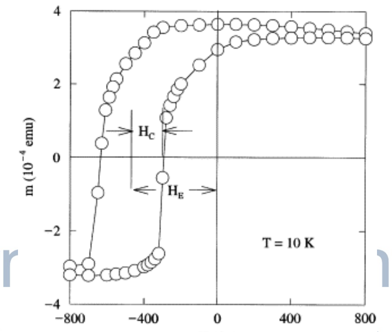

Fig. 1. Typical shift in a FeF_2/Fe bilayer at T=10 K after field cooling [2]. The exchange bias, H^{E}, and the coercivity, H^{C}, are indicated.

A number of new synthesis techniques have recently open the possibility of an improved control on NPs and therefore, the building of many combinations of RE-free magnetic phases. In this work, we present a short review of nanostructured materials exhibiting anisotropic coupling leading to "exchange bias" and "spring magnets" [3], based on ferrimagnetic (FI) oxides (Fe3O4, CoFe2O4, NiFe2O4, BaFe12O19), and AF oxides (CoO, NiO, Fe2O3). Their main magnetic properties are also examined. In some cases, these phenomena have also been observed on consolidated nanostructured phases [4].

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

DESIGN AND PROTOTYPE OF ALTERNATIVE HOUSING SYSTEM, WITH AUTO ASSEMBLED LOW COST PIECES

M. Espitia, D. Corredor, H. Bustos, A. Muñoz, A. Rivera, N. Rodríguez, P. Castaño, R. Peraza.

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The technologies that are traditionally used for construction, implement materials such as; reinforced concrete, ceramic brick, and tile that conceive a problem of affordability for vulnerable communities due to their high costs [1], on the other hand, these construction systems apply consecutive methods and stages that prevent self-construction [2]. This work presents the prototype of an alternative system of construction, using self-assembling polymeric pieces, focused on housing of social interest for vulnerable community; to achieve this, we used the software solidworks, where the design, geometry and assembly of the pieces of the house was created, a structural simulation was made using Etabs and finally the prototype was printed in 3D. In order to generate a constructive housing system, by means of self-assembling pieces with recycled polymers reinforced with natural fibers, which has an optimal functioning, is easy to construct, and improves the quality of life of the communities with a positive impact on the user and the environment. From the above it was determined that the prototype housing is an alternative system of construction, since it has a low cost, because the parts are made from recycled materials and thus contribute to the environmental impact, also the construction times are shorter because it does not require consecutive stages, it is very easy to build, it does not require trained labor, and the model supports the static loads imposed on this type of dwelling.

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT-2017"

DESIGN AND PROTOTYPE OF ALTERNATIVE HOUSING SYSTEM, WITH AUTO ASSEMBLED LOW COST PIECES

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

Chromium retention in the system of binary grafting of N-vinyl-caprolactam and dimethylacrylamide onto chitosan, synthesized by gamma radiation.

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Chitosan and crosslinked chitosan were grafted with vinylcaprolactam (VCL) and dimethylacrylamide (DMAAm) by ionizing radiation. Both systems were characterized with FTIR, TGA and contact angle. The retention of chromium (VI) in the synthesized binary grafted samples was studied at different concentrations and retention time and their behavior studied by Langmuir and Freundlich isotherms.

Grafting of VCL/ DMAAm onto CS (CS-g-(VCL/DMAAm))

Solutions of CS (1 %) in acetic acid (10%), with different ratio of VCL/DMAAm were irradiated in argon atmosphere at different doses and at dose rate of 10 kGy/h. The grafting percentage was calculated by the equation [(Wf-Wo)/Wo]100.

Grafting of VCL/DMAAm onto chitosan gel ((net-CS)-g-(VCL/DMAAm))

Cs gel (net-CS) was prepared by chemical reaction with formaldehide as crosslinking agent. The CS gel (net-CS), was grafted with NVCL/DMAAm 15%/ 5% v/v in methanol solution, in argon atmosphere at different doses (2.5 a 10 kGy).

Chromium retention (adsorption isotherms)

The Cr (VI) retention was estimated with aid of the Langmuir and Freundlich isotherms in the systems: (net-CS 1%), (net-CS 3%), ((net CS 3%)-g- NVCL/DMAAm (15/5) and (CS 1%)-g-NVCL/DMAAm by plotting the log Qo as a function of the initial concentration of CrO_4^{-2}. the Freundlich constant was calculated with the experimental results.

Conclusions

The best results in the chromium retention were found in the systems CS-g- NVCL/DMAAm (200%graft) with the absorption of 45 mg/g of grafting sample.

Similar results were found in the binary graft onto CS gels with a grafting percentage between 5 to 21%, with the absorption of about 47 mg/g of sample. Both systems have a good correlation for the Freundlich and Langmuir (0.9 to 0.994) in case of Net-g- VCL/DMAAm, 21 % grafting.

Acknowledgements.

The authors thanks to Francisco García, Luis Miguel Valdes, Luciano Diaz and Martin Cruz, from ICN UNAM for technical support and to the project CONACyT 280431: Laboratorio Nacional de Investigaciones en Forense Nuclear, for the support in the analysis of present studies.

INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

Particulate β-Sheet Nanocrystal-Reinforced Supramolecular Elastomers

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Akon, Ohio 44325, USA

Many synthetic supramolecular thermoplastic elastomers (TPEs) are analogs of natural silks in the sense that both types of materials contain β-sheet crystalline domains that serve to crosslink and reinforce the elastic network. However, one of the key differences between the synthetic and natural analogs is the aspect ratio of β-sheet crystals. The nanocrystals in silks are particulate, with the sizes in all three dimensions less than 10 nanometers (e.g., 2.1x2.7x6.5 nm^3 in spider dragline), while the crystalline domains in synthetic supramolecular TPE display fibrous morphology with the longest dimension ranging from hundreds of nanometers to micrometers (Figure 1).

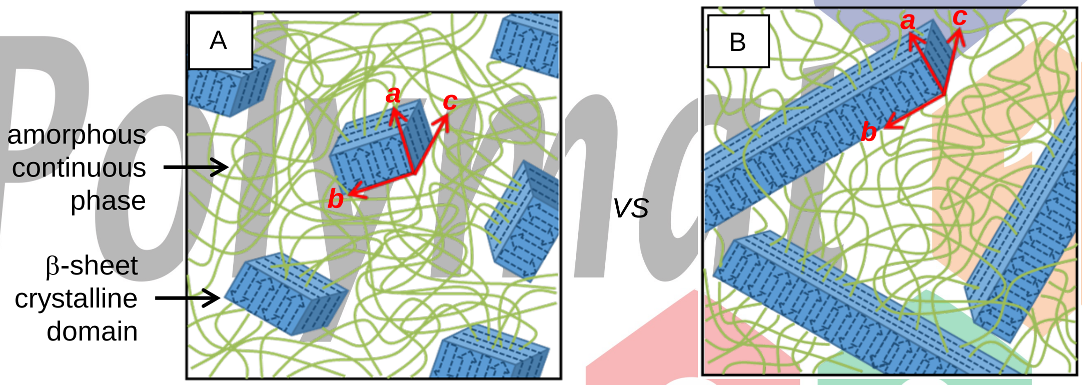

Figure 1. Schematic illustration of β-sheet nanocrystallites (A) and fibrous crystalline domains (B) dispersed in an amorphous phase. The *a*, *b*, and *c* axes correspond to the direction of covalent bonding, hydrogen-bonding, and β-sheet stacking, respectively.

To provide reinforcement, these crystalline domains must be strong and stiff. In order to attain the strength and stiffness at such a small length scale, it is necessary to use strongly associating molecular motifs. Thus, those capable of forming multiple cooperative hydrogen bonds are adopted by both nature and man. However, the strong association also provides a thermodynamic incentive for a high degree of association that exceeds the aforementioned nanometer scale. In silk, the size of the crystallites is generally believed to be attributable to their specific amino acid sequences. In the absence of specific amino acid sequences, how to achieve the nanometer size is an interesting challenge for synthetic TPEs.

In this presentation, I will first show that particulate β-sheet nanocrystals with the longest dimension well-below 100 nm can be attained without an elaborate amino acid sequence. The small size is attributed to the grafting topology. The topology renders a rapid increase of entropic loss as the degree of association increases to stop the growth of the β-sheet. Second, I will show that the particulate nanocrystals display a remarkable ability to simultaneously provide stiffness, extensibility, and strength to the synthetic elastic network and do so highly efficiently at a low volume fraction of the material. The herein studied butyl rubber-based thermoplastic elastomers containing 3.6 volume % of β-sheet nanocrystals are stiffer, stronger, and more extensible than vulcanized butyl rubber reinforced by 20 volume % of carbon black and poly(styrene-*b*-isobutylene-*b*-styrene) reinforced by >33 volume % of polystyrene domains. The high reinforcing efficacy of the β-sheet crystals is attributable to two phenomena associated with their small sizes, a stick-slip mechanism for energy dissipation and an auxiliary layer of polymer brush that contributes to increasing the modulus.

N-heterocyclic carbene complexes derived from theobromine for antitumor drugs

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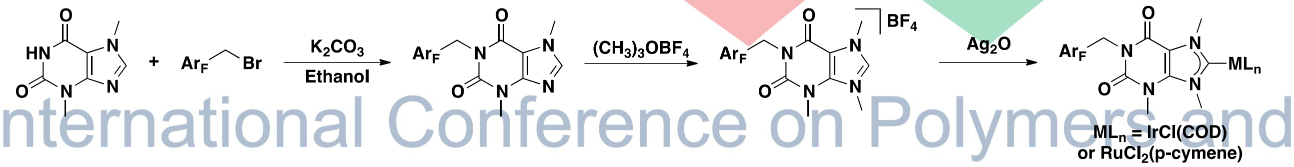
The design and development of new drugs, more active and with less side effects, is commonly achieved by optimizing the structure-activity relationship (SAR). In this sense, the use of transition metals for pharmacological application has been of interest in the past years. Among them Pt is probably one of the most known and studied, because of its high anticancer activity. Up to this moment, three compounds based on Pt have been employed as chemotherapeutic agent, namely cisplatin, carboplatin and oxaliplatin. However, the use of these drugs has been related to several side effects, such as infertility, alopecia and anemia. In order to overcome these drawbacks, many research groups have focused their efforts on developing new compounds based on others transition metals. In this regard, Ru has emerged as a good alternative to Pt since Ru is cheaper and exhibits slow ligand exchange rate. Currently, there are two ruthenium species in clinical trials and there is a great effort in the study of the mechanism and interaction of these species with DNA.[1,2]

Following our interest in the development of novel antitumor drugs, we envisioned that by combining the biological activity of theobromine with the antitumor potential of Ru and Ir complexes we could enhance the activity of their related drugs. In order to accomplish our purpose, we prepared a series of N-heterocyclic (NHC) complexes. As shown in **Scheme 1**, the complexes were synthetized in three steps. The first one allowed us the incorporation of fluorinated benzyl fragments in the backbone of the theobromine. The reaction of these precursors with trimethyloxonium tetrafluoroborate produced the corresponding azolium salts. Finally, the coordination to Ir and Ru was performed through a transmetallation reaction. The antitumor tests are currently developing in our laboratory.



Scheme 1

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A Simple Pathway to Perfect Nanoscale, Metallodendrimers

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Can supramacromolecular dendrimers be constructed from a series of simple polyfunctional monomers in one step and quantitatively? In fact, there are very few complex organic materials that can be assembled from a monomer in a one-step, assembly process. This initially started using simple, perfect polycarboxylates to be the counterions for different simple metalloconstructs; thus, generating a very accurate size, shape, and structure possessing only polyanionic counterions. This perfect aligned, directed structural rigidity and diverse modes of different metal connectivity have given interesting novel new avenues to the construction of three-dimensional, supramacromolecular materials predicated on similar, as well as dissimilar polytopic ligands. Over the last five years using simple architectures possessing preplanned directionality, a perfect entrée to the quantitative synthesis of precise macromolecular Archimedean architectures has been realized and subsequently shown to be able to spontaneously equilibrate under simple dilution conditions. The structural implications, based on controlling the concentration within the assembly process, will be demonstrated. The construction of novel 3D architectures will be confirmed; then the introduction of molecular fission/fusion will be introduced to demonstrate how this can lead to nano-scale unimolecular micelles, generated in quantitative yields.

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PHYSICO-MECHANICAL CHARACTERIZATION OF RECYCLE POLYMERES COMPOSITE WITH NATURAL FIBERS.

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In order to manufacture high-performance materials, natural fibers have been studied in recent years as reinforcement of composites, replacing mainly synthetic fibers [1], in fact it has been found that natural fibers are an attractive material for the High growth rate, low cost and good physical, mechanical and thermal properties [2] [3]. This work shows the effect of the fibers of guadua, fique and coconut with and without chemical treatment, using 5% sodium hydroxide and 15% as compatibilizer, on the physical and mechanical properties of a polymer matrix of polyethylene and polystyrene Reinforced with 10% and 20% fiber by weight. In order to achieve this, it was used Scanning Electron Microscopy (SEM) and mechanical tests of compression, flexure and impact to the composite, resulting in the observation of the adhesion of the fibers to the matrices, the homogeneity and the porosity of the compound, on the other hand, the incorporation of fique fibers generated an increase in the stiffness of the compounds, in turn the guadua fiber reinforced composite showed good flexural strength in isotropic and discontinuous distribution, while the samples reinforced with coconut fibers In the polyethylene compound generate an increase in the resistance to the compression and the impact, improving the deformation properties of the material. The treatment with sodium hydroxide cleans the surface of the fibers and significantly influences the mechanical properties, ultimately confirming the potential of natural fibers to be used as reinforcement in composite materials.

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POLYMERS FOR BIOMATERIALS APPLICATIONS

Harald D.H. Stöver, **Casey Gardner, Rachelle Kleinberger, Samantha Ros, Sheilan Sinjari, Nicholas A.D. Burke**

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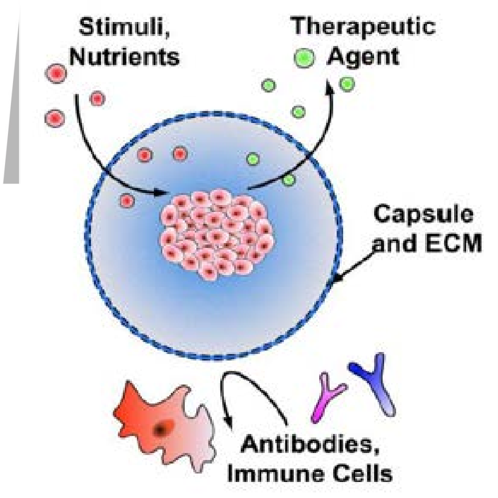
Synthetic hydrophilic polymers are promising building blocks for many emerging biomaterials applications. This talk will describe the design and use of reactive polyelectrolytes to form cell compatible hydrogels for cell transplantation and as model extracellular matrices.[1, 2, 3]



In particular, I will discuss the key role of such polymers in immuno-protecting transplanted cells in cell-based therapies of diabetes and other chronic endocrine disorder. This will include requirements for immuno-isolation of transplanted cells, and formation of hydrogels that can serve the diverse needs of this application. The talk will describe the central role of charges in these polyelectrolytes, and discuss different means of controlling anionic/cationic charge ratios and of introducing reactive groups to enable crosslinking in presence of cells.

In addition, I will outline emerging uses of synthetic spherical microgels as model extracellular matrices to probe cell-cell interactions.

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EFFECTS OF THE SLIP CONDITIONS ON THE PULSATING FLOW OF BLOOD WITH CHOLESTEROL

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Abstract: 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 oscillating flow is assumed to be of small amplitude and can be adequately represented by a weakly stochastic process, for which a quasi-static perturbation solution scheme is suggested, in terms of a small parameter. This flow is analyzed with the Tanner constitutive equation model with the viscosity function represented by the Reiner-Philippoff model. 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 TRF 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 to the material properties in the system.

Keywords: Pulsating and Oscillating pipes, Stochastic Noise, Tanner and Reiner-Philippoff constitutive equation, Perturbation solution, analytical solution

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Hybrid hydrogel based xylan polysaccharide matrix for immobilization and growth of fibroblast cell

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Fibroblasts are ubiquitous cells that constitute the strom of virtually all tissues and play vital roles in homeostasis [1]. However, some applications of free fibroblast are still hindered due to their difficulties in separation and reuse as well a slow stability upon exposure to heat, extreme pH values and organic solvents [2]. Both poly(2-hydroxyethyl methacrylate) (PHEMA) and polysaccharides has been widely studied to be suitable materials as matrices for cell immobilization [3]. Under this perspective, ceramic/polymer hybrid scaffolds offer improved mechanical properties and biological activity compared to a ceramic or polymer material alone [4].

In this study, a hybrid hydrogel was prepared by chemical crosslinking in two steps with the intended use of cell immobilization and growth. Firstly, the xylan-type hemicellulose was functionalized with acryloyl chloride in order to introduce vinyl groups. In the second step, the functionalized xylan was mixture with different quantities of mesoporous silica SBA-15 and 2-hydroxyethyl methacrylate (HEMA), the vinyl groups in xylan and HEMA were crosslinking by free radical polymerization. The effects of SBA-15 and HEMA concentration in the structure, mechanical properties and hydrophobicity of the hydrogels was characterized as well as, and the viability, proliferation, adhesion and morphology of fibroblast was also investigated.
The FTIR and RMN characterization showed, the presence of xylan, HEMA and SBA-15 in the hydrogel. According the rheological analysis, SBA-15 enhanced the mechanical properties and also favored cell adhesion and proliferation.

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

Non-covalent interactions in Polyaromatic N-Heterocyclic Carbenes. Catalysis and Host-Guest chemistry

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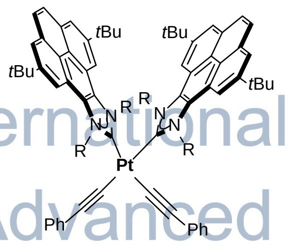
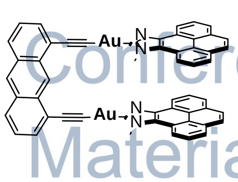
In the course of our most recent research, we demonstrated how homogeneous catalysts with polyaromatic functionalities possess properties that clearly differ from those shown by analogues lacking these polyaromatic systems. The differences arise from the ability of the polyaromatic groups to afford non-covalent interactions with aromatic molecules, which can either be substrates in a homogeneous catalysed reaction, or the same catalysts to afford self-assembled systems.[1] This presentation summarizes all our efforts toward understanding the fundamental effects of π-stacking interactions in homogenous catalysis, particularly in those cases where catalysts bearing polyaromatic functionalities are used. The study reveals several important implications regarding the influence of ligand-ligand interactions, ligand-additive interactions, and ligand-substrate interactions, in the performance of the catalysts used.[2] The nature and the magnitude of these supramolecular interactions were unveiled by using host-guest chemistry methods applied to organometallic catalysis.[3]

The development of a wide variety of N-heterocyclic carbene ligands with extended polyaromatic functionalizations also allowed us to prepare a large variety of metallo-supramolecular complexes, including metallotweezers,[4] metallo-rectangles,[5] metallo-folders[6] and bowl-shaped metallo-structures.[7] Depending on their structural features, these species were used for the recognition of a variety of organic substrates, such as electron-deficient aromatic substrates, polycyclic aromatic hydrocarbons and heavy metal cations.



Metallo-folder



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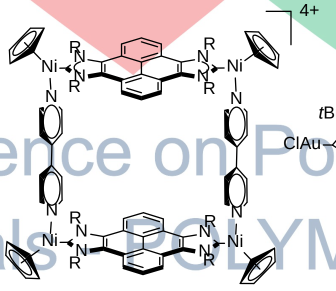

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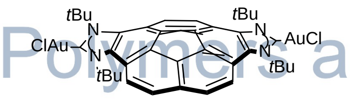

metallo-bowl

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INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

Formation of Molecular Hydrogels and Marginal Solubility

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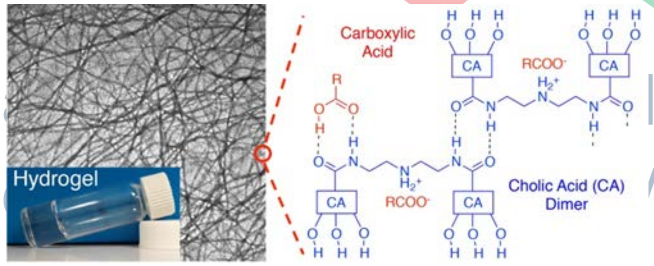
Molecular and polymeric hydrogels are useful materials for a variety of applications including the biomedical and pharmaceutical fields. Bile acids are natural compounds exist in the body of human and most animals. In their salt form or after suitable chemical modifications, they can interact with each other in a specific solvent to form gels with self-assemble fibrous network, thus the molecular gels. Cholic acid, a primary bile acid, was connected covalently through a secondary amine link to form a dimer which can bind with a series of carboxylic acids in water to form hydrogels though acid-base interactions and hydrogen bonding. This dimer is sparingly soluble in water but shows improved solubility upon the addition of selected carboxylic acids. Under conditions of a marginal solubility of the complex, they form monodisperse nanofibers in water at a stoichiometric ratio. These nanofibers are separated at low concentrations but entangle with each other at high concentrations to form hydrogels with well-dispersed and randomly-arranged 3D fibrous networks. Alternatively, sparingly soluble bile acids may form molecular hydrogels with added bases and water-soluble bile salts will become less soluble when acidified and form hydrogels. This work points to the conditions needed for gelation in water. The molecular hydrogels may be potentially useful in tissue engineering, cell culture, and mechano-optical sensing.



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CRACK INITIATION AND PROPAGATION UNDER CONSTANT DISPLACEMENT LOADING USING CT SPECIMENS, FOR THE POLYMERS ABS AND PMMA

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Crack initiation and propagation tests have been carried out under constant displacement loading on two polymeric materials: ABS (Acrylonitrile Butadiene Styrene) and PMMA (Polymethyl methacrylate), using the CT (compact tension) specimen according to the ASTM E647-00 Standard. A self-constructed equipment has been used for the constant displacement loading at the frequency of 0.25 Hz and a maximum displacement of 380 mm. The stress intensity factor has been obtained for different characteristic crack dimensions "a" for the two polymeric materials; furthermore, from the obtained stress intensity factors was evaluated the energy release rate G for the corresponding experimental tests. Finally, the fracture surfaces were analyzed by scanning electron and optical microscopes in order to investigate the general causes at the origin of crack initiation and propagation under the described loading conditions.

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ULTRASONIC FATIGUE TESTS ON METILMETACRYLATE POLYMER USED IN THE MEDICAL INDUSTRY

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Ultrasonic fatigue tests were carried out on PMMA polymer material, which is used for dental applications. The resonance condition was obtained by the numerical simulation and modal analysis of finite elements and the ANSYS-15 software, which allows determining the dimensions of the hourglass shape for the test specimen. The manufacturing process of this polymer was also performed to control the properties of the test material. Fatigue tests were applied on a patented ultrasonic fatigue machine (patent no. 323948, 2014, Mexico), which was developed by Dr. Gonzalo Domínguez Almaraz and is characterized by a new and simple test control using the LabVIEW platform. The test specimens were immersed in a solution to simulate the effect of the spittle with the corresponding pH and to limit its temperature degradation under the very high frequency load. Thermographic analysis has been implemented in order to control the test temperature in real time. Finally, the ultrasonic fatigue strength was determined for this polymer material together with a general investigation of crack initiation and propagation under the described conditions of the test.

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Acknowledgements: We want to express our gratitude to the University of Michoacan in Mexico (UMSNH) for the facilities received in the development of this study.

DEVELOPMENT AND VALIDATION OF A MODEL OF THREE POINTS BENDING IN ULTRASONIC FATIGUE OF NAFION MEMBRANE 115.

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In order to carry out ultrasonic fatigue tests on the Nafion 115 proton exchange polymer membrane, a mechanism was fabricated to hold the membrane at two points, which in turn required calibration of the displacement against the initial stress applied by the punch in charge of completing the three points flexion in the ultrasonic fatigue machine. During the experimental tests, ultrasonic fatigue was investigated under the three-points flexural modality in the Nafion 115 proton exchange polymer membrane used in fuel cells. The test temperature was controlled with aim to restrain this parameter (the highest testing temperature was 60°C), keeping this parameter high below in regard the glass transition temperature of this material (110 ° C). Experimental results show that the fatigue strength under this modality is close to half a million cycles for 0.478 MPa of applied load; this mechanical property is close to 5.5 million cycles when the applied load decreases to 0.468 MPa.

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Lithium (poly)pirazolylaluminates

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On the search of bimetallic systems that induce cooperative effects in homogenous catalysis, poly(pyrazolyl)aluminates and related aluminates seem to be attractive candidates. As poly(pyrazolyl)borates, they would be easily tune in terms of steric and electronic requirements through appropriate substituents on the pyrazolyl rings and on the aluminum center.[1] Although the first report on such a ligand system dates the seventies,[2] it was not until a few years ago that our group reported the first authenticated sodium poly(pyrazolyl)aluminate with Al–CH_3 bonds.[3] More recently, a series of aluminates with Al–H bonds were reported,[4] aiming to transfer the aluminate to different metal halides. The tris(pyrazolyl)aluminate $[\{Li(THF)\}\{Al(Ph_2pz)_3H\}]$ was only successfully transferred to a Zn center, but with undesirable hydride transfer from aluminum to zinc giving $[\{ZnH\}\{Al(Ph_2pz)_3H\}]$. Other metal halides gave bimetallic pyrazolates, $[M_2X_2(Ph_2pz)_2(THF)_3]$ with M = Mg, X = Br; M = Co; X = Cl. As well as the first row transition metal halides of Mn, Fe, Ni, and Cu produced intractable powders. A better performance of the poly(pyrazolyl)aluminate ligand system might be achieved using alkyl groups on the aluminum center instead of hydrogen to prevent hydride transfer, and electron richer transition metal centers. Another interesting aspect that emerged during our investigations on sodium poly(pyrazolyl)aluminates is the identification of C–H interactions to the metal center by X-ray crystallography that seem to play an important role in the assembly of infinite polymers, dimers and stabilization of reaction intermediates.[5] Herein we disclose the synthesis and characterization of the lithiumbis(pyrazolylaluminates) $[Me_2Al(^tBu_2pz)_2Li(THF)]$ (**1**) and $[^iBu_2Al(^tBu_2pz)_2Li(THF)]$ (**2**) that apart from their potential to prepare new complexes with transition metals trough the transfer of the aluminates, offer an opportunity to study an isolated (C–H)···Li agostic interaction in discrete complexes. The previously DFT calculations of **1** are used as a context to highlight the importance and role of the agostic bonding to stabilize the lithium center.[6]

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Fotoacoustic method for evaluation of starch biofilms

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One a day, edible and biodegradable packaging and coatings represent a broad field of application for polymers in response to the need to prolong the shelf life of foods and keep them in good conditions One of the polymers most used for this purpose is the starch, due to its availability, low cost and ease of handling in thin films [1]. The addition of plasticizers in the starch-water mixture in filmmaking enhances the flexibility of the material by reducing intermolecular forces [2].

On the other hand, the photoacoustic is a versatile methodology that can be used for the rapid and correct characterization of thin biofilm. The principle of this method is the generation of acoustic waves that provoke the vibration of the sample giving rise to temperature variations and pressure fluctuations in the sample [3].

The behavior of biofilms exposed to the photoacustic can be related with its composition and physical properties. In this work, corn starch biofilms were prepared with glycerol as plasticizer. The biofilms were characterized in its mechanical properties and water vapor permeability, using traditional mechanical methods and a closed photoacoustic cell.

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Synthesis and electrochemical characterization of bismuth vanadate thin film produced by co-sputtering

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Semiconductors based on bismuth oxide present a band gap in the visible light, these materials are candidate for photoelectrochemical applications, and one of the most important uses is as photoanodes for water splitting for H_2 generation.

We report the synthesis of bismuth vanadate (BiVO4) thin films deposited by reactive magnetron co- sputtering; metallic vanadium and bismuth oxide (Bi_2O_3) targets were used to deposit vanadate bismuth on FTO (fluorine doped tin oxide), glass (fused silica) and silicon substrates. In order to obtain the monoclinic crystalline phase [1], it was necessary to heat the samples at 400°C in static air for 2 h. The X-ray diffraction results confirmed the formation of the monoclinic $BiVO_4$ phase. The optical and electronic properties of the films were evaluated by UV-Vis spectrometry and Mott- Schottky plots, finding that the optical band gap is ~2.5 eV and the films presented an n-type conductivity with a flat band potential of -0.56 V.

Moreover, we deposited three different thickness (170, 200 and 250 nm) because it is important to find the optimum thickness for maximum photocurrent that was of 1.16 mA/cm^2 at 1.23 V vs NHE for the film of 250 nm.

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The influence of hydration degree of sodium montmorillonite on the flexural strength, conversion degree and rheological properties of Bis-GMA/TEGDMA resin

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In this work nanocomposites were prepared using a mixture of Bis-phenol A glycidyl methacrylate and triethylene glycol dimethacrylate (Bis-GMA/TEGDMA, 70/30 w/w, Resin) and sodium montmorillonite (MMT) as inorganic filler in concentrations of 0.1, 0.2, 0.3 and 0.4 phr. Two groups were prepared: the first one by adding hydrated MMT to the resin (Resin-hMMT) and the second one by adding clay slurry to the resin (Resin-sMMT). The properties of these two groups were compared with the control group (Bis-GMA/TEGDMA without clay). The mechanical properties (flexural strength and flexural modulus) have been evaluated according to the established standards for dental materials application; the conversion degree of nanocomposites based on Bis-GMA/TEGDMA by FTIR; the state which the clay sheets are found in the polymer matrix has been studied by using XRD; the morphology of the nanocomposite has been analyzed with SEM and finally the interaction of the clay sheets with the polymeric matrix through rheological tests. For both groups (Resin-hMMT and Resin-sMMT) at a concentration of 0.3 phr and 0.2 phr, in the flexural strength tests, there were increases of 34% and 41% respectively, without significant variation in the flexural modulus. The values obtained for the conversion degree were higher with respect to the control at all concentrations and both groups except at a concentration of 0.4 phr for Resin-hMMT, this fact showed that there was no interference of the clay particles in the polymerization process [1]. For a concentration of 0.3 phr for the two groups the results obtained by XRD showed that Bis-GMA/TEGDMA can penetrate the interlaminar space of the MMT causing a polymer intercalation in the clay sheets [2]. Scanning electron microscopy exhibited a rough surface for the two groups containing 0.3 phr of clay, indicative of an electrostatic interaction between the nanoparticle and the polymer [3]. Similarly, rheological tests also showed that there is an interaction between the clay and the polymer matrix due a better distribution and dispersion of the nanoparticle.

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Rheological properties of starch from different sources for industrial application

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Starch is the most important polymer in the industry because of its easy production and physicochemical properties. This polymer is the second most abundant in the nature and its applications range from the food industry, pharmaceutical, chemical, sanitary, coatings, paints and biodegradable packaging among others [1, 2]. The main sources of starch are: corn, wheat, and rice, however, these are too the most important cereals in the world for the feeding of the population. Therefore new sources of starch are still the object of researches.

The starch have interesting physicochemical properties that affect the behavior of products. Some of these properties are: thickening capacity, gelling, high water absorption capacity, stabilizing function, emulsifying faculty, and increases of viscosity in solutions [2]. The rheological properties are related whit functionality of starch and industrial applications.

Therefore, in this work starches from diferent botanical sources were extracted. The isolate method was neutral to avoid the damage to the native structure of the starches. The starches were characterized in its pasting and rheological properties. The results show dependence of viscosity by shear rate and temperature, this behavior is similar to report in other researches [3]. To model the behaviour of starch the power law was used. The general behavior of starches gels was pseudoplastic.

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Combination of periodontal ligament mesenchymal stem cells and chitosan, lysine and polyurethane scaffold promise for cartilage repair

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Introducction

Osteoarthritis is a degenerative joint disorder commonly found in clinical practice, and is the leading cause of disability in the elderly [1]. New biological therapies that can effectively treat joint degeneration. In that sense the combination of stem cells isolated from periodontal ligament of oral cavity are considered a promising candidate for cartilage regeneration, due to their self-renewal capacity and potential to differentiate into chondrocytes, as well as other cell types [2] Scaffolds containing Chitosan/PU/lysine in the following ratios have been manufactured by freeze drying. 100/0/0 to 50/50/80. Periodontal ligament stem cells were isolated from impacted third molars of young healthy donors; anti-body CD44 and anti-body Stro-1 [2] was positive and anti-body anti human CD45 negative have been used as phenotype markers and live and dead assays have been used for viability assay and MTT for proliferation at different periods of time, the construct were cultured by 21 with chondrogenic medium and analyzed by histology with alcian blue staining [2]

Results

A significant increase in cell viability and proliferation could be observed in lysine containing scaffolds. This study confirms that lysine may act as a favorable substrate for cell adhesion and proliferation, the constructs was positive for alcian blue staining.

Conclusion

The combination of lysine-polyurethane scaffolds and periodontal ligament stem cells offer a promising alternative for the development of construct for tissue regeneration in osteoarthritis.

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Synthesis of poly(N,N-dimethylacrylamide-co-2-hydroxyethyl methacrylate) hydrogels.

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Many contaminats from wastewater have a negative impact on health and environment, even in low concentrations. Several methods had been proposed for their removal, one of them is using hydrogels as adsorbents for wastewater treatment[1-4]. In this work, we describe the hydrogel swelling behavior of a non-ionic copolymer of N,N-dimethylacrylamide and 2-hydroxyethyl methacrylate copolymer (poly(HEMA-co-DMAa)), as function of pH and temperature. Detailed characterization of the crosslinked copolymer and its hydrogel structure were performed; after the synthesis, polymerization was confirmed by FTIR spectroscopy. Swelling measurements on cylindrical-shaped dried hydrogels (approximate dimensions: diameter 4.34 mm; long 19.4 mm; weight 309.2 mg) were been and the effect of pH and the temperature on the swelling properties was studied. The results showed that LCST of poly(HEMA-co-DMAa) hydrogel was to 321 K and a complex was formed at pH = 8; and charged species promoted an increasing in hydrogel water content at pH above or below this value. FTIR spectrum corroborated hydrogel stability. In conclusion, a promising smart hydrogel able to uptake contaminats in a wide range of pH was obtained, and the design of this novel hydrogel was based on the non-toxicity of HEMA and the overall stimuli-responsive behavior of DMAa; additionally, the poly(HEMA-co-DMAa) hydrogels would have less environmental impacts due to their biocompatibility and non-cytotoxicity.

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Grafted poly(ethylene) for thermo-responsive controlled drug delivery

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Polymers are macromolecules formed by smaller particles called monomers and are classified (among several classifications) in natural, semi-synthetic and synthetic but another important class with increasing significant application can be added: smart polymers which encompasses a wide spectrum of different compounds with unique potential [1-2]. The feature that made these polymers "smart" are their ability to respond to slight changes in the surrounding environment such as temperature, pH shift, increase ionic strength, electric and magnetic field, light and others; also, its uniqueness is not only in the physical changes they present (shape, surface, solubility, sol-gel transition, etc.) but also these being reversible [3].

Low density poly(ethylene) (LDPE) is highly hydrophobic because of this, is difficult to be combined with other polar polymers which is why ideally its surface should be chemically modified. Surface enhanced for polymers graft has become a powerful lookout in order to adapt the chemical and physical properties of interfaces for a desire application giving advances and knowledge to surface and interface science [4].

In the present work, the chemical modification of a LDPE thin film using grafting a copolymer of DMA-co-VCL at different molar relationship in order to create a new smart polymer is presented; the modified LDPE is used for the controlled delivery of a selected drug. [5-6]

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Green synthesis of metallic nanoparticles using *Paulownia tomentosa* and their antibacterial activity

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The application-based study of noble metals nanoparticles has received great attention, among them the silver nanoparticles (AgNps) have a significant consideration nowadays, even emerging areas as biomedicine suggest that among different nanoparticles, silver nanoparticles owns a relatively safe use in medicine due to its healing, anticancer, antibacterial and antimicrobial potential.[1-5] AgNPs ought to be synthetized by various methods such as chemical, physical or even biologicals; leading capping of different (even toxic) chemicals species on the nanoparticle surface, affecting adversely in biological applications.[2-4] Due to the environmental impact implied in the synthesis of these materials a cost-effective, safe and environmental friendly sound alternative method, a "greener" one that use eco-frinedly reactants such as leafs and flowers extracts with inherit reducing capacities.[3]

For green synthesis of AgNps from silver nitrate ($AgNO_3$), leafs of *Paulownia tomentosa*, a deciduous, fast growing, hardwood tree native from China, were used and different synthesis conditions were studied in size distribution and morphology of the formed nanoparticles.

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METAL CHELATION IN MEDICINE: EVALUATION OF THE MACROMOLECULAR CONTRAST AGENT FIBPEP-(GD-AAZTAC$_4$COOH)$_4$ FOR THE PRECOCE PROSTATE CANCER DIAGNOSTICS

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Noninvasive *in vivo* detection of fibrin using diagnostic imaging modalities may improve clinical decision on possible therapeutic options in atherosclerosis, cancer and thrombus-related pathologies [1,2]. The aim of this study was to assess the potential of a novel contrast agent derived from AAZTA (6-amino-6-methylperhydro-1,4-diazepine tetraacetic acid) [3] ligand possessing a pendant pentanoic acid radical conjugated with the fibrin-binding peptide (FibPep). These macrocomplex was used to visualize thrombi in mices using magnetic resonance imaging (MRI). The longitudinal paramagnetic relaxivity (r_{1p}) that can be interpreted as the efficiency for generate contrast, was 79.1 Mm^{-1}.s^{-1} at 20 MHz. This value is significantly higher in comparison (9.4 mM^{-1}.s^{-1}) with the precursor ligand, AAZTAC$_4$COOH, in the same magnetic field. The *in vivo* results demonstrated that this new contrast agent have higher affinity to bind to fibrin clots originated from prostate tumors, in comparison with the controls one (healthy prostate). Besides, these results demonstrated that this new probe is highly sensible to detect prostate cancer, cell line PC-3 (normally present in the more advances evolution stages of the metastasis) in mices. The results show that after 6.0 min was possible clearly visualize the region affected by the tumor. Besides, this contrast agent is rapidly eliminated (after 60 min), principally through the kidneys. Moreover, the *post-mortem* studies, realized by the quantification of residual metal on the organs was realized using ICP-OES, and confirmed that the majority concentration of the gadolinium was eliminated trough renal excretion. Therefore, given the results is possible to conclude that the macrocomplex, FibPep-(GdAAZTAC$_4$COOH)$_4$ may provide a new tool to precoce prostate cancer diagnostics by MRI tomography.

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DISEÑO DE UN DISPOSITIVO PARA LA FABRICACIÓN DE ESPUMAS METÁLICAS DE ALUMINIO POR EL MÉTODO DE INFILTRACIÓN

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Se ha definido a una espuma metálica como cualquier tipo de material metálico que contiene poros, estos tipos de materiales presentan una interesante combinación de propiedades, tales como alta rigidez, baja densidad, aumento de absorción a la energía de impacto, etc. Existen diversos métodos de fabricación: pulvimetalurgia, espumado de metal fundido, infiltración de preforma, etc. [1]. En este trabajo se diseñó un dispositivo para fabricar espumas de aluminio por el método de infiltración de una preforma de NaCl. Este dispositivo consiste en una cámara donde se lleva a cabo la infiltración, una boquilla de inyección de gas, un sujetador y una cuchara que sostiene al dispositivo como tal, el NaCl usado como material para la preforma presenta tamaño de partícula de 2 mm y 4 mm. Los resultados obtenidos fueron espumas en excelentes condiciones y con buenas propiedades, teniendo densidades que van desde 0.95 a 1.01 gr/cm^3.

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MATERIAL PROPERTIES OF THIN FILMS BASED ON PEROVSKITES /BFO/ USING THE METHOD OF SPRAY PYROLYSIS FOLLOWED BY USE OF ANNEALING WITH CO2 LASER

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$BiFeO_3$ (BFO) is the only known material that presents ferroelectricity and antiferromagnetism at the same time and under normal conditions of pressure and temperature. The Curie transition temperature is high (T_C = 1103 K) as well as the Neel temperature (T_N = 643 K). In addition, these two properties interact mutually, which turns the material into a magnetoelectric material. Antiferromagnetism is not perfect so there is weak ferromagnetism. This feature suggests various applications such as information storage devices. However, there are a number of technical difficulties to be solved, including the difficulty to synthesize the pure phase since some secondary phases such as $Bi_2Fe_4O_9$ and $Bi_{25}FeO_{39}$ are typically present. In this work thin films of BFO were prepared by spray pyrolysis followed by a heat treatment applied with a CO_2 laser to nucleate the BFO phase. The use of the laser allows to accomplish heat treatments in tiny areas as well as localized tempering. This versatility of the laser allows to modify in many ways the transformation kinetics in the crystalline phase of the films. As a result of this work the production of the BFO phase by the application of the laser is shown along with the corresponding microstructure in the films.

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MATERIAL PROPERTIES OF THIN FILMS BASED ON PEROVSKITES USING THE METHOD OF CENTRIFUGATION FOLLOWED BY USE OF ANNEALING WITH CO2 LASER

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Material properties of thin films of perovskite have recently been intensively studied, due to the large potential of this material in the field of solar energy, photocatalysis, etc. Solid films are widely used as a transparent material of n-type conductivity and a hole blocking layer in perovskite solar cells. These elements are the most researched and promising, in particular due to the rapid increase in the coefficient of efficiency (efficiency) from 3.8% to 19.3% over the past 5 years [1, 2]. Essential for perovskite solar cells is the formation of a thin film with a low level of pores (cracks) of a nanometer size, which helps to reduce recombination losses and improve efficiency. In this paper we present a method for depositing a continuous thin perovskite film for use in solar cells, including centrifugation of the perovskite precursor followed by laser annealing with CO2 laser radiation at a wavelength of 10,6 µm. The effect of laser annealing on the grain size in the thin film and the centrifugation rate on its thickness was studied. Laser annealing is a constantly growing new technology, which is increasingly used in micro- and nanoelectronics. Laser annealing can lead to better crystallinity, lower surface roughness, larger grain size, better uniformity, reduced recombination centers, and increased continuity. Thus, effectively matched parameters of laser radiation can improve the characteristics of solar cells.

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Systematic Hydrophobic Modification of Starch with Commercially Available Substituted Succinic Anhydrides and Maleated Vegetable Oil

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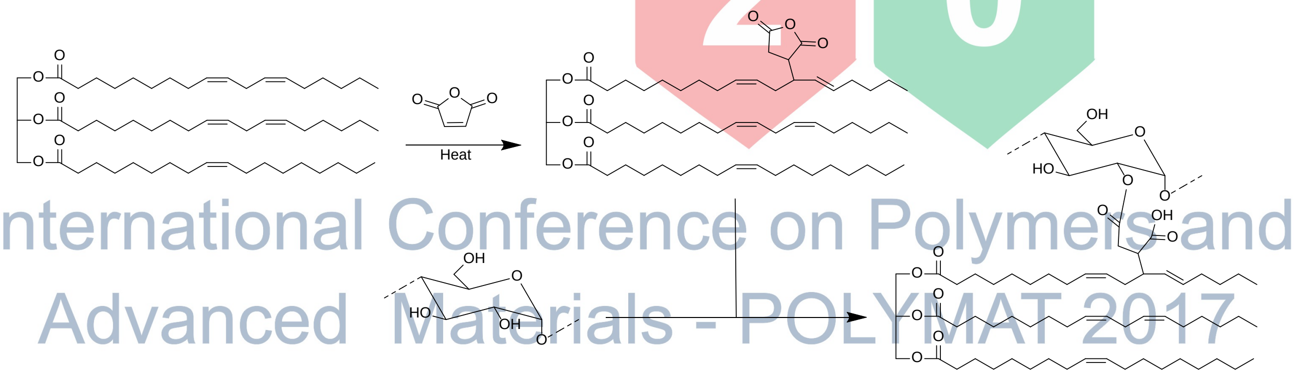
Starch, as the second most abundant biopolymer, is a cost efficient, readily available and renewable carbohydrate. Native starch is composed of amylose and amylopectin forming granules that are non-dispersible in cold water. Cooking of the starch, a process known as gelatinization, breaks down the granule structure, allowing the dispersion of free polymer chains in solution. After gelatinization the starch chains are more readily available for chemical modification. The addition of a substituted succinic anhydride to starch can introduce hydrophobic character due to the presence of alkyl chains or aromatic rings, and an anionic group results from opening the anhydride group. The modification of starch allows tailoring of its properties. Substituted succinic anhydride-modified starch has found uses in food and industrial applications. A drawback of these materials is that they are partly derived from petroleum products.

This presentation focuses on the synthesis of novel vegetable oil-modified starch products. The synthesis of maleated vegetable oil was first investigated by different methods and experimental conditions; it was then optimized to tailor physical properties and functionality of the resulting products. Second, the reactivity of maleated vegetable oil with starch was compared with that of commercially available substituted succinic anhydrides. Starch modification was completed in slurry reactions, in a melt mixer, and in a twin screw extruder. The products were characterized by ^{1}H NMR spectroscopy and gel permeation chromatography.



Synthesis of maleated vegetable oil and its reaction with starch.

INTERACTION STUDIES OF FUNCTIONALIZED PAMAM DENDRIMERS WITH SOMATOSTATIN-14

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Somatostatin is a peptide with hormonal activity. It has natural antiproliferative action, therefore could be used in antineoplastic therapy [1]. This effect can be improved by conjugation of cytotoxic drugs in one of its amino acids [2]. However, their poor half-life due to their susceptibility to enzymatic degradation in the biological environment limits their use.

To overcome this problem, it is possible to use nanomaterials as nanocarriers with the aim of protecting these molecules and they have their pharmacological action successfully. Within these materials polyamidoamine dendrimers (PAMAM) are the most versatile. Their structure consists of polyamidominas and primary amines on their surface, that gives them unique chemical characteristics and allows their modification through simple reactions. However, it is necessary to functionalize their surface with harmless molecules because under physiological conditions the positive charge of PAMAM generates non-specific cytotoxicity [3, 4].

In order to generate a supramolecular complex with antitumoral activity, fourth generation PAMAM dendrimers were functionalized with polyethylene glycol and folic acid and the interaction of these nanomaterials with somatostatin-14 was studied. The characterization of the nanocarriers was carried out by ^{1}H NMR spectroscopy and the cytotoxicity of the functionalized PAMAM were evaluated at different concentrations in HEK cell cultures. In addition, the interactions were analyzed by NOESY NMR and fluorescence spectroscopy.

These results showed that the functionalization with polyethylene glycol and folate was about 50% of the surface amines and they are non-toxic at the different concentrations studied. On the other hand, the NOESY spectra ratify the interaction between the peptide and the modified dendrimers and the fluorescence studies indicated that the functionalization of PAMAM increased the association between the dendrimers and the peptide compared to unmodified PAMAM. Therefore, these results show the possibility of generating a complex with pharmacological application. Already known these interactions will be possible to determine how they are affected if a cytotoxic drug is conjugated to the peptide later.

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USE OF MODIFIED CLAYS AND CLAY-POLYMER MATERIALS FOR TRICHLOROPHENOL SORPTION

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Due to the problem generated by trichlorophenol as pollutant in aqueous effluents, this work proposes the use of modified clays and clay-polymer materials for the adsorption of this compound. For this purpose, composites were synthesized from a natural bentonite from the Puebla-Tlaxcala region, modified with a cationic surfactant Hexadecyltrimethylammonium (HDTMA), and a commercial montmorillonite type bentonite, modified with the surfactant Dimethyldialkylammonium (C14-C18), respectively, and both of them supported in an alginate polymer matrix. Synthesized composites were characterized by means of infrared spectroscopy (IR) and scanning electron microscopy (SEM).

In addition, kinetics experiments were carried out with clays and composites, and from the obtained results, it was verified that the Ho and McKay model was the one that best fitted the experimental data acquired. From this model, it has been found that the removal capacity for both materials, organoclays and the clay-polymer composites, increased when the mass/ volume ratio changed.

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PREPARETION AND CHARACTERIZATION OF SINGLE AND COAXIAL PLA-PROPOLIS MEMBRANES BY ELECTROSPINNING

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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 as the active agent in the fibers [1].

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Abstract preparation

Organic co-polymers with potential applications in solid-state organic

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Current trends in artificial lighting have boosted the demand for white organic light-emitting materials, because in most cases white-light emitting diodes are made of combination of individual compounds emitting in red, green and blue areas of spectrum. Organic luminescent materials are generally preferred over their inorganic counterparts owing to their low cost, solution processability, flexibility and etc. That is why they have found wider and wider applications in the field of artificial lighting, display systems and fluorescence bio-material tools. Although considerable progress has been made in this field, development of purely organic white-light emitting materials of simple structure still remains very urgent task.

Perinones are fused heterocycles traditionally used in the plastic industry as pigments and colorants. They demonstrate high thermal stability and uv-resistance because of their conjugated structure. However, frequently synthesis of the perinones required hush conditions. Recently, our group reported the new highly effective route to the synthesis of perinones under mild conditions. [1,2] Thus, a series of different perinones, including structures with polymerizable carbon-carbon double bond, has been obtained. Most of them were able to emit visible light quite intensively in solution, solid state and even being incorporated into the polymer chains via radical co-polymerization with such traditional monomers such as styrene and methyl methacrylate. The luminescence properties of the novel perinones and the co-polymers will be discussed in this presentation.

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SYNTHESIS OF FUNCTIONAL POLYISOBUTYLENE-BASED MATERIALS BY “CLICK” CHEMISTRY

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Poly(isobutylene-*co*-isoprene) (PII) copolymers have multiple applications due to their unusual physical properties. The range of properties displayed by these materials could be further expanded by introducing a low concentration of ionic moieties bound along the polymer chains, to produce ionomers. Unfortunately there are currently very few examples of ionomers derived from PII. “Click” chemistry techniques are interesting for polymer modification, because of their tolerance to different types of functional groups and their high yield. The synthesis of carboxylated PII derivatives with different alkyl chain lengths was achieved using thiol-ene “click” chemistry, by radical-promoted addition of carboxylated thiols (mercaptanoic acids) with different alkyl chain lengths across the 1,4-isoprene units of PII. The synthesis of quaternary ammonium, carboxylate, and sulfobetaine ionomers was also achieved from azidated PII substrates. The Cu (I)–catalyzed azide-alkyne [3+2] cycloaddition was successfully applied to couple alkynyl amines and carboxylic acid esters with azide-functionalized PII. Quaternization of the amine-functionalized PII with an alkyl halide produced ammonium ionomers, while sultones yielded the corresponding sulfobetaine derivatives. The different PII derivatives obtained were characterized by ^{1}H NMR and FT-IR spectroscopy. The conversion of the isoprene units reached 80-100%, depending on the reaction conditions used.

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SELF-IMMOLATIVE POLYGLYOXYLATES: STRUCTURE, PROPERTIES, AND FUNCTION

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The development of degradable polymers is of significant interest across a wide range of fields from coatings to nanomedicine and tissue engineering. Much progress has been made with conventional polyesters such as polylactide and polycaprolactone. However, the ability to control the degradation of these polymers in different environments is limited and they may degrade more rapidly or more slowly than desired. Many stimuli-responsive polymers have been developed over the past couple of decades, but these polymers typically require many stimuli-mediated events to achieve complete backbone degradation. This presentation will describe our recent work on polyglyoxylates, a new class of self-immolative polymers, that undergo end-to-end backbone depolymerisation in response to the cleavage of a single end-cap from the polymer terminus, thereby affording amplification of the stimulus-mediated event [1]. Polyglyoxylate properties could be tuned by varying the structures of the glyoxylate monomers to afford different pendant groups on the polymers or by performing post-polymerization functionalization. In addition, block copolymers could be prepared using linker end-caps having additional functional groups and these were assembled into stimuli-responsive nanoscale vesicles and micelles [2]. A diverse library of end-caps was developed that were responsive to stimuli including light, heat, pH changes, reducing agents, reactive oxygen species, and enzymes [3]. Unlike conventional stimuli-responsive polymers, it was possible to change the stimuli to which the system responded simply by changing the end-cap. The function of these polyglyoxylates was demonstrated through the incorporation and triggered release of drug molecules from surfactant-stabilized nanoparticles, micelles, and vesicles. In addition, polyglyoxylates were applied as coatings to release chemicals in response to stimuli. Overall, this work demonstrates the versatility and applicability of self-immolative polyglyoxylates across a range of fields.

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THEORETICAL STUDY OF A MULTI-THERMORESPONSIVE COPOLYMER CONSTITUTED OF N-ALKYL-SUBSTITUTED POLY(METH)ACRYLAMIDES

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Abstract: Multi-thermoresponsive triblock copolymers with tunable critical solution temperatures (LCST and UCST) can develop different inverse micellar states with a well-defined core-corona structure in aqueous dissolution only by temperature effect. Due to the above, in this work we explore the micellar states that exhibit the PEMA-b-PNIPMAM-b-PNNPAM triblock copolymer on watery environment employing dissipative particle dynamics (DPD) simulations and coarse-grained models. The dynamic behavior that exhibits the multi-thermoresponsive copolymer in aqueous environment was explored in detail on temperature interval of 280K-323K, Figure 1.

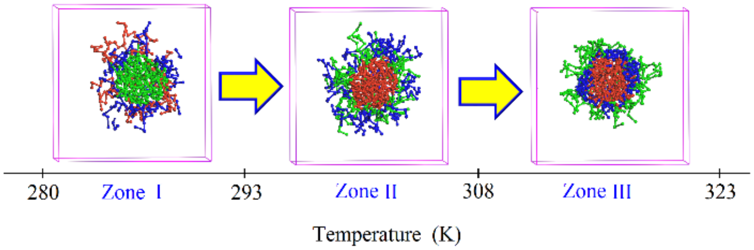

Figure 1. Snapshots of the micellar behavior generated during the thermal study: (a) polymeric micelle with PNIPMAM-core and corona double (PNNPAM, PEMA); (b) polymeric micelle with PEMA-core and (corona double PNNPAM, PNIPMAM) and (c) polymeric micelle with PEMA-core with PNNPAM-layer and PNIPMAM-corona.

The mesoscopic simulation outcomes reveal that the PEMA-b-PNIPMAM-b-PNNPAM copolymer exhibit three specific micellar states (core-shell) as a function of temperature, the micellar states are reversible totally. Finally, we conclude that our simulations can follow the kinetic behavior and micellar evolution in specific chemical environments by purely temperature effects.

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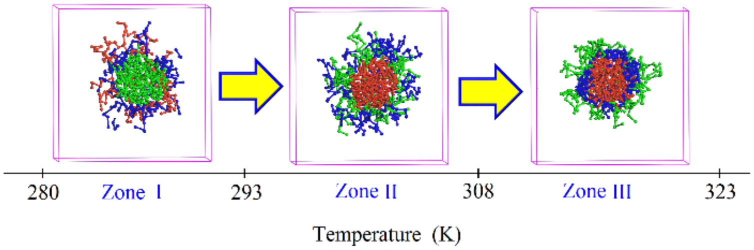
Abstract: Multi-thermoresponsive triblock copolymers with tunable critical solution temperatures (LCST and UCST) can develop different inverse micellar states with a well-defined core-corona structure in aqueous dissolution only by temperature effect. Due to the above, in this work we explore the micellar states that exhibit the PEMA-b-PNIPMAM-b-PNNPAM triblock copolymer on watery environment employing dissipative particle dynamics (DPD) simulations and coarse-grained models. The dynamic behavior that exhibits the multi-thermoresponsive copolymer in aqueous environment was explored in detail on temperature interval of 280K-323K, Figure 1.



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PREPARATION AND CHARACTERIZATION OF NANOCOMPOSITE HYDROGELS BASED ON ALGINATE, POLYVINYLPYRROLIDONE AND CARBON NANOTUBES

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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 [1]. 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_3/H_2SO_4 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 [2].

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Synthesis, characterization and kinetics of PMMA-SiO_2 Pickering emulsion polymerization

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Pickering emulsion polymerization, is a kind of emulsion polymerization which use the phenomena of Pickering stabilization discovered by the English chemist Spencer Umfreville Pickering where solid particles can reside at the interface of droplets and bubbles, thereby providing resistance against coalescence and Ostwald ripening [1] and has advantages over traditional methods since organic stabilizers are not needed, it does not require high energy inputs, allowing effortless scale-up for industrial applications and an excellent process to fabricate composite polymers particles armored with a layer of solid, potentially functional, small particles [2,3].

The underlying physics of these process has been studied and discussed from different perspectives, particle size, morphology and hydrophobicity and how these affects the final characteristics since current technology does not allowed armored latex with an overall solid content of over 50%, so there is a need for a thorough mechanistic understanding of the process [4].

In this work, PMMA-SiO_2 latexes, with different %w/w of SiO_2/PMMA, were synthetized by Pickering emulsion polymerization and characterized by structural and morphological techniques; also, a general mathematical model, with at least one adjust parameter [5] is presented in order to describe the kinetics of the process using new ideas on diffusion-controlled coefficients [6,7].

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

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In recent years, there has been an increase in the use of environmentally friendly materials, which translates into greater environmental awareness among the population and a greater demand for these materials, in particular polymer matrix composite materials, use natural fibers to reduce their environmental impact, their density and improve their specific properties [1]. In the present work, high density polyethylene (HDPE) matrix composites were prepared, which is a highly commercialized polymer. The composites were reinforced with agave fiber of the species *Agustifolia Haw*, from the bagasse generated by the mezcal production industry. The fiber was treated with a 5% NaOH solution before being introduced into the matrix, for improve the interfacial adhesion. It was tested with three different concentrations of the fiber: 5, 7.5 and 10% by weight. The composites were tested to evaluate their linear coefficient of thermal expansion at 35 ° C, according to the ASTM E831-14 standard. Regarding the matrix, a greater linear coefficient of thermal expansion was observed in the composites with 7.5 % of fiber; 7.7x10^{-2} and 8.3x10^{-2} μm mm^{-1} K^{-1}, respectively. While the composite with 5% and 10% fiber content, it presented a behavior lower to that of the matrix, 6.7x10^{-2} and 7.3x10^{-2} μm mm^{-1} K^{-1}, respectively. The increase in the thermal expansion could be attributed to the hydrophilic character of the fiber, which favors the dimensional changes, whereas the decrease in the thermal expansion can be due to a good adhesion between fiber and matrix, preventing the dilatation of the matrix [2].

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SYNTHESIS AND CHARACTERIZATION OF ALGINATE-/ORGANOPHILIC CLAY COMPOSITES FOR THE REMOVAL OF AZO-DYE FROM WATER

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In this study, two different sodium alginate (SA)/organophilic clay composites were synthesized to compare their adsorption capacity for the removal of an azo synthetic dye. Composites were prepared in aqueous solution of calcium chloride and with two different types of clay. The first one, a natural clay modified with a cationic surfactant, hexadecyl trimethylammonium bromide (HDTMA-Br); the second one, a commercial organomontmorillonite modified with a cationic dialkyl dimethylamine salt. Synthesized composites were characterized by means of infrared spectroscopy (IR) and scanning electron microscopy (SEM). Moreover, composites were employed in batch systems for the adsorption of Allura red-dye from solutions with different concentrations at 25 °C.

In addition, their adsorption kinetics and isotherms were evaluated. From these set of experiments, it was determined that the highest adsorption capacity for Allura red-dye was found for the composite with HDTMA-modified clay. In addition, adsorption kinetics process best fitted the pseudo-second-order model. Meanwhile, experimental data showed a better adjustment to the pseudo-second-order model (Langmuir-Freundlich) for both composites. Also, the adsorption process showed an intra-particle diffusion mechanism for the first system; whereas in the case of the second system, was the rate-controlling step. The obtained results suggest that composites could be effective adsorbents for the removal of anionic dyes from wastewater.

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Cyclodextrin-based supramolecular poly(N-isopropylacrylamide) hydrogels prepared by frontal polymerization

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Frontal polymerization (FP) was successfully applied to the synthesis of poly(N-isopropylacrylamide)-grafted-acryloyl-β-cyclodextrin supramolecularly crosslinked hydrogels. It was established that acryloyl-β-cyclodextrin (AβCD) allowed performing successful frontal polymerizations with N-isopropylacrylamide even in the absence of any covalent crosslinker, which is something generally required. This focus has been achived by exploting some paritcular proprieties of cyclodextrins (CDs): this molecules tend to aggregate in water giving rise to supramolecular structures [1], wich are exploited in lecterature to form supramolucular hydrogels [2]; is well know that poly(N-isopropylacrylamide) (PNIPAAM) can fit into the cavity of γCD giving rise to a polypseudorotaxane (PPR), but it cannot passthrough βCD or αCD [3]; isopropylamide group form an inclusion complex with βCD, it being able to enter the cavity but not to slide from one face to the other [4]. As a consequence CDs present just as pendant groups but cannot be threaded by the macromolecular chains, can give rise to supramolecular crosslinking by both effect of self-assembly and formation of the inclusion complex with the PNIPAAM isopropylamide group, without any formation of PPR.

The most interesting effect was observed on the swelling behavior of hydrogels. It was found that the swelling properties of the resulting hydrogels can be tuned by varying the amount of AβCD. Namely, when little amounts of this non-covalent crosslinker were used, superabsorbent hydrogels were obtained. Hydrogels containing a covalent crosslinker were also prepared for comparison. These latter exhibited swelling ratios that are much lower than the others. This fact clearly demonstrate that supramolecular crosslinking may be a great added value in frontal polymerization in that it allows obtaining stable fronts, prevents fingering formation and permits large swelling even in absence of ionic monomers.

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ELECTROSPUN MICRO AND NANOFIBRES OF ORANGE ESSENTIAL OIL AND POLYVINILIC ALCOHOL

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Electrospun micro and nanofibres were obtained from an emulsion of polyvinyl alcohol (PVA) at a concentration of 10% and orange essential oil at 4, 8 and 12% w/w). Scanning electron microscope images showed tubular, continuous fibers, whose diameters are dependent on the concentration of the PVA and orange essential oil. Fourier transform infrared spectroscopy indicated that the obtained fibers were composed of both components. The study demonstrated the potential to encapsulate liposoluble compounds in polymeric fibers using the electrospinning technique.

Electrospinning is a method of obtaining nanofibers [1]. The assembly for the execution of this technique consists of a capillary injector, through which a polymer solution its ejected [2] and a high voltage source that has two electrodes, one of which must be connected to the injector and the other directly to the collecting plate where the fibers are deposited [3]. The technique can be set up horizontally or vertically. The electrospinning technique allowed the formation of PVA nanofibers in which orange essential oil was encapsulated. Initially simply the possibility of forming PVA nanofibers was identified, after which it was found that the morphology of the nanofibers varied as a function of the concentration of PVA in the solution, presenting fibers with varying diameter of values between 0.1206 and 0.3599 µm.

The electrospinning technique permitted the encapsulation of orange essential oil in PVA microfibers, with an average diameter of PVA +4, 0.1638 ± 0.0002 µm; PVA + 8, 0.5261 ± 0.0002 µm and PVA + 12, 0.8091 ± 0.0002 µm. The encapsulation was verified by FTIR spectroscopy, highlighting the potential of the electrospinning technique through the identification of the double bonds corresponding to the unsaturation of orange essential oil. It was determined that the fibers obtained had a low water content since 99% of the solvent was evaporated during electrospinning.

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Manufacture and characterization of a polypropylene composite with waste ceramics from the investment casting process

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A new composite material was studied using virgin isotactic polypropylene [1] and waste ceramics [2-5] from the investment casting process. The base composition of the refractory is 80 %wt. of SiO_2 -Al_2O_3 (mullite), 16 %wt. of $ZrOSi_2$, among other compounds. The average particle size obtained was 170 μm. Additionally, a maleic anhydride compatibilizing agent was added to study the interaction of matrix adhesion and ceramic particles. The composite was made by obtaining pellet by extrusion at 200 °C at 150 rpm. Subsequently, it was injected in a temperature range of 220 to 250 °C to obtain specimens and obtain its mechanical properties and hardness according to ASTM. Characterization of the fracture surface was performed by scanning electron microscopy (SEM). The samples were also analyzed by X-ray diffraction (XRD), infrared (FTIR), thermogravimetry (TGA) and calorimetry (DSC). The results show that there is an effect of the residual ceramics in the polypropylene generating a reduction in its plastic behavior and maintaining its mechanical resistance. In addition, the presence of the α and β phases of the isotactic polypropylene was observed, where the percent crystallinity and crystal size were determined using the Scherrer equation.

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Effect of the amylose content on the mechanical behavior of starch biofilms

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Starch is an abundant polysaccharide found in nature. Physically, it is a complex granular structure that consists on crystalline and amorphous areas, which vary its shape in accordance to its botanical source. Starch is composed by two macromolecules: amylose and amylopectin. Amylose is a linear molecule formed by glucose units with α-1,4 linkages regulary represents 17 to 28% of the starch, whilst amylopectin represents 72 to 83%. Recent studies have demonstred that starch has the capacity to form films, this property is significantly interesting to satisfy the need to replace the no-biodegradable packings that represent a heavy ecological issue [1].
The content of amylose plays an important role in the formulation of biofilms based on starch. This compound can improve the mechanical traits of biofilms; such as elasticity, stiffness and tensile strenght [2]. These features can have several applications in the industrial scope, it can be used as a coating material but mainly as a substitute of some petroleum based plastics.

Therefore, the objective of this research was to compare the rheological and mechanical properties of biofilms utilizing different formulations based on starches with different content of amylose in order to elucidate which one offers the best physical characteristics. The viscosity was determined by an Anton Paar MCR 102 rheometer, the mechanical properties were studied by tensile strenght and the amylose content was quantified by spectrophotometry. It was found an effect of the amylose content on the mechanical properties and behavior of biofilms.

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Molecular simulation for better understanding and prediction of disordered polymer materials

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Molecular simulation is becoming an indispensable tool in the discovery and development of advanced polymer materials. Yet, unique challenges exist in both model construction and improving the prediction reliability. This presentation will discuss our recent computational efforts in simulating disordered polymer materials, in particular, polymer networks and polymer-plasticizer mixtures.

(a) Molecular modeling of crosslinked polymer networks often follows arbitrary pathways for network generation, with different precursor topology from experimental systems. We use coarse-grained molecular simulation to study the effects of precursor choice on the predicted network structure and properties[1]. Three sets of precursors with different molecular architectures are designed such that they would form identical networks at the limit of perfect conversion. Little difference is observed between the resulting networks in typical properties including the radial distribution function, macroscopic statistics of network connectivity, and glass transition behaviors. However, the stress-strain relationship in tensile deformation clearly depends on the formation pathway when compared at the same crosslinking density. The elastic modulus of the network is found to correlate strongly with the number of elastic strands in the network, except at the highly-crosslinked limit where substantial discrepancy is observed between networks from different precursors. Although these final networks contain a similar average density of structural defects, the choice of precursor has significant impact on their spatial distribution, leading to the precursor dependence of their mechanical properties.

(b) Despite the widespread use of plasticizers in the polymer industry, the mechanism of plasticization remains poorly understood. Industrial selection of plasticizers largely relies on semi-empirical rules and even for successful candidates, it is often difficult to answer why they outperform other molecules in terms of effectively reducing the glass transition temperature and elastic modulus of the material. In addition to plasticization efficiency, plasticizer migration is an issue that is causing increasing attention. The loss of plasticizers over time not only causes the deterioration of material properties, it is also an environmental and safety concern. We use molecular simulation at both the full-atom and coarse-grained levels to understand the plasticization mechanism. From this knowledge, a number of molecular descriptors will be identified for a semi-quantitative prediction of the efficiency of any plasticizer based on its chemical structure. In addition, predictions will also be made on the thermodynamic compatibility between the plasticizer and its host polymer, as well as the diffusion coefficient of the plasticizer in the latter.

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Abstract preparation

RAFT Aqueous Dispersion Polymerization via Host-Guest Supramolecular Chemistry

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Polymerization-induced self-assembly (PISA) has been developed recently to access block copolymer (BCP) self-assemblies directly due to the advantage of much higher concentrations compared to traditional post-polymerization self-assembly techniques.[1-5] The aqueous dispersion polymerization requires water-soluble monomers that form water-insoluble polymers. Thus, the technique is not suitable for water-immiscible monomers. We aim to achieve an aqueous dispersion PISA process of water-immiscible monomers using host-guest supramolecular chemistry. One-step PISA by dispersion polymerization of hydrophobic monomers directly in water was studied, based on cyclodextrin (CD)-mediated host-guest complexation. The polymerization could be realized by reversible addition-fragmentation chain transfer (RAFT) polymerization of CD/styrene complexes in water with an end-functionalized polyethylene glycol (PEG) as a macro-chain transfer agent (macro-CTA). Through the polymerization, CDs dissociate from polystyrene (PS) blocks because of the hydrophobic interactions between neighboring phenyl moieties. Accordingly, the resulted amphiphilic PEG-*b*-PS diblock copolymers could self-assemble in situ into nanoparticles with various morphologies. By targeting different copolymer compositions, various spheres, worms, nanoplates, ribbons, and nanotubes were obtained controllably. This technique can be very easily extended to n-butyl acrylate and many other hydrophobic monomers. We believe that the CD-mediated aqueous dispersion polymerization of water-immiscible monomers could be a powerful technique for the construction of nanomaterials with different morphology and different function.

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Abstract preparation

A DESCRIPTION OF AMYLOPECTIN AT THE MOLECULAR LEVEL IN DMSO BY USING PYRENE EXCIMER FLUORESCENCE

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The fluorescent dye 1-pyrenebutyric acid was covalently attached onto amylopectin to yield Py-Amylopectin and its ability at forming excimer was characterized in DMSO by steady-state and time-resolved fluorescence. Py-Amylopectin was found to form excimer very effectively, twice faster than pyrene-labeled poly(methyl acrylate) (Py-PMA) which is a very flexible polymer. That Py-Amylopectin would form excimer more effectively than Py-PMA was rationalized by considering that the side chains of amylopectin formed single or double helices in DMSO. This dense conformation of amylopectin brought the pyrene labels close to one another resulting in strong excimer formation. Fluorescence blob model (FBM) analysis of the fluorescence decays acquired with Py-Amylopectin led to the conclusion that each pyrene label could contact, on average, a pyrene label located up to 20 residues away. Molecular mechanics optimizations or MMOs were conducted to quantify the interhelical distances that would match a separation of 20 residues between helices formed by the side chains. This study led to the conclusion that the helices of amylopectin in DMSO must be separated by about 28 Å. In turn, a 28 Å interhelix separation would suggest that amylopectin in DMSO would have a density of 0.17 g/mL, one-to-two orders of magnitude larger than reported in the literature. This discrepancy led to the proposal of the solution cluster model for amylopectin whereby the interior of amylopectin shows dense clusters of helices held together by flexible linear oligosaccharide segments that swell in solution resulting in the overall low density of amylopectin described by techniques other than fluorescence. The solution-cluster model appears to rationalize most, if not all, experimental observations reported about amylopectin in the literature and can be employed to visualize the complex internal architecture of amylopectin.

High spin ground states of the graphene nanoflakes and related molecules

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Graphene has emerged as a new promising material for molecular electronics.[1] It has very high charge carrier mobility, Hall effect at room temperature, excellent mechanic properties.[2,3] The principal drawback of graphene, is zero band gap which creates difficulties for the application of graphene in electronic devices. This drawback, however, can be mitigated using the graphene nanoflakes and the graphene nanoribbons instead of graphene in electronic devices. The graphene nanoribbons and the nanoflakes (GNF) are the strips of graphene of different shapes with the wide of less than 50 nm.The the multiplisity of the ground state of the GNF is governed by the Ovchinnikov's rule [4] which states that the total spin of the ground state is proportional to the difference between atoms of different "color".

We have discovered high spin systems that do not obey this rule, opening up new possibilies in the field of organic ferromagnetiics, we also provided an explanation of this phenomenon using complete active space calculations. It has been found that the violation of the famous Ovchinnikov's rule is related to strong exghange repulsion in GNFs.

The same method of calculations was applied to explore the ground states of the graphene nanobelts, Möbius strips and higher order Möbius strips derived from graphene. The calculations demonstrated strong polyradicalic and sometimes, high spin character of the ground states in all studied systems. According to our results the total spin of the ground state do not depend on the number of twists in Möbius strips and higher order Möbius strips. The strain energy increases with number of twists as it could be expected, however the increase is not uniform. The increase of the strain energy is more notable when passing from even number of twists to odd number of twists, than the otherwise.

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EFFECT OF PARTICLE SIZE ON THE PERMEABILITY OF CHITOSAN MEMBRANES

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In recent years the use of chitosan polymer has been observed in activities related to the preservation of the environment and to the care of human health. Due to its chemical structure it is possible to make membranes for potential applications.

Membrane adsorbents have emerged as powerful and attractive tools for the removal of hazardous materials such as dyes and heavy metal ions, mainly in trace amounts, from water resources. Among membrane adsorbents, those prepared from or modified with chitosan biopolymer and its derivatives are cases of interest because of chitosan advantages including biocompatibility, biodegradability, nontoxicity, reactivity, film and fiber forming capacity and favorable hydrophilicity. The present study aims to elaborate chitosan membranes and compare the permeation efficiency of chitosan membranes of different particle size (53, 62 and 74 µm) to estimate the permeability of nickel ions and sucrose molecules in solutions model. Infrared spectroscopy was used to evaluate the structural stability of the membranes, factor of swelling, membrane thickness and permeability were determined. In addition, a low cost permeation unit was designed for experimentation with the elaborated membranes. Transparent, flexible and resistant membranes were obtained, the model solutions were analyzed by polarimetry and refractometry. The results show a higher permeation efficiency in the larger particle membranes.

The purpose of the research is to use a biodegradable material to remove heavy metals and emerging pollutants from wastewater, using a low energy consumption technique and, on the other hand, to generate cheap, effective and applicable solutions to specific problems

Acknowledgements

VIEP-BUAP

In Situ Forming Mechanically Robust, Cell-Instructive Hydrogels for Mesenchymal Stem Cell Delivery

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The local delivery of mesenchymal stem cells is being examined for a number of therapeutic applications, including in situ regeneration of soft connective tissues such articular cartilage and the intervertebral disc,[1] and for the induction of angiogenesis to treat ischemic conditions.[2] Given their high water content and ability to be delivered via minimally invasive means, in situ forming hydrogels are ideal for these purposes. The design of such hydrogels requires consideration of the gel-forming chemistry, the internal cell-material interactions, local tissue response, as well as the mechanical environment of the tissue surrounding the stem-cell laden hydrogel. In this talk, I will describe the design of hydrogels we are presently examining for such applications.

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Acknowledgements (10 pt)

Funding for these studies from the Heart and Stroke Foundation of Canada and from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

Synthesis of biocatalyzed benzyl butanoate with lipases in organic solvents

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Key words*:* Enzymes, flavoring, benzo butyrate, HPL

INTRODUCTION

There is a growing demand for synthetic and natural flavorings which are mainly used in the food, cosmetic and pharmaceutical industries. However, the traditional synthesis of these at present is considered not environmentally responsible since during its production are used corrosive chemicals, high temperatures and pressures, in addition to organic solvents flammable and highly polluting. In this sense, biocatalysis is a fundamental pillar, since it allows the use of enzymes to biocatalise these, under mild conditions of temperature, pressure and avoiding the use of acid catalysts.

MATERIALS AND METHODS

Using commercially available porcine pancreas lipases, Candida rugosa and Mucor miehei and a 2k experimental design, the production of benzyl butanoate from butyric acid and benzyl alcohol was optimized as shown in Figure 1. Monitoring of the reaction Was carried out using HPLC-DAD equipped with a C18 column and a mobile phase of 70/30 acetonitrile / water v / v composition acidified with 0.1% formic acid. Typically, the reactions were carried out in a 125 mL flat bottom flask with magnetic stirring, 40 ° C, 250 rpm, time periods of up to 72 hours, varying the enzyme substrate ratio and the type of enzyme. The product was isolated by column chromatography using silica gel as the stationary phase and a 30/70, v / v mixture, hexanes / dichloromethane as the mobile phase.

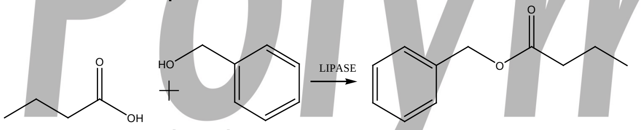

Figura 1. Reacción química

RESULTS AND DISCUSSION

Using the areas under the curve of the chromatograms Figure 2, it was possible to determine the conversion values for each of the biocatalyzed reactions, finding optimum reaction conditions for the conversion up to 70% of benzyl butyrate, Candida rugosa lipase as a biocatalyst at a concentration of 1g enzyme / 10 mmol of The substrates, 40 ° C, 250 rpm and toluene as the reaction solvent.

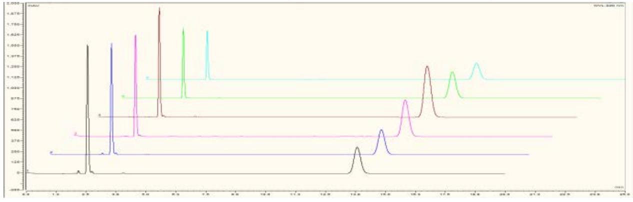

Figura 2. Monitoreo de cinética de reacción por HPLC.

Después de aislar el producto principal por cromatografía y recuperarlo por evaporación al vacío se encontró un rendimiento máximo final de hasta un 68.17% en base a peso y la pureza del mismo se evaluó por H^{1}RMN.

AGRADECIMIENTOS

FCQ-UACH and CONACyT are thanked for their support through project # 232163.

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SYNTHESIS OF CdSe NANOPARTICLES INMERSED IN AN ORGANIC MATRIX OF AMYLOPECTIN BY MEANS OF RF SPUTTERING

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CdSe nanoparticles immersed in an organic matrix of amylopectin have been synthesized by means of the rf magnetron-sputtering growth technique. The target was elaborated employing a mixture of CdSe and amylopectin high purity powders. X-ray diffraction (XRD) shows the cubic zinc blende crystalline phase of the nanoparticle and the amorphous structure of the amylopectin film. The average radius of the grains, calculated using the Scherrer formula in XRD peaks, is of the order of 8 nm. Results of resonant Raman scattering show that no confinement effects of optical phonons are observed in these CdSe nanoparticles. The band gap of CdSe nanoparticles measured from optical absorption measure- ments is 1.9 7 0.1 eV.

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Theoretical study of the electronic properties of Flavylium salts functionalized with Pyrene and Naphthalene groups.

Cesar Castro-García[1], Nora-Aydeé Sánchez-Bojorge[1], Luz-María Rodríguez-Valdez[1], Gerardo Zaragoza-Galán[1]

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The increase in energy demand has led to the search for alternative energies, and the use of them has been increased. , The state of Chihuahua present the highest of solar radiation incidence in the country, this is the reason for why researches are focused to this type of technologies, specifically in Grätzel´s solar cells. The function of the dyes in these solar cells is to absorb sunlight and use it to excite electrons. The light that comes from the sun is a set of electromagnetic radiations, ranging from ultraviolet, to infrared rays.[i] Therefore it is important that the dye absorb in this range of wavelengths. In the present work electronic and photo physical properties are analyzed for Flavylium salts functionalized with pyrene and naphthalene groups as electron-donors (figure 1),to determinate the presence of electron transfer phenomenon photo induced, since the Flavylium salts acts like strong photo oxidants in their exited state. An application for this kind of compounds, electron donor-acceptor, is the incorporation in Grätzel solar cells, since these compounds are added to this kind of device their efficiencies are improved and show very high yields. Density Functional Theory (DFT) was used for the determination of the electronic and structural properties of Flavylium salts derivatives. DFT was used with Minnesota family functional and the PBE0 functional, with 6-31G (d) basis set. The maximum absorption wavelength was compared with experimental data with the purpose to justify the methodology used. The results show that the functional PBE0 gives a good approximation to the experimental maximum wavelength for these structures. The Flavylium salts absorb inside the visible spectra at around 417 nm, its favors their use as dyes in DSSC.

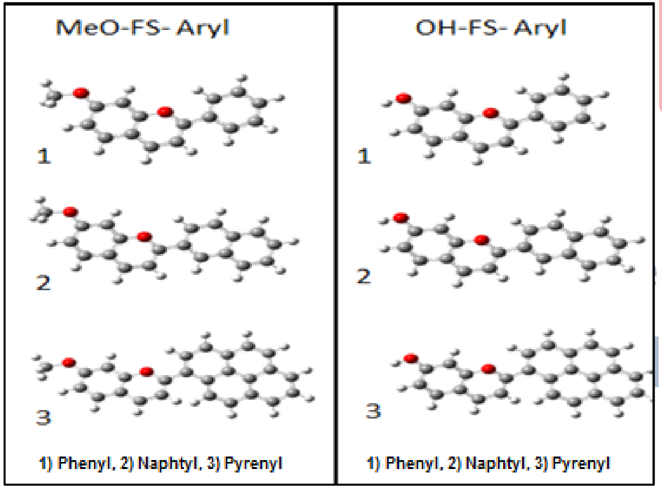

Figure 1) Analyzed systems with different substituents.

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Organic salts derived from the flavylium ion as new fluorophores.

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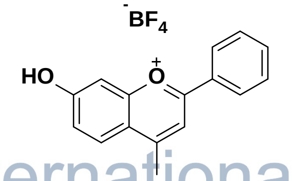
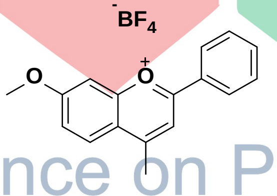
Anthocyanins are a group of colorful and bioactive natural pigments with numerous important physiological and ecological functions in plants. [1] They are responsible for the red, blue and purple colors of most fruits, flowers and leaves. [2]The main hypotheses about the presence of anthocyanins in plants are that they occur in response to stress, such as excess light, drought or pests. [3] In general, these have a protective role for plants in the presence of light; transforming excess of radiation into heat by competitive absorption of light. Implicit in the photoprotection hypothesis is the expectation that anthocyanins possess extremely non-radiative properties, ways for the dissipation of excitation energy from the excited state of electrons. [2]

In this contribution the synthesis and reactivity of 2-phenyl-4-methyl-7-hydroxy-1-benzopyrylium (OHFS) and 2-phenyl-4-methyl-7-methoxy-1-benzopyrylium (OMeFS) are reported. Compounds OHFS and OMeFS were synthesized by condensation of benzoylacetone and corresponding 2-hydroxy-4-oxo-benzaldehyde in acidic conditions (H2SO4 and HBF4). All the obtained products were subjected to NMR, UV-Vis and chromatographic studies to elucidate the structure and to recognize its purity. Yields and purity of flavylium salts were strongly affected by nature of the acid employed for the synthetic protocol. The flavylium salt derivatives exhibited strong absorption and emission in the region of 400-600 nm. Furthermore, benzopyryrylium unit in OHFS and OMeFS displayed remarkable response towards H+ concentration. In conclusion, a new family of organic cationic molecules was synthesized and their optical properties as pH fluorescent sensors were studied.



2-phenyl-4-methyl-7-hydroxy-1-benzopyrylium
OHFS



2-phenyl-4-methyl-7-methoxy-1-benzopyrylium
OMeFS

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Chitosan-hydroxyapatite chips for non-surgical periodontal therapy

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Periodontitis is a recurrent pathology in the oral cavity, where the bacteria is the main etiological factor. These periodontopatogens create their habitat in the gingival sulcus generating periodontal pockets. The standard treatment of this disease consists of the removal of supra- and sub-gingival periodontopatogens deposits by mechanical instrumentation of the root surface (Dental scaling and root planing), aimed to avoid the periodontal attachment loss and bone destruction, which may lead to edentulism. The usage of antimicrobial substances (antibiotics) favors the reinsertion periodontal fibers; however, the efficiency is limited to the antibacterial action. Then, it is desirable to have a material with this property as well as with anti-inflammatory and regenerative properties contributing to strengthening the reinsertion biological processes, improving patient's periodontal conditions. In this work, the efficacy of chitosan-hydroxyapatite chips of controlled release as adjuvants in the periodontal reinsertion on patients with moderate to serious chronic periodontitis is evaluated. Chitosan was obtained directly from waste shrimp skeletons following the chemical method; hydroxyapatite was recuperated from the *Pterygoplichthys spp*. fish bone. FTIR was used to confirm the presence of both molecules. A randomized controlled clinical assay with 30 healthy (except periodontal disease) patients was developed. Non-surgical periodontal therapy as well as a random selection of the periodontal pockets was done. The insertion loses and the pocket depth was measured at the beginning and at 21 days of the chips application. At this time, the gain was bigger where the chips were used as compared with the conventional treatment, 1.54 ± 0.34 ($p < 0.05$).

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STUDY OF CARBON NANOTUBES DISPERSION WITH MESO-PYRENE-BORODIPIRROMETHENE

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4,4-difluoro-4-bora-3a,4a-diaza-s-indacene dyes (abbreviated as BODIPY) are composed of two units of pyrrole which are connected by a methene in the 2-position and a boron atom coordinated by the N-heteroatom. BODIPY dyes are highly absorbent in the visible and ultraviolet spectrum, have high fluorescent quantum yields, thermic and photochemical stability and high solubility in organic solvents[3].

Carbon nanotubes (CNT) have high thermal resistance, good mechanical and electrical properties. However, Van Der Waals interactions cause nanotubes to become agglomerated. A strategy to disperse carbon nanostructures is non-covalent functionalization with dispersants bearing units capable of interact with CNT surface. Pyrene labeled molecules are excellent CNT exfoliants due strong pi-pi interactions between pyrene and sp^2 carbon atoms in CNT.

In this contribution, the synthesis and spectroscopic characterization of meso-pyrene-bodipy (Py-BODIPY) is reported. Py-BODIPY was tested as CNT dispersant in organic solvents and hybrid materials were studied by Raman spectroscopy.

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SOUND ABSORPTION PERFORMANCE OF AN AGAVE FIBRE BIOCOMPOSITE MATERIAL

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ABSTRACT:
In the present study the acoustic absorption characteristics of a biocomposite panel reinforced with *angustifolia haw* agave fibre was carried out in a reverberation room. Short agave fibres 10 mm long were was selected to make compacted panels of 0.6x0.6 m long by 0.25 m thick. Panel composition was made with a 2:1 latex polymer/agave fibre ratio and a curing time of 28 days. Acoustic absorption tests on real scale samples were performed by reverberation chamber method according to standard ASTM C423-17. Results indicate that the biocomposite panel made of latex and agave fibre exhibit a noise reduction coefficient (NRC) equal to 0.45, que es un valor menor al de varios panels asilantes acusticos comerciales que existen en el mercado.

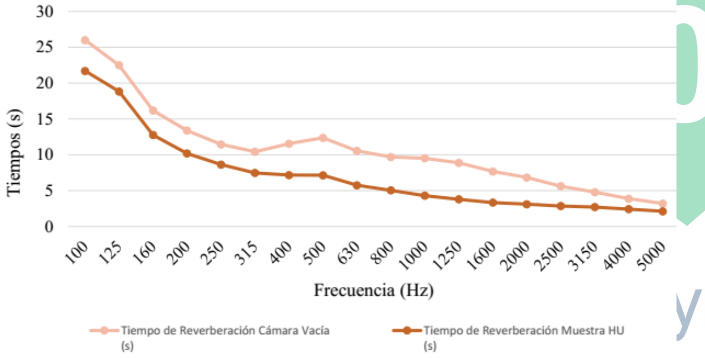

Figure 1. Times in reverberation room for reinforced biocomposite panel and empty chamber.

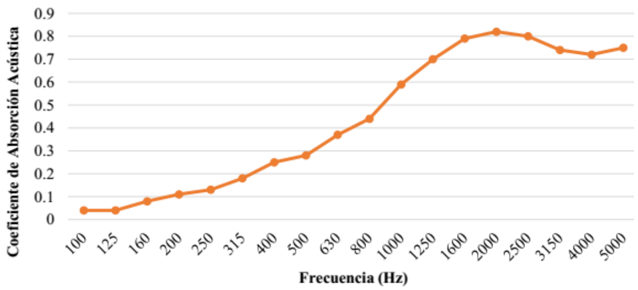

Figure 2. Absorption coefficient per thirds of octave taken on reinforced biocomposite panel made of latex-agave fibre under standard ASTM C 423 in a reverberation chamber.

Applications of the Orthogonal Reactivity and Multicoponent Reactions in the Synthesis of Complex Fluorophores

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In this presentation, we will describe the efforts made toward the preparation of BODIPY (Borondipyrromethenes)-based building blocks. These building blocks have proven to be remarkably versatile to label a host of different compounds. Depending on the functionality appended, the BODIPY derivatives can react with: boronic acids, organostannanes, organozinc derivatives, alcohols, phenols, 1,3-dicarbonyl compounds, amines, phosphines, carbohydrates, polyaryamines. Additionally, they can be manipulated to bear functional groups that display orthogonal reactivity and that can be activated under judiciously chosen reaction conditions. As a result, it is possible to carry out in an independent fashion on the same starting material, transition-metal-catalyzed cross-coupling reactions such as Liebeskind-Srogl, Suzuki, Stille and Sonogashira reactions [1]. An additional transformation in which these derivatives participate is the Knoevenagel reaction. Furthermore, the building blocks can be transformed into new compounds that have extended conjugation thereby emitting in the NIR region of the electromagnetic spectrum. In this fashion, we have prepared a new set of BODIPY analogues with substitution on the 8-,2-,3-,5-, and 6-positions. On the other hand, we have started to exploit the synthetic applications of formyl-containing BODIPYs in the preparation of complex fluorophores [2]. Thus, we have prepared a family of BODIPYs with formyl groups in different positions and used them in both the Passerini and Ugi multicomponent reactions to generate, in one step, derivatives with rich functionality in good to excellent yields.

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THERMAL INSULATION CHARACTERISTICS OF A BIOPOLYMER COMPOSITE REINFORCED WITH ANGUSTIFOLIA HAW AGAVE FIBER

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ABSTRACT:

One of the main factors of global warming is energy generation and households consume a lot of energy to get thermal comfort. This trend is increasing rapidly in cities, estimating that more than 30% of the available energy is being consumed in thermal conditioning. A possible solution to this problem is to include thermal insulation barriers that prevent the exchange of heat between the interior and exterior of buildings. In Oaxaca, Mexico, one of the main industries is the mezcal from *angustifolia haw* agave. About 10,000 tons of agave bagasse and wastes are generated annually contaminating soils and being very difficult to degrade.

In this study the use of latex reiforced agave fiber biocomposite as thermal insulation material is presented. Measurements of thermal conductivity, thermal resistance and specific heat were performed at different densities. Results show that thermal conductivity of biocomposite is about 0.037 W/m°C, a comparable value to expanded polystyrene, one of the most common commercial insulators. Best results were shown for the 60/40 fiber-latex composition as shown in table 1 and figure 1.

Table 1. Thermal properties of biocomposite latex-agave fibre

BIOCOMPUESTO FIBRA DE AGAVE 1 CM/LÁTEX			
MEZCLA	K	R (m² °C/W)	Ce (J/kg °C)
60/40	0.037	0.34	1905.59
50/50	0.040	0.31	2083.10
40/60	0.047	0.27	1995.45

Figure 1. Thermal conductivity at different compositions of biopolymer latex-agave fibre.

EFFECT OF SYNTHESIS PROCESS VARIABLES ON MORPHOLOGICAL AND MECHANICAL PROPERTIES OF VITREOUS CARBON SCAFFOLDS FOR TISSUE ENGINEERING APPLICATIONS

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Vitreous carbon foams have been shown to promote bone cell adhesion, mineralization and proliferation. However, their low mechanical resistance as well as their high manufacturing cost restrict their utilization in the biomedical area. The purpose of this study was to develop bone tissue engineering scaffolds from vitreous carbon foams, which were fabricated through the template route using an economical and renewable precursor. Towards this, cellulose sponges were impregnated with a sucrose-based resin and then carbonized under inert atmosphere. The effect of the concentration of the components of the resin (HNO3 and sucrose) on the mechanical and morphological properties of the resulting foams was determined. Moreover, the ability of the synthesized foams to promote cell adhesion was evaluated in vitro using human osteoblasts. Our results show that it was possible to produce vitreous carbon foams with highly interconnected polyhedral cells (cell size ~1000 µm). Scaffold morphology was strongly affected by the concentration of the catalyst in the resin (HNO_3) due to its foaming effect, which lead to porous and irregular surfaces on the carbonaceous materials. Also, increasing the concentration of sucrose in the precursor resin favored the mechanical resistance of the resulting foams, reaching values close to the commercial foams. In conclusion, vitreous carbon foams with trabecular bone-like morphology were obtained from a non-toxic and renewable precursor. The fabricated foams were shown to be highly cytocompatible and to promote human osteoblast adhesion. Although the compressive strength of the foams is much lower than that of native bone, their high porosity will allow their reinforcement using an additional biocompatible phase (coating/filler). Therefore, the vitreous foams synthesized here could be used as the porous component of a composite biomaterial system for the treatment of bone defects.

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Synthesis of Phenolic foams for hydroponics substrate usage.

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Hydroponics is a technique that uses a substrate and a nutrient solution for growing crops, this helps in avoid using land, optimize space, minimize water consumption, increase watering interval, among other benefits. Substrates have special characteristics such as good support, inert, humidity retention, innocuous, and aireation. Phenolic foams (PF) have been used as floral support due to its characteristics, but now, PF are used in hydroponics, hydrating them with nutrient solutions which allows crops to obtain the necessary nutrients and grow in optimal conditions. Phenolic foams are polymers that have open cells and are a result of a reaction using Resol resin, a surfactant, and other agents. (Figure 1)

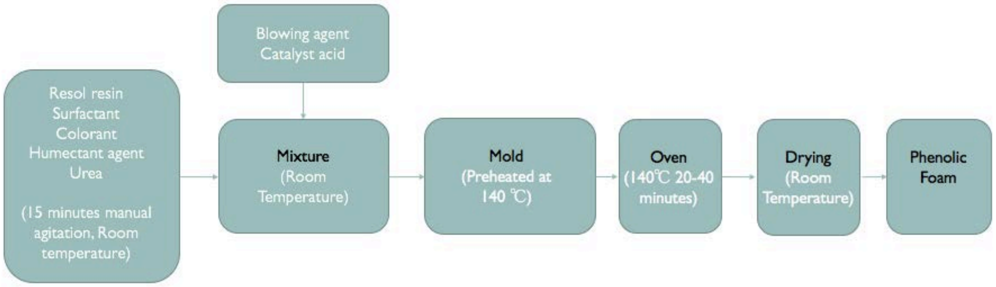

Figure 1. General diagram of phenolic foam synthesis.

The agriculture sector is one of the most important sectors in the world, that is necessary for food production, but that have many negative consequences to the Earth; such as contamination of bodies of water, exploitation of the soil, use of excess chemicals, excessive use of water, erosion among others. It is important to find alternatives that perform the same function but that impact less the planet, hydroponics is a good alternative for the agriculture sector. PF used as substrate in hydroponics fulfills the functions of a good substrate and helps on the road to sustainability through the hydroponic technique.

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Facultad de Ciencias Químicas e Ingeniería-Universidad Autónoma del Estado de Morelos, for allowing us to make the synthesis, provide the materials, equipment, and knowledge.

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SYNTHESIS AND THEORETICAL STUDY OF FLAVYLIUM SALTS

Gerardo Zaragoza-Galán, **Bethsy A. Aguilar-Castillo, Nora A. Sánchez-Bojorge, Luz M. Rodríguez Valdez, David Chávez-Flores, A. Camacho-Dávila**

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The 2-phenyl-1-benzopyrylium is the basic chemical structure –named, flavylium cation $[AH^+]$- and chromophoric core of the most widely encountered family of natural pigments found in the plant kingdom: the anthocyanins, which confer colour to plants and fruits. These chemical systems possessing chemical species attached to the flavylium cation can be used in applications ranged from those at the macro scale: dye sensitive solar cells to those at the nanoscale: pH molecular probes. Here we report a one-step procedure for the synthesis of flavylium salts substituted with specific moieties attached to the C ring (pyrilium ring) at position 2. A one-step preparation of flavylium salts containing Naphtyl and Pyrenyl moieties is described hereafter. Flavylium salts were successfully characterized by NMR and ESI-MS spectroscopies. The **FS** derivatives were obtained via Aldol condensation in acetic acid media, then; in the context of the green chemistry philosophy, we can consider these compounds to compete with the traditional functional organic materials in terms of electronic properties along with a sustainable and easier synthesis. To obtain a better understanding of the electronic properties of the synthetic flavylium salts, we have described the optical properties linked with the density functional theory (DFT) calculations of the synthesized compounds. Molecular simulation of -naphtyl derivatives displayed a coplanar conformation between naphthalene and benzopyrylium moieties. In contrast, DFT analysis exhibited a non-coplanar arrangement of pyrene and benzopyrylium units. These former statements in coherence with the absorption experiments where the naphtyl-flavylium dyads shows a red-shifted maximum absorption band with respect to pyrene dyads, led us to conclude that these bathochromic effects are associated with a more planar conformation.

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Rapid Solidification of AlSiFe-X Alloys (X= Cr, Ti and Mn)

V. A. Aranda Villada[1a], I. A. Figueroa[1], G. Gonzalez[1], J. A. García Hinojosa [2], G.A. Lara-Rodriguez[1], O. Novelo[1]

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The Al-Si alloy is one of the most used alloys in the automotive industry [2], however, Fe is an element that has high solubility in Al, in the liquid state. This impurity or alloy element tends to produce a sharp increment in hardness, thus embrittling the alloy. In this work the ternary AlSiFe master alloys was produced and 1, 3 and 5% of Cr, Ti and Mn were added in order to evaluate their effects on the mechanical properties. The master alloy with its correspondence small element additions were produced by means of argon arc melting. Once the ingots were produced, ribbons of a thickness of 25 micros were produced by melt-spinner. The mechanical and structural characterization was carried out by Vickers microhardness test and Scanning electron microscopy (SEM). In the as cast structure, the results showed a fragmentation of the needles shaped iron intermetallics for each alloy. Therefore the microhardness of the investigated alloys decreased. On the other hand, when the alloys are ribbon shape produced the hardness varied considerably.

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Acknowledgements

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Mechanical analysis of open pore Al-Mg foams

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Open pore Al-Mg base foams using the infiltration method were produced. NaCl particles were used as preform with sizes ranging from (A) 2.38 mm a 2 mm and (B) 1 mm to 710 µm, the porosities obtained were 62 % to 65 %. The mechanical properties were investigated by means of compression test using ASTM E9 standard. Four compositions alloys were produced in order to obtain lighter and more resistant foams than its pure elements; the alloys were Al, Al-10Mg % wt, Mg-10Al % wt and Mg. According to the results, it was found that foams with pore (B) showed better mechanical properties than foams with pore (A). Finally, the Al-10Mg alloy was 27 % lighter and 3.5 times more resistant than the foam of pure Al.

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Addressing the Toxicity and Instability of Halide Perovskite through Chemical Design

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Organic-Inorganic lead halide perovskites have recently emerged as one of the most promising families of photovoltaic materials. From the original report in 2009,[1] power conversion efficiency (PCE) of solar cells based on these materials has risen from 3.8 to 22.1%.[2] The pivotal material for this development has the formula $MAPbI_3$, where MA stands for methyl ammonium. $MAPbI_3$ and related materials have exhibit superb photophysical properties and amenable syntheses.[3] However, the toxicity of lead and the lack of stability of these materials towards light and moisture remain the main obstacles for big-scale implementation.[4-6]

In this talk we will discuss our group efforts to address these issues through chemical design. In particular, two approaches will be discussed. The first approach will deal with our exploration of new lead-free perovskite architectures and the second one will describe our work with functional organic linkers that might enhance the stability and optical properties of perovskite-like materials.

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EFFECT OF AMMONIA IN THE FORMATION OF SILICA PARTICLES BY SONOCHEMICAL METHOD

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Currently, the particles of silica have great relevance in the investigation due to their novel applications based on the characteristics such as form, size and porosity. The control of these allows its adequate implementation. There are different methods for the preparation of these particles, where the reaction time is from 2 to 12 hours and irradiation power up to 500 W. In this study, particles of silica were synthetized by sonochemical method using tetraethyl orthosilicate (TEOS) as Si precursor and ammonia as hydrolyzing agent in presence of ethanol. By varying the reaction conditions we can modify the characteristics of produced particles. We modify the volume of ammonia (from 2.5 to 25 mL) in order to knowledge the effect of this parameter in the quality, size or form of nanoparticles produced. We produce silica particles in 1.5 hours in an ultrasonic processor (130 W, 20 KHz). The characterization by transmission electron microscopy reveals high quality and sphericity of particles but the effect of ammonia is few significate in size but very significate in the size distribution. These results allow obtain silica particles in reduced time and scalable to industrial level.

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GLASS FORMATION OF SOME ZrCuAlNi BULK METALLIC GLASSES

C. E. Borja[1], **I. A. Figueroa**[2], **O. Lozada-Flores**[2], **G. A Lara-Rodriguez**[2], **J. A. Verduzco-Martínez**[1]

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The glass forming ability of some ZrCuAlNi bulk metallic glasses is presented and discussed. The alloy compositions were theoretically determined with the miracle model [1] and kinetic fragility index [2] model. Cylindrical and conical ingots were produced using suction casting technique. It was found that both alloys have a critical glassy diameter, D_c, of 3 mm. The gamma parameter, γ, supercooled liquid region, ΔT_x, and reduced glass transition temperature, T_{rg}, parameters of the obtained glasses indicated high glass forming ability. Both glasses have a fragility index, $m = 40$. The use of both models did help predicting glass forming compositions in the alloy family investigated.

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Session3-Borja_Carlos

VISCOELASTIC BEHAVIOR(TTS MASTER CURVE) OF COPOLYMER/CLAY NANOCOMPOSITES

Rubén Castillo-Pérez[1,2*],**Mireya Lizbeth Hernández-Vargas**[1,2], , **Bernardo Fabián Campillo-Illanes**[1,3], **Osvaldo Flores Cedillo**[3].

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The aim of the present work is to study of the rheology of copolymer and clay nanocomposites containing 1%wt, 2wt%and 3%wt of bentonite nanoclay. The nanofiller effect on the dynamics of acrylic polymer was studied using frequency-dependent oscillatory shear measurements at multiple discrete temperatures T>Tg, as a result for obtaining master curves, using the time–temperature superposition principle. This superposition principle is used to determine temperature-dependent mechanical properties of linear viscoelastic materials from known properties at a reference temperature.The results illustrate the construction of master curves for the copolymer sample, called polyacrylic, and nanocomposites incorporating nanofiller up to 3wt%. The depiction of the master curves used temperature of 10°C as reference, and three regions in the viscoelastic spectrum of non-Newtonian liquids are observed. First, at large frequencies and shorter times, the material resists deformation due to opposition of the polymer molecular chains, these regions is known as glassy zone; second, as the frequency achieve intermediate values, the material decreases its opposition, due to a greater relaxation time to the polymer chains, and it's called transition zone (leather/transition); and finally at lower frequencies and longer times, the material tends to behave like a rubber, called rubbery/plateau. Thus, a study of the viscoelastic behavior in a wide spectrum of frequencies allows predicting the processability of the material and their behavior in future applications.

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Photoluminiscent activity of nanostructured system from *eysenharditia polystachia* and SiO_2 nanoparticles

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The studies on designing and synthesizing new nanomaterials for detection have always been an interesting topic due to environmental, biological, chemical and effectively for imaging in biotechnology applications [1,2]; in order to measure different physical and biochemical parameters to be used for the basis of mathematical modeling of protein kinetics, biochemical networks and test of computational models already developed [3,4].

The design of surface-functionalized fluorescent silica nanoparticle from *Eysenhardtia Polystachia*, a medicinal tree known in Mexico as *"palo azul"* [5,6], as a potential biomarker is presented. Photoluminiscent activity (PL) of four different solvent extractions of palo azul (ethanol, methanol, methanol-ethanol and deionized water) were evaluated including molecular dynamic simulation to recognize molecular interaction of the extracted compounds and the solvent. The surface-functionalized systems were fully characterized regarding it's PL activity and the systems were compared against rhodamine 6G for comparison against a commercially used dye for imaging techniques [7].

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MANUFACTURE OF PURE OPEN-CELL MG FOAMS FOR CO2 CAPTURE

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Abstract

Carbon dioxide (CO2) is a major greenhouse gas, commonly formed by the combustion of fossil fuels. Recently, several systems such as zeolites, activated carbon, ceramic alkaline, calcium and magnesium oxides have been proposed for the CO2 capture. Open-cell Mg foams present a large surface area, which can be oxidized to form Mg oxides with attractive possibilities to use them as structured CO2 captors. Open-cell Mg foams with mean pore size of 350 microns, relative density of 0.33 and surface area (BET) of 5.42m2/g were used to carry out the surface oxidation and CO2 capture experiments. The CO2 capture capacity was studied at low temperatures (between 40 and 60 ° C) and with a relative humidity ranging from 40 to 80%. Optical microscopy and XRD techniques were used to characterize the structure of the foams and to identify the superficial oxide formed over the cells. The final products, formed after the isothermal CO2-H2O capture experiments were identified by scanning electron microscopy (SEM) and infrared spectroscopy (FTIR). The products formed after the isothermal capture process were thermally decomposed by mean of thermogravimetric analysis (TGA), this in order to quantify the amount of CO2 captured for the MgO layer. The results showed that the Mg foams with a superficial thicknesses layer of 8 microns of MgO showed the highest CO2 capture capacity (0.87 mmol / g) analyzed at 60 ° C and 80% of relative humidity. The mechanical properties (yield strength, ultimate strength, elastic modulus etc.) of the Mg foams and the considerable CO2 capture capacity obtained in this work, supports the possibility of using them for functional applications as structured CO2 captors.

Acknowledgements

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Coupling between graphene and intersubband collective excitations in quantum wells

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Recently, strong light-matter coupling between the electromagnetic modes in plasmonic metasurfaces with quantum-engineering electronic intersubband transitions in quantum wells has been demonstrated experimentally [A. Benz et.al., ACS Photonics **1** (2014) 906, J. Lee et.al., Nature 511 (2014) 65]. These novel materials combining different two-dimensional electronic systems offer new opportunities for tunable optical devices and fundamental studies of collective excitations driven by interlayer Coulomb interactions. In this work, our aim is to study the plasmon spectra of a hybrid structure consisting of conventional two-dimensional electron gas (2DEG) in a semiconductor quantum well and a graphene sheet with an interlayer separation of *a*. This electronic bilayer structure is immersed in a nonhomgeneous dielectric background of the system. We use a simple model in which the graphene surface plasmons and both; the intrasubband and intersubband collective electron excitations in the quantum well are coupled via screened Coulomb interaction. Here we calculate the dispersion of these relativistic/nonrelativistic new plasmon modes taking into account the thickness of the quantum well providing analytical expressions in the long-wavelength limit.

POLYACRYLIC/SiO$_2$ NANOCOMPOSITES: A STUDY OF VISCOELASTIC BEHAVIOR (TTS MASTER CURVES)

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This research focuses on the study of the rheology of polyacrylic and SiO$_2$ nanocomposites containing 1%wt, 2wt% and 3%wt of nanoSiO$_2$. The nanofiller effect on the dynamics of polyacrylic was studied using frequency-dependent oscillatory shear measurements at multiple discrete temperatures $T>T_g$, in order to obtain master curves, using the time–temperature superposition principle. This superposition principle is used to determine temperature-dependent mechanical properties of linear viscoelastic materials from known properties at a reference temperature. The results show the construction of master curves for the copolymer sample, called polyacrylic, and nanocomposites incorporating nanofiller up to 3wt%. The construction of the master curves were carried out using a temperature of 10°C as reference, and three regions in the viscoelastic spectrum of non-Newtonian liquids are observed: a) At large frequencies (shorter times) the material prevents deformation due to opposition of the polymer molecular chains, these regions is known as glassy zone; b) as the frequency has intermediate values, the material decreases its opposition, due to a greater relaxation time to the polymer chains, called transition zone (leather/transition), and at c) at lower frequencies (longer times), the material tends to behave like a rubber, called rubbery/plateau. Thus, a study of the viscoelastic behavior in a wide spectrum of frequencies allows predicting the processability of the material and their behavior in future applications.

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Hydrotalcites as bactericidal agents of *Corynebacterium ammoniagenes*

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Diaper rash is often not consider a disease but an irritation of the skin, caused by a wet or dirty diaper that has been in contact with the dermis for a long time. If the diaper is not changed, serious hygiene problems are generated in the area, as the bacterium contained in the urine, *Corynebacterium ammoniagenes,* generates ammonia, which is a potent skin irritant. Furthermore, the covered area by the diaper reaches the suitable humidity and temperature for the bacteria growth. This phenomenon can be controlled by using bactericidal agents, such as silver and copper. Moreover, zeolites or clays can be used as a new alternative of innocuous bactericides. Among the clays, the hydrotalcites have been shown to be effective bactericidal materials [1-2]. The cations that are incorporated into the hydrotalcite structure may present bactericidal properties, such as copper and zinc. In this work, the antibacterial effectiveness of hydrotalcites with different chemical compositions against *Corynebacterium ammoniagenes* was evaluated using two *in vitro* methods. The first method consisted of the modified Kirby Bauer methodology and, the second refers to the evaluation of bacterial growth by turbidimetry using the broth dilution method. The hydrotalcites were characterized by X-ray diffraction, infrared spectroscopy, scanning electron microscopy, dispersive energy X-ray spectroscopy and inductive coupling plasma emission spectroscopy. The zinc-aluminum hydrotalcite was the material that presented the best bactericidal effect, with a bacterial reduction rate of 80% for *Corynebacterium ammoniagenes*.

Keywords: Layered double hydroxides, bacterium, diapers, bactericidal solid.

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SYNTHESIS AND CHARACTERIZATION OF MULTILAYER HYBRID MEMBRANES FOR GUIDED TISSUE REGENERATION (GTR)

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The materials that are used for manufacturing bone scaffolds must possess osteoconductive, osteoinductive and biocompatible properties [1]. In addition, GTR allows the bone formation through the use of membranes with barrier functions able to prevent the soft tissue infiltration in the repair zone [2]. The development of hybrid materials is considered in this research [3]. The aim of this study is to relate good physical and mechanical properties of a synthetic polymer (PVA) with a biocompatible natural polymer, *e.g.* collagen (COL). The collagen is able to promote and stimulate the biological degradation. Furthermore, the synthetic polymer mixed with collagen type I will acquire the necessary characteristics such as: biodegradability, biocompatibility and bioactivity. The materials will be reinforced with bone-like ceramics, such as hydroxyapatite, whereby cells are expected to recognize this biomaterial rapidly, propitiate osteconduction, bone growth and act as a barrier to different cellular components than bone cells. Thus, in this work hybrid materials were synthetized varying the ratio compositions between 50%-10% PVA-COL. It was observed that at higher percentage of PVA, the membranes improve their mechanical properties, however, it was observed that their plasticity must to be improving. Thus, the effect of the addition of Glycerol and Ethylene Glycol during the synthesis was studied. In order to modify the degradation time, the membranes were cross-linked with 1-ethyl-3-(-3-dimethylaminopropyl) carbodimide (EDC). Then, the membranes surface and hydroxyapatite morphology were studied through SEM. On the other hand, the characteristic bands of COL and PVA in IR technique were observed. Also, XRD characterization was used with the aim to confirm the crystal structure of the hydroxyapatite. In conclusion, the characterization results provided evidence that it is possible to synthetized new hybrid membranes, which present better mechanical and biological properties than their pure counterparts and also they present a potential application in bone regeneration issues.

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Fluorinated benzimidazole-based ligand as an approach to histidine-rich oxidative enzyme active sites

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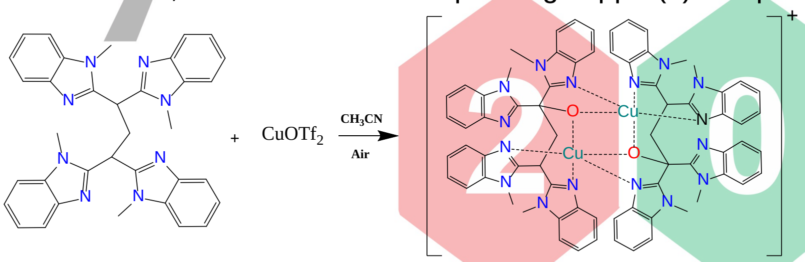
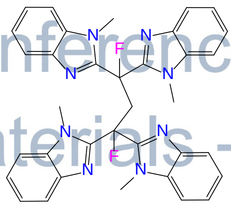
Biomimetic catalysts for oxidation reactions are of great interest in inorganic chemistry, specially when dioxygen and first-row transition metals are employed [1]. The use of benzimidazole ligands in the desing of metal complexes that are able to oxidize C-H bonds has not been extensively explored. In our research group, we recently showed the intramolecular C-H bond hydroxilation of the tetrabenzimidazole-based copper complex which resulted in a mixed valence dicopper species, likely through dioxygen activation [2]. This behavior is similar to that observed in monooxygenase enzymes like particulate methane monooxygenase [3]. In order to avoid the autooxidation of the starting compound, the new fluorinated tetrabenzimidazole derivative was synthesized and characterized, as well as the corresponding copper(II) complex.





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

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The nanocomposite materials have great advantages compared to other plastics and composites, because when the properties of the polymers with a nano-sized reinforcement component are combined there is an improvement in their specific properties. In the present work, maize starch was used as the matrix of the nanocomposite, a natural biopolymer that is exploited for its biodegradability and low costs. The 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. The addition of silica nanoparticles (Aerosil-vs Nis-silice) to the maize starch base structure was done to improve its mechanical and thermal properties. Different formulations were prepared by varying the amount of filler to be obtained, these being 2.5, 5 and 7.5% by weight. To evaluate the effects on the dimensional changes of the test specimens due to exposure to different temperatures, a thermomechanical analysis was performed to determine the linear coefficient of thermal expansion and the glass transition temperature in a TMA Q400, TA Instruments equipment under the standard ASTM E831-14. Mean values of thermal expansion coefficient were 0.0598 μ/mm °C for pure corn starch based plastic, and 0.0580, 0.1104 and 0.2196 μ/mm °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.

INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT 2017"

ONE–STEP AQUEOUS SYNTHESIS OF CADMIUM SULFIDE NANOPARTICLES WITH DIFFERENT SOLUBLE POLYMERS

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In the last years, semiconductor nanoparticles have emerged as an important class of materials that offers great promise to a diverse range of applications ranging from energy conversion to biomedicine. The synthesis of these nanoparticles is an important aspect of the research, due their water-solubility, simple chemical modification well dispersed and stabilized nanoparticles by utilizing soluble polymers, surfactant or capping agent. In comparison with the original organometallic synthesis, the resulting alternative routes are safe, simple, inexpensive, reproducible, versatile, and yield nanoparticles with well-controlled size, shape, and size/shape distribution.

Cadmium sulfide nanoparticles were prepared with one-step aqueous synthesis method. Different soluble polymers, i.e. dextrin, maltodextrin and polyethylene glycol, were used and the effect of different concentrations was analyzed for their effectiveness in limiting the particle growth. The morphology and the crystalline structure were measured by transmission electron microscopy (TEM) and x-ray diffraction (XRD), respectively. Particle size of the particles obtained from these experiments correlates well with the optical absorption spectroscopy and Scherrer´s formula from XRD patterns. Thus the presence of polymer on the surface of cadmium sulfide plays a significant role in reducing the size of the particle. XRD analysis revealed single crystal cadmium sulfide nanoparticles of size 3 nm in case of dextrin capping.

Process of marking by an inorganic material in a ferrous metal base, using the irradiation of a CO_2 laser

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This work developed a brand with the assistance of CO2 laser equipment. Using the marking technique by sintering and crystallization of glassy powders forming a ceramic-vitreous matrix in a ferrous metal base.

The ceramic-vitreous matrix adheres to the substrate forming a layer with mechanical properties: such as corrosion resistance, wear resistance, fracture strength as well as toughness and aesthetic functions. The ceramic-vitreous matrix will be obtained by a mixture of various inorganic raw materials conformed by silicate, metallic oxides of cobalt, zinc, alumina, frits, and feldspars.

The application was made by enameling, in this process depends on two important factors: the nature of the surface of the substrate and the type of glass-ceramic used. For enameling, two processes are used: 1) Porcelain enamel moist. 2) Dry-silicon porcelain enamel. During the synthesis process to create the glass-ceramic matrix CO2 laser radiation will be used, reaching a temperature at approximately 870 ° C.

This marking process using the radiation density of the CO2 laser is made up of four main regions which can be identified: a) the pure metal region. B) The region where the constituent metals are dominant compared to the vitreous ceramic components. C) The region where the vitreous ceramic constituents are dominant compared to those of metal, d) the compound for the ceramic-vitreous material. Each region of the composite structure has a specific adjective in the process: the ferrous metal base functions primarily as a structure for the support of the ceramic-vitreous matrix.

Due to the different vitreous-ceramic compounds and the thermal properties of the metal substrate, residual stresses are generated affecting the adhesion of both. As a result a vitreous-ceramic will be developed capable of generating the smallest residual stresses to ensure the development of a line layers to identify as a brand.

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CRYSTAL STRUCTURE OF CADMIUN TARTRATES AND ITS POTENTIAL APPLICATIONS

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Three metal-organic coordination polymers: $\{[Cd_3(C_4H_4O_6)_3(H_2O)]\cdot H_2O\}_n$ **I**, $\{[Cd_3(C_4H_3O_6)_2(H_2O)_2]\cdot 5.5H_2O\}_n$ **II** and $\{[Cd_2(C_4H_4O_6)_2(H_2O)]\cdot 3H_2O\}_n$ **III** were obtained under hydrothermal conditions and characterized by IR spectroscopy and single crystal X-ray diffraction. The structural analysis reveals that all compounds exhibit new 3D open frameworks filled with water molecules, which according to thermogravimetric analysis evolve at temperatures significantly lower than onset temperatures for decomposition [1]. Compound **I** exhibits an 8-c net; uninodal net (eci net) with Schläfli symbol $\{3^6\cdot4^{12}\cdot5^{10}\}$, where Cd atoms are connected by μ_4,κ^6-mode and μ_4,κ^5-mode tartrate ligands. Compound **II** is a rare example of a tartrate trianion complex formed by μ_5,κ^6-mode ligands creating a (6,3)-connected net with Schläfli symbol $(4\cdot6^2)_2(4^2\cdot6^{10}\cdot8^3)$. Compound **III** exhibits a 3,3,4,4-connected, 4-nodal net with Schläfli symbol $\{4\cdot8^2\}\{4\cdot8^4\cdot10\}$, built up by dimers of two octahedral Cd atoms linked by μ_4,κ^6-mode and μ_3,κ^5-mode tartrate ligands. None of the compounds reported here are topologically related, evidencing the versatility of the tartrate ligand for the framework formation of coordination polymers. Molecular sieve properties of compounds I and II were explored by gas adsorption. The results of this study show gate-opening effect in compound **I** and high adsorption capacity en compound **II**. Compound **III** shows a change in the photoluminescence response with hydration degree.

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Synthesis of multifunctional materials based in the ligand itacoperinone with different transition metals (II)

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Multifunctional materials is a blooming topic, because this kind of materials posses two or more properties which may coexist or even interact between them. Thus we can observe phenomena never seen before, as, for example, magnetochirality or photomagnetization, that can result in breakthrough technologies. One of the interesting tendencies in the development of such multifunctional materials is based on application of the organic radicals. Although the open shell systems are generally not stable but they may present interesting properties which are not possibly observed in much more stable closed shell species, such as magnetism, for example, that was considered as metals phenomenon exclusively.

Recently, the synthesis of coordination compound with photomagnetic properties has been reported by our group [1]. Hereby we would like to present the initial results on synthesis of another coordination compounds based on the Itacoperinone ligand (IP). IP itself demonstrated quite unusual photoluminescence and paramagnetism behavior for the perinone kind molecules. [2] Therefore, we made an attempts to coordinate IP with such magnetic metals as Ni (II), Co (II) and Fe (II) in order to increase magnetization and obtain new multifunctional materials.

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PD-CATALYZED MECHANISTIC SWITCH IN C-H BOND FUNCTIONALIZATION OF ARYL HALIDES.

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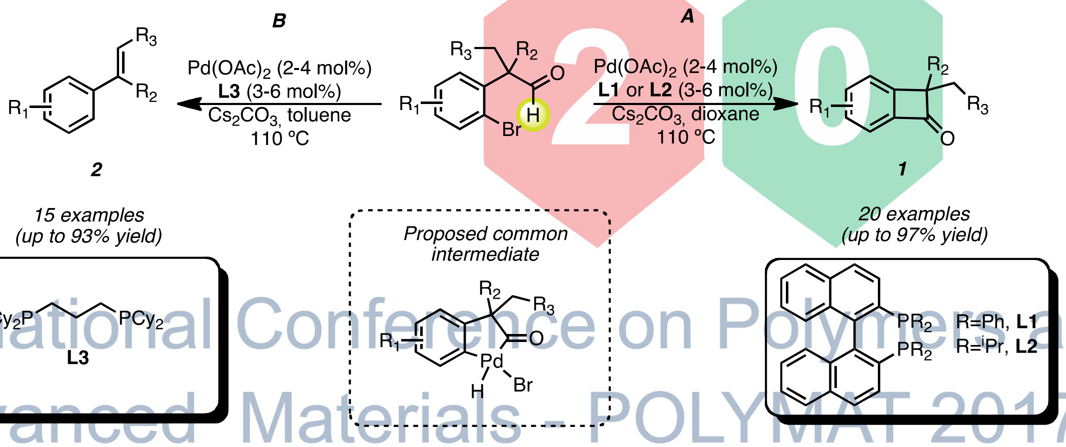
Pd-catalyzed C-H bond-functionalization reactions hold great promise to revolutionize synthetic strategies from both atom and economical fashion [1]. Herein, we describe an interesting ligand dichotomy in the Pd-catalyzed intramolecular C-H acylation of aryl bromides and aryl chlorides [2]. For aryl bromides, the use of rac-BINAP gives access to benzocyclobutenones compounds that have been used extensively as powerful synthetic intermediates in organic synthesis (Figure, route A) [3]. A subtle modification on the ligand backbone to a more flexible and hemilabile 1,3-dicyclohexylphosphinopropane lead to a new catalytic manifold for preparing configurationally pure styrenes derivatives (Figure, route B) [4].



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Desulfurization of dibenzothiophene and sulfone derivate via cross coupling reactions with nickel compounds

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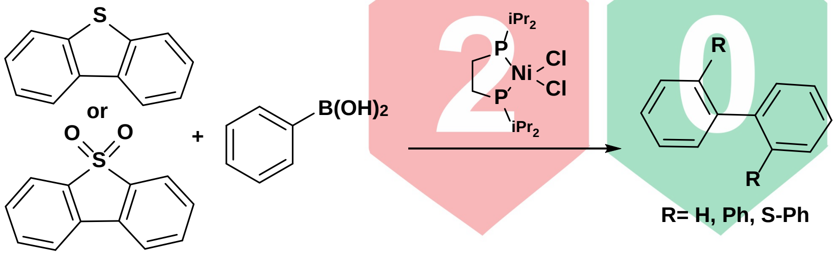
Hydrodesulfurization (HDS) is the industrial process employed for removal the organosulfur compounds present in petroleum, treating the crude oil with high hydrogen pressures and temperatures (250 atm, 300-450°C) in presence of nickel or cobalt doped molybdenum sulfide heterogenous catalyst. [1] However, dibenzothiophene and mainly its 4,6-substituted compounds are persistent in petroleum after this process. Therefore, sulfur removal of them through ''deep desulfurization'' is a high demanding task, which a satisfactory and practical solution has not yet been found. [2]

Reaction between dibenzothiophene and the sulfone derivate with phenyl boronic acid was performed mediated by the nickel precursor [Ni(dippe)Cl_2] in relatively mild conditions (70-100 °C), obtaining sulfur-free products. Furthermore, it has been realized reactions using water as co-solvent, where water has the role of hydrogen source. The yields of desulfured products are from moderates to good.



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SYNTHESIS, CHARACTERIZATION AND NMR REACTION MONITORING OF THE CATALYTIC ACTIVITY OF A NEW RUTHENIUM (II) COMPLEX

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There is a significant need for new catalyst with improved performance and environmentally friendly. In other words, catalyst with higher activity, superior selectivity, and enhanced stability are highly pursued [1]. Catalysis under mild conditions is of great importance to various chemistry areas, particularly for the development of novel active compounds and for natural products modifications, among others [2]. In this study, the synthesis, characterization, and study of catalytic activity by high field NMR of a new ruthenium (II) compound – $[Ru(\eta^6\text{-}p\text{-cymene})(dppb)Cl]PF_6$ (**1**) wherein dppb = 1,4-bis(diphenylphosphine)butane, – is presented. The synthesis reactions were carried out within an argon atmosphere using standard Schlenk techniques. NMR analyses of the catalytic activity were carried out in 5 mm NMR tubes in a Bruker Ascend 600 MHz equipment. Samples comprising substrate/base/catalyst at a 200/20/1 ratio were poured into conventional 5 mm tubes and monitored *in situ* and in real time fashion at 40, 50, and 60 °C, using integration of static with rapid injection in the NMR spectrometer [3]. The complex was active in the hydrogen transfer reaction, achieving conversions superior to 90% for different substrates within 4 hours at 60 °C, which suggests under mild conditions. Therefore, *in situ* monitoring the reactions through ^1H NMR was a valuable technique to establish the possible catalytic mechanism of Ru (II) precatalyst.

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METALLOCYCLIC COPPER(II) COMPLEX WITH A GLYCINE-SCHIFF BASE LIGAND: SYNTHESIS AND STRUCTURE

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Our working group has been interested in making contributions to coordination and bio-inspired chemistry. Complexes of different transition metals (such as copper, iron, zinc, rhodium, ruthenium, manganese, etc.), and ligands of different nature (such as cyclophanes, triazenides, etc.), have been tested in some activities, typical of biologicals systems, such as catalysis, antioxidant and antimicrobial processes [1-3]. Recently, we have focused our interest in metal complexes bearing (amino acids)-Schiff base ligands. We have obtained a copper complex which structure was elucidated by X-ray crystallography. In the solid state, the metallic complex shows a very interesting array: a four-(metallic center/ligand) cycle. The synthesis and structure of the copper(II) complex are presented.

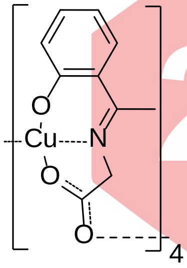

Figure 1. General structure of metallocyclic copper(II) complex

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Arylative Cyclization of Alkynoic Acids and Arylation of Indoles Promoted by Gold

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In recent years has emerged an interest to expand the chemistry of gold typically governed by the oxidation state I, by engaging it in redox processes. This has led to the development of a variety of strategies aiming at circumventing the high redox potential of the Au(I)/Au(III) couple. Initial efforts involved the addition of strong external oxidants with the concomitant problems of toxicity, low functional group compatibility or atom-economy. [1] More recently milder approaches have been described relied on the use of arenediazonium salts as electrophiles.[2] In particular, our group showed that arenediazonium chlorides are able to oxidize [AuCl(L)] (L = SMe_2, PPh_3) complexes to [$ArAuCl_2$(L)], under thermal conditions.[3] With the aim of exploring the reactivity of these species, we have studied the arylative cyclization of alkynoic acids along with the arylation of indoles. Interestingly, we have found that the arylative cyclization proceeds with a different regioselectivity compare to the cycloisomeration process catalysed by Au(I), and that the arylation of indoles occurs at the C-3 position according to a S_EAr mechanism.

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Carbon based materials as selective catalyst for the CO_2 electrochemical reduction

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The direct electrochemical CO_2 reduction reaction (CO2RR) to fuels and chemicals has attracted attention given its potential use for CO_2 to -chemical valorization using renewable energies as a driving force. The technological viability of this process, however, relays on the development of affordable and stable catalyst that can overcome the challenges regarding low energy efficiency and product selectivity. Work on heterogeneous electrocatalyst for the electroreduction of CO_2 to CO has been mostly focus on metals such as gold and silver. Herein, we present alternative catalyst based on N-coordinated non-noble metal doped carbon materials (MNCs).[1] The presence of insolated active sites composed of MetalNx moieties, enhances the selectivity towards CO2RR by suppressing the competitive process of the hydrogen evolution reaction.[2]

For this contribution we present a study of five different metal centers (Mn, Co, Cu, Ni, and Fe) and show the selectivity of the process is affected by the metal incorporated to the carbon structure. In particular, materials containing Fe and Ni outperform Ag and Au catalyst. Furthermore, we show that the catalyst performance is also dependent on the reaction conditions such as the electrolytes pH. We observe that while the hydrogen evolution reactions is inhibited at high local pH values, the CO production is not afectd by the proton concentration a thus it is indepenet on the pH. These results present the opportunity of tuning the reaction's selectivity via the electrolytes pH.

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Evolution of mechanical properties during aluminum wire drawing with and without lubrication

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One of the main problems in the wire drawing process is the radical change of mechanical properties of the material. Between the variables relevant to this process is the strain rate and the presence of lubricants. For this reason, this work carried out a study on how these variables affect the mechanical properties during a wire aluminium wire drawing.

Firstly, the wire was deformed six times with an area reduction of 20-29% at different drawing speed (80, 160, and 240 mm/min) and using Zinc stearate as a lubricant. After, tensile tests were carried out in order to characterize the mechanical behavior of the wire for each reduction step. Subsequently, the samples were examined metallographically where can be observed grains extremely aligned in the drawing direction.

Properties were determined as the Modulus of Elasticity, Yield Strength, Ultimate Tensile strength, Resilience and others. These were plotted and analyzed in order to extablish the effect of drawing speed and the use of lubricant on the mechanical properties.

Keywords: ***wire drawing, lubricating, drawing speed*.**

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SYNTHESIS AND CORROSION INHIBITION MECHANISM OF AMMONIUM-BASED IONIC LIQUIDS ON API 5L X60 STEEL IN SULFURIC ACID SOLUTION

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The prevention of corrosion is vital not only for increasing the lifetime of pieces of equipment and transport systems in the industry, but also for decreasing the dissolution of toxic metals from the metal components into the environment [1, 2]. In corrosive aqueous media, the use of corrosion inhibitors (CIs) is common due to the fact that these compounds do not affect the industrial processes, in addition to their low cost and easy application [3]. The number of available CIs is very high, where those of the organic type are just an example and their chemical structure is related to their inhibition efficiency [3]. On the other hand, in the last years, a new class of chemical products has shown the possibility of having a promising future in the corrosion protection branch due to their physicochemical properties, which make them unique, i.e. the ionic liquids (ILs). Their application in different areas has enabled the researchers to enrich their knowledge of this type of compounds that consist of a cation and an anion. Furthermore, the broad variability of the possible anions and cations present in the ILs offers the opportunity to adapt their properties to specific requirements, mainly when they are meant to be used as CIs [4]. In this sense, there are studies on ammonium-derived ILs as CIs for API 5L X52 steel exposed to hydrochloric and sulfuric acid solutions with good inhibition results [5, 6]. According to the aforementioned, in the present work, four new ionic liquids (ILs) derived from ammonium were evaluated as corrosion inhibitors of API 5L X60 steel in 1 M H_2SO_4 by means of the potentiodynamic polarization and weight loss techniques. The results confirmed that the inhibition efficiency displayed by the four ILs is a function of their concentration and molecular structure. The obtained inhibition efficiency ranged from 51 to 89%. The analysis of the potentiodynamic results showed that these compounds inhibit the corrosion of steel, classifying them as mixed-type CIs. The adsorption process of these new CIs on the API 5L X60 steel surface, which obeyed the Langmuir isotherm, was found to be physical and chemical. The SEM and EDX analyses confirmed the protection of steel in the corrosive medium.

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Abstract preparation

Heat transfer and flow dynamics in a biomass cookstove geometry

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In this work, the tridimensional hydrodynamic and thermal behavior for an air flow rate through four different biomass cookstove geometries is analysed from a numerical point of view. As a first approach, just the internal volume of the stoves is considered for this study. Mass, momentum and energy conservation equations with proper boundary conditions are solved using the ANSYS software. In particular, at the inlet of the stove a uniform and constant velocity is imposed and it is also assumed to be at a temperature of 100°C. Steady state solutions for the velocity and temperature fields are shown in different planes and for different velocity magnitudes. Preliminary comparisons with other similar studies [1,2] are also discussed.

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Hydroponics substrates- an option for sustainable agriculture.

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Agriculture is a necessary activity for the human being, reason for which they have looked for alternatives to obtain a sustainable agriculture. As each activity leads to an environmental impact, hydroponics is a proposal to reduce this impact by avoiding the use of soil, reducing the amount of water used in irrigation, and preventing the contamination of aquifers.

In order for any plant to reach its full genetic potential of producing the beautiful foliage, flowers or fruit its programmed to create, it must be provided with everything it needs in just the right proportions, and, at just the right time. With the science of hydroponics, this is possible by applying proper watering and feeding regimens, environmental control and plenty of quality lighting. [1] The hydroponics consists of a medium or substrate and a nutrient solution enriched with the nutrients necessary to obtain the plants with an adequate quality. The substrates must possess certain characteristics or properties to be able to be used in the hydroponic crops.

Table 1. Principal properties of hydroponics substrates

Property-description
1. Moisture retention-determines the possibility that the plant has the nutrients available so that it can perform its metabolic processes.
2. Capillarity- substrate has the ability to absorb and distribute the nutrient solution through the micropores in all directions.
3. Aeration capacity - proportion of the volume of oxygen that is available in the substrate, after it has been saturated with water and has finished draining.
4. Support (physic stability)- substrate compactation and decomposition may causes a reduction in the porous material and aeration capacity.
5. Light-weight- this determines the resistance of the hydroponics montage, it is easier to manage lighter weights.
6. Well draining- substrate should not be innundated because that´s against plants oxygenation.
7. Innert- substrate shall not content any element that can alterate the nutrient solution or make a reaction with biological species that can produce crops infections.
8. Cost- determining factor for utilization.

Table 2. Principal substrates used in hydroponics

Substrate name	**Cost**	**Advantage(s)**
1. Coconut Coir **2. Agricultural Grade Perlite** **3. Expanded Clay Pellets** **4. Common Pea Gravel** **5. Phenolic foam**	1. 40 MXN /Kg 2. 28 MXN/Kg 3. 40 MXN/Kg 4. 25 MXN/Kg 5. 20 MXN/piece 6. 150 MXN/piece 7. 240 MXN/piece	1. pH, moisture retention 2. Moisture retention, light-weight 3. Light-weight, innert 4. Aeration capacity 5. Support, lifetime

6. Polyacrilate (Sodium/Potassiun) **7. Rockwool** **8. Vermiculite** **9. Peatmoss**	8. 60 MXN/Kg 9. 33 MXN/Kg	6. Lifetime, moisture retention 7. Moisture retention, light-weight 8. Mositure retention, aeration capacity 9. Moisture retention, aeration capacity

In the way to achieve agriculture sustainability is important to use alternatives that helps environmental impact reduction, hydroponics is an eco-friendly alternative. Having several substrates for the technique, is important to know the advantages of each taking into account costs and availability.

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Metal Oxide effect on the microstructural and mechanical properties of aluminum based alloys

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Excellent combination may result trough the combination of low melting point, good mechanical properties and low density (2.7 g/cm3) such as aluminum based alloys, these characteristics are currently needed mostly in structural applications such as aeronautics, military and transportation [1-4]. In this work, the addition of metal oxide particles (ZrO_2 and CuO_2) in Al matrix is presented. In the alloy synthesis, samples were obtained by stir casting process, by adding 0.15g, 0.25g and 0.50g of metal oxides to 50g of high purity aluminum (99.98%). Vicker´s hardness in Al+CuO2 alloy shows slight variation with an average grain size of 21 ± 1.2 µm with respect to the unreinforced matrix, which presented 31 ± 1.1 µm. While with the addition of 0.25 g and 0.50 g metal oxides the average grain size slightly decreased by 4.4 ± 0.7 µm below the unreinforced matrix which possesses uniform granular structure. The alloys Al + ZrO_2 have similar behavior, where the hardness value had decreased to 10.2 ± 1.1 HV. From SEM results, it was observed that metal oxides induce modification of dendritic structure and grain refinement. X-ray diffraction characterization, shows the intermetallic compounds formation such as: $ZrAl_3$, Al_2CuO_4 and CuO. Metal oxides addition (ZrO_2 and CuO_2) in Al matrix offers the possibility of improving reinforcement in their properties for specific requirements. Suggested use for this alloy may be in the manufacture of automotive components where controlled deformation is needed to increase performance and structural security with low density. Although, the benefits are promising, it is important to note that the addition of nanostructures is difficult in achieve a complete homogenization.

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POLYSTYRENE DEGRADATION BY ULTRASONIC STRESS.

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Polystyrene (***PS***) is a common polymer that is used daily in several applications, such as furniture or electro-domestic covering wraps, disposable tableware, dielectric stuff and thermo-isolators. Nevertheless, the versatility of this material has increased the amount of ***PS*** wastes. Due to this fact we investigated a different way to recycling those wastes, employing *Ultrasonic Stress* (***US***).

Research began by collection of PS scraps (e. g. packing materials, styrofoam cups and polymerized old styrene reactive). After purification and viscosimetric analysis were found two kinds of ***PS***: *Low Molecular Weight* (***LMW-PS***) and *High Molecular Weight* (***HMW-PS***). Samples of each type of ***PS*** were diluted (50mg in 2mL) in various solvents such as acetone, chloroform, tetrahydrofuran and toluene. Finally were sonicated at room temperature and with 42 kHz and 1.2 MHz frequencies, for periods between 15 and 60 min.

Sonicated samples of ***LMW-PS*** and ***HMW-PS*** were characterized by FTIR, NMR and HPSEC to associate any change. The study had demonstrated that ***PS*** polymer chains suffered scissions, causing decrease in ***MW***. ***LMW-PS*** was less affected than ***HMW-PS***, in both cases toluene was the best solvent.

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STRUCTURE AND MECHANICAL PROPERTIES IN CORRUGATED STEEL RODS G42 QUENCHED AND SELF-TEMPERED IN LINE BY QTB PROCESS

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The QTB process (Quenched and Tempered Bar) is a relatively new heat treatment in the industrial production of long steels with cylindrical geometry and whose importance is that it is possible to obtain products with characteristics comparable to those of micro alloyed steels without the need to add a large amount of elements to the chemical composition. This process offers numerous advantages: mechanical strength according to international standards, good elongation levels, weldable materials and low production costs [1]. Nowadays there is little information regarding the microstructural characteristics formed by this process and the mechanical properties that confers to the material.

This research project is linked to the industrial steel sector with the company *Gerdau Corsa*, which is dedicated to the production of long steel: T profiles, round profiles, corrugated rods, etc.; in this last product the study is focused.

In this work the structure formed as a result of the QTB process is analyzed, generally can be described by three annular zones arranged radially in the product: martensitic outer ring, transition middle ring and ferritic – pearlitic core. The mechanical properties of the material are defined by the characteristics of these zones and by the fraction of each them. It has been found that the yield strength (YS) and ultimate tensile strength (UTS) depends on the thickness of the martensitic ring, whereas the elongation is related to the core morphology: percentage of phases and grain size. The effect of austenization temperature and tempering temperature on the final characteristics of the product is studied. In addition, a laboratory analysis of a steel with defined chemical composition for grade 42 (provided by the industrial plant) has been done in order to obtain the critical transformation temperatures by varying the cooling rate for the construction of a CCT (Continuous Cooling Transformation) diagram sketch; this through a dilatometry study and Jominy tests. The microstructures obtained in the laboratory and in the industrial complex are analyzed in Optical Microscopy and Scanning Electron Microscopy and subjected to Vickers micro-hardness tests.

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$Ni(x)$-Na_2ZrO_3 catalysts for CO_2 storage and H_2 production through CH_4 reforming process

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In the past decades, CH_4 and CO_2 emissions have been responsible of climate change, as both gases are the major contributors to the greenhouse effect [1]. Regarding to diminish CO_2 effects, many technologies have been proposed for CO_2 capture and storage (CCS) [2], using different alkali and alkaline-earth metal-based ceramics as chemical sorbents [3]. Another option to avoid greenhouse effect is diminishing both gas emissions and converting them into an alternative and cleaner energy source. In this regard, H_2 production would be a viable option [4]. Thus, in this work Ni-doped sodium zirconate (Ni-Na_2ZrO_3) ceramics were synthetized with different amounts of Ni (between 0 and 10 wt.%) and characterized by powder XRD, SEM-EDS and N_2 physisorption. Structural and microstructural characteristics of Na_2ZrO_3 based-ceramic were maintained in all Ni-containing samples. Therefore, all Na_2ZrO_3 materials were tested for CO_2 capture (thermogravimetric assessments), desorption processes (TPD analysis) and then for H_2 production (catalytic tests). In CO_2 adsorption, Ni addition slightly inhibits CO_2 capture, as the nickel added blocks Na_2ZrO_3 surface. Although a decrease in the CO_2 capture was registered, Ni addition benefits the H_2 production during the CH_4 reforming process. All Ni-doped samples presented a better catalytic behavior than that obtained with pure Na_2ZrO_3. The Ni effect for this catalytic process was evidenced by the production of higher amounts of H_2 and a drastically reduction in the temperature where syngas mixture was obtained, especially for the Na_2ZrO_3 material doped with 10 wt.% of Ni. Additionally, the regeneration and cyclic abilities for the Ni-doped Na_2ZrO_3 (10 wt.%) sample were evaluated. Results showed that it is possible to accomplish cycles of CO_2 capture and CH_4 reforming processes, obtaining a considerable regeneration of the original material. Regarding to the cyclability, it was observed that this property is affected due to a partial Ni reduction after the CH_4 reforming steps. However, when a pre-oxidation stage was performed the catalytic activity and H_2 production were recovered.

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Acknowledgements

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Desmoldantes base agua para Poliuretano en la Industria Zapatera

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La industria zapatera en México ha sido por muchos años, líder en el mundo. En este sector de la industria y en lo relacionado a la fabricación de suelas y piezas inyectadas base poliuretano, se utilizan los llamados desmoldantes, los cuales en general dejan una película delgada entre la pieza inyectada y el molde, estos desmoldantes son base solvente, se utilizan por ejemplo los denominados "Stoddard"® que es una mezcla de hidrocarburos entre C_7 y C_{12} y que se evaporan entre 150 y 200°C. Este desarrollo pretende fabricar este tipo de materiales, que cumplan la misma función anteriormente indicada, pero base agua. Este proyecto busca eliminar hasta cierto punto el uso de solventes y evitar la contaminación por vapores que se van a la atmósfera, se busca también que nuestros desmoldantes sean amigables con el medio ambiente y que comercialmente sean atractivos para la industria zapatera en general. Se está trabajando en formulaciones que contienen: ceras polietilénicas, derivados de poli-dimetil siloxano y ceras de bajo peso molecular parcialmente oxidadas y que puedan tener la función de ser desmoldantes acuosos. Se pueden indicar como referencias, solo los catálogos y fichas técnicas de varias compañías que fabrican este tipo de productos base solvente.

INTERNATIONAL CONFERENCE ON POLYMERS AND ADVANCED MATERIALS "POLYMAT-2017"

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FLOW-DYNAMICS OPTIMIZATION IN A DELTA-SHAPE FIVE-STRAND BILLET CASTING TUNDISH

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Abstract

In the present study a multiphase flow-dynamic was analyzed by numerical modeling into a non-symmetry five-strand billet casting tundish for steel. The aim was to optimize cleanness of the semi-finished product since the steel industry has focused lately on automotive steel grades. As in previous studies [1-9] a fully-turbulent flow was considered by using k-e model. The model also considered isothermal and steady states which permit to keep flows thermo-physical properties unchangeable with time. Three cases were considered: 1) Tundish+ Impact pad, 2) Tundish+ Impact pad+ a pair of baffles and 3)) Tundish+ Impact pad+ a pair of dams.

It was found that case 3 worked the best, improving the flow-dynamics of steel and also the nonmetallic inclusion removal. Nevertheless, despite case 1 showed the less slag layer aperture, this presented the bypassing phenomena for the closest exits to the steel input. The late, makes this case non-recommendable for high-valued steel grades.

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EFFECT OF SIMPLE SHEAR DEFORMATION ON MICROSTRUCTURE AND FATIGUE STRENGTH OF A 6061-T6 ALUMINUM ALLOY

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C. Reyes-Ruiz[1], J.M. Cabrera[2], V. Favier[3], N. Ranc[3] C. Braham[3], I.A. Figueroa[1] and G. Gonzalez[1].

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Equal channel angular pressing (ECAP) is a severe plastic deformation (SPD) technique that has been applied to a wide amount of materials due to its capability to produce of an ultra-fine grain (UFG) microstructure [1-3]. At the first stages of the process, the ECAP technique does not generate a homogeneous plastic deformation, and the UFG microstructure has not been reached. However, mechanical improvements after one ECAP pass are interesting for industrial applications [4,5]. The present work had as main objective to characterize and analyze the effects of simple shear deformation on microstructure and fatigue life of an aluminum alloy 6061-T6. The deformed specimens were subjected to a high fatigue cycle regime. The ECAP process showed some improvements in fatigue life limit, at the earliest stages of the process. Scanning Electron Microscopy (SEM) analysis of the fatigue fracture surface showed a different crack propagation mechanisms, that depended on the amount of deformation and crystallographic texture, generated by the process.

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HYBRID-CLAY COMPOSITE AS CONTROLLED-RELEASE OF N-P-K FERTILIZER

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NO_3^-, PO_4^{-3} and K^+ are macronutrients that the plants can absorb as NPK, but their inappropriate application methods and consequent pollution of soil and water reservoirs represent the main handling issues. The over application of fertilizers can be reduced through the use of control-release porous additives to trap and deliver such kind of agrochemicals. According to the American Association of Official Control Plant Food [1], slow or controlled fertilizers have to provide nutrients for plants in the following ways: i) retarding and regulating of nutrient availability, ii) providing adequately the plants requirements and iii) remaining for a long period of time. In this work, new control-release fertilizers (CRF) were formulated from anionic clays containing NO_3^- and PO_4^{-3} and from potassium (K^+) cationic clay. The clays were agglutinated with a calcium alginate biopolymer solution. These materials were tested in a hydroponic crop of lettuce. The anionic clays were prepared by the coprecipitación method reported elsewhere [2]. A bentonite cationic clay was utilized to intercalate K^+. Therefore, an appropriate amount of clays was encapsulated with calcium alginate as container and slow delivery of the nutrients. The N-P-K release tests were carried out in aqueous solution with and without crop. Indeed, the calcium alginate, as “clay container”, contributes to diminish between four and ten times the kinetic of nutrients delivery. Furthermore, during the hydroponic crop test with lettuce, the CRF presented a better performance and improvement of the lettuce growth than that observed by the conventional hydroponic nutrient mixture. This research opens a new formulation approach of controlled-release fertilizers.

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Encapsulation of alpha-tocopherol in gelatin nanofibers by electrospinning process.

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Electrospinning is a technique that has allowed the development of new fibrous structures from synthetic or naturally polymers for the development of materials applicable to the food, pharmaceutical, biomedical industry, among others. Electrospun micro and nanofibers offer many advantages over other methods, such as higher superficial area per unit volume [1], higher porosity [2] and variable composition to obtain the required physicochemical properties of the resulting fibers [3].

Nanofibrous films were fabricated from blend emulsion of gelatin type A (GA) and a-tocopherol by electrospinning. Scanning electron microscopic images showed that the continuity of the blend fibers was improved with an increase in the gelatin (GA) concentration. Fourier-transformed infrared spectroscopy indicated that the obtained fibers were composed of both a-tocopherol and gelatin constituents. This study demonstrated a potential to fabricate nanofibers from natural food biopolymers using the electrospinning technique.

Electrospinning is a novel technique that allowed the formation of alpha-tocopherol- gelatin nanofibers. We conclude that the gelatine type used and its concentration, as well as the polarity of the polymer residues, had an important influence on the fiber formation process and in its structure. High voltages used in electrospinning process generated more uniform fibers, while low voltages did not allow the formation of the fibers, use of 15 KV for the positive pole and 15 KV for the negative pole allowed alpha-tocopherol- gelatin nanofibers. Encapsulation of alpha tocopherol in gelatin nanofibers was confirmed by FTIR and DSC identifying the structural components corresponding to the molecules of alpha-tocopherol and gelatin.

It is concluded that electrospinning is an innovative technique, for the development of new materials. In this case the electrospun material was applied as skin moisturizing mask, whose content like gelatin as alpha-Tocopherol, permitted a cellular repair process in the skin.

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Encapsulation of alpha-tocopherol in gelatin nanofibers by electrospinning process.

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Deposition of thin films based on silicon by PECVD

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In 1970-80 S. R. Ovshinsky, D. E. Carlson, C. Wronski and the group of W. E. Spear and P- G. Lecomber developed and promoted the fabrication of a series of devices based on amorphous silicon and hydrogenated amorphous silicon. In particular, these scientists developed the first solar cells based on amorphous semiconductors. Much work has been reported of the production thin films by sputtering, chemical vapour deposition and plasma enhanced chemical vapour deposition, PECVD. At the beginning of the 80's it became clear that PECVD provided a number of advantages, particularly for the deposition of amorphous material over large areas. My intention is to present a description of the PECVD process and some details of the work carried out in this field by our colleague Marel Monroy.

Acknowledgements: Ernesto Garcia y G. Santana

Electronic Structure of Small Endohedral Fullerenes

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Endohedral fullerenes are fullerenes that contain other species inside of them. In this presentation we study the electronic structure of X@C_{28}, X@C_{36} and X@C_{44}. The metals chosen are those found by mass spectrometry experiments. Calculations have been carried out at DFT level using PBE functional and def2-TZVP basis for all atoms. The reported geometries are the lowest minima after a potential energy surface scan. We analyse the geometry, electronic and energetic properties for each system. We also carried out charge distribution and NICS calculations. An analysis of the stability of the 3 systems is presented.

Marel: Science Woman and Dreaming Light

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Body Dr. Marel showed her vocation for physics science from early age. She was a naughty little girl, with a beaut smile and an very active mind. The books and films of science fiction awoke her great creativity and liking for science.

Her golden dream was study physics at UNAM and arrive to stay. When she entered to semiconductor nano-structures world, she found her passionate research field. Then she secured the love bonding between Marel, Science and UNAM forever. Marel wanted to contribute with her silicon nanocrystals to the care of the environment. Her scientific contributions carried his personal touch; firm steps to generate knowledge. Marel was a brilliant woman as a human being. She always enjoyed to share her innovative ideas with her research group.

She never gave up difficult challenges and pushed others to achieve her goals. In addition, Marel enjoyed much of the opportunities to feed back and transmit her knowledge. Her passion for the research of photovoltaic materials and solar cells spread to all her staff. During her time at the IIM-UNAM, she left a dynamic of great rhythm and struggle until the end.

Marel analyzed the interaction of photons-energy with matter many times. These interactions help to see everything around us. However, we can see sequences of events in our dreams and memories etched in ourself, where there are no photons interactions. Marel left engraved an infinite number of unforgettable moments that were glorious in space-time, we just have to close your eyes and contemplate. We will always remember Marel by her great smiling, teachings and scientific contributions as a person full of light and energy.

Part of the academic and personal life of Marel will be presented in this talk.

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Reducing sugar production from corn stover and stem of faba bean by alkaline treatment followed dilute acid hydrolysis

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Faba bean and corn are predominant crops in Mexico State with an annual production of 32,033 and 26 million dry tons respectively; for faba bean this production represents approximately 55% of national harvest [1]. After harvesting the main residues generated are stalks, leaves and stover, which are disposed wrongly and contributing to environmental contamination. There are many treatments that can be transformed polysaccharides in agricultural wastes into reducing sugars. Among all them, acid hydrolysis has been reported as an efficient method to obtain high amount of sugars in a rapid and economic way, however, the efficiency of acid hydrolysis is limited by the physical barrier of lignin. Alkaline treatment has the potential to partially remove of lignin, allowing unaltered cellulosic fraction, which can be used to obtain monomeric sugar in subsequent enzymatic or acid hydrolysis processes [2], but studies referred to alkaline treatment followed acid hydrolysis are still few. The aim of this work was to evaluate the effect of alkaline treatment over sugar production yield from Faba Bean Stalk (FBS) and Corn Stover (CS) by dilute acid hydrolysis. Alkaline treatment was carried out at 100°C and 1%w sodium hydroxide for 60 minutes reaction time and using a ratio between liquid and solid phase of 15:1. Acid hydrolysis was performed with 5%v phosphoric acid and 100°C, employing raw and alkaline pretreated FBS and CS and a solid-liquid ratio of 1:15. After different times samples were taken and filtered in order to separate phases. Hydrolysates obtained after acid hydrolysis were used to quantify the amount of reducing sugar by dinitro salicylic acid method. Fourier Transform Infrared Spectroscopy (FTIR) analysis of alkaline treated samples showed a decrease in the intensity of the vibrational bands of lignin (1510 and 1590 cm^{-1}), while characteristic vibrations of cellulose (1000-1200 cm^{-1}) and hemicellulose (1240 and 1740 cm^{-1}) decreased their intensity and amplitude after acid treatment. For each test, the amount of reducing sugar increased as a function of time and sugar production data was adjusted to first order kinetic model.

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Study of Charge Transfer in Porphyrin with TiO_2 nanoparticles

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The growing level of environmental awareness over the last decades have stimulated an intense research into a solution of the energy crisis[1]. The need to replace fossil fuels with alternative and environmentally friendly energy sources has spread the use of renewable energies, harvesting the energy of the sun is a reasonable solution. However, photovoltaic technologies are mainly based on inorganic materials, which can contain toxic materials like CdTe, in addition to the high cost of production[2]. On the other hand, organic photovoltaics are inexpensive and environmental friendly. The efficiency record for organic cell is 11.9 ± 0.4 % in contrast to 28.8 ± 0.9 (GaAs thin film cell) for inorganic cell[3].

Porphyrin sensitised solar cells (PSSC) with TiO_2 are a promising solution for the need of green energy in the near future. The study investigates the charge dynamics recombination behaviour of Porphyrin using a range of steady state and time resolved techniques. The understanding of the dynamics will enhance the performance of PSSC with TiO_2. In this study, different porphyrins have been synthesized and optically characterised[4], the results showed that the compounds 3 (–OH, A_4), 9 (-OH, A_3B) and 11 (-COOH, A_3B) have the capability to be used in solar cells due to the proximity between LUMOs states and TiO_2 conduction band states. This a key part in the recombination dynamics of PSSC.

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Determination of kinetic and thermodynamic parameters of reducing sugar production by dilute acid hydrolysis of corncob

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Corncob is one of the most abundant agricultural residues around the world, it annual production exceeds 25 million dry tons in Mexico and commonly is disposed in open dumps contributing to environmental damage [1]. Corncob is comprised mainly by cellulose and hemicellulose, carbohydrates that can be used in biotechnological processes if they are transformed previously into monomeric sugars. Acid hydrolysis has been employed to depolymerized holocellulosic fraction in a rapid and efficient way; however, more researches are needed in order to improve the process performance and to determine kinetic and thermodynamic parameters. In this work, corncob was hydrolyzed with dilute phosphoric acid at different operational temperatures, acid concentration and reaction times, after acid treatment the amount of reducing sugars was determined in liquid phase employing dinitro salicylic acid method and the remainder solid was neutralized with hot distilled water and analyzed by Fourier Transform Infrared Spectroscopy (FTIR) as well as by X Ray Diffraction (XRD) in order to evaluate structural changes due to phosphoric acid contact. Results showed that the increase in sugar production yield can be associated with an increase in hydrolysis temperature and acid concentration, the maximum sugar production was 54.31 g sugar / 100 g corncob obtained at 110ºC, 7%v phosphoric acid and after 300 minutes reaction time, this value corresponds to holocellulose-monomeric sugar conversion of 74.77%. Moreover, sugar production data was adjusted to first order model, thus, kinetic and thermodynamic parameters were calculated. The major activation energy and the highest frequency factor were found with the minimum acid concentration. FTIR analysis showed a decrease in both amplitude and intensity of the main vibrational bands of cellulose (1200-1000 cm^{-1}) and hemicellulose (1740, 1240 cm^{-1}), while vibrations associated to lignin increase slightly their intensity (1510, 1590, 1432 cm^{-1}) [2].

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Synthesis of novel supramolecular dendritic systems for controlled drug delivery

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In this work, two novel supramolecular systems based on dendritic structures bearing β-cyclodextrin (βCD) for the intracellular delivery of Doxorubicin (Dox) were designed for future applications in the treatment of breast cancer.

The first part consisted on the synthesis, characterization and study of the kinetics of Dox-prodrugs hydrolysis, which are sensitive to acidic pH. Dox was linked to an adamantine unit (Ad) to give an Dox(Ad-Dox) complex with hydrolyzable bonds in acidic media (hydrazone, amide and ester), in order to select the linker with the best *in vitro* behavior. The Ad will allow the formation of an inclusion complex with βCD [1].

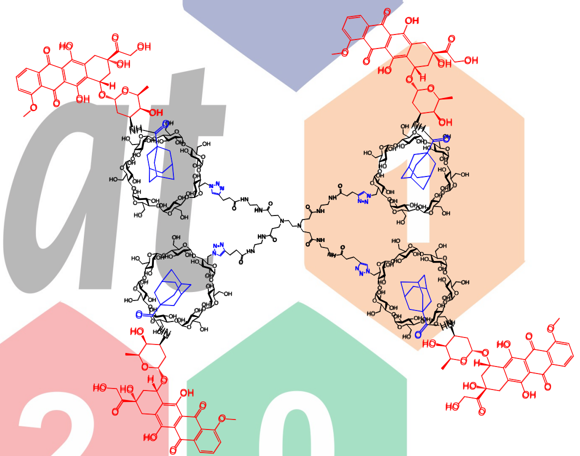

Figure 1. βCD-conjugated PAMAM G0 dendrimer

Herein, we propose the construction of two novel dendritic supramolecular systems, combining the primary face of the βCD with the PAMAM-G0 (**Figure 1**) and PAMAM-G1 dendrimers in order to increase the therapeutic load and control the release of the drugs [2]. According to the rational design, we evaluated only the Ad-Dox prodrugs that show a good cytotoxic activity *in vitro* in breast cancer cell lines.

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PREPARATION AND CHARACTERIZATION OF EXPANDED POLYSTYRENE WASTE NANOPARTICLES BY THE EMULSIFICATION-SOLVENT EVAPORATION METHOD: A DESIGN OF EXPERIMENTS APPROACH

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Expanded polystyrene (EPS) is is one of the most widely produced polymer products in the world due to its versatile application in different fields, mainly for insulation and packaging materials [1]. Many industries use EPS because of its versatility, dimensional stability, cleanliness, and low cost [2]. Nevertheless, the disposal of waste plastics poses a serious problem, because plastics are not biodegradable and cause environmental pollution. Therefore, alternative methods for EPS waste recycling are required. In this study, a recycling process was developed for the treatment of EPS waste in the preparation of nanoparticles with wide potential of technological applications. Recycled EPS nanoparticles were prepared by the emulsification-solvent evaporation method [3]. EPS wastes obtained from packaging material were processed and preliminary studies allowed to determine the suitable components and conditions for the preparation method. The obtained nanoparticles were characterized using dynamic light scattering and laser Doppler velocimetry. This study also evaluates the influence of critical factors such as polymer and stabilizer concentrations as well as the speed and time of stirring, on particle size and process yield, by applying a design of experiments (DoE) approach. Nanoparticle formulations were obtained with a narrow size distribution (PDI < 0.25) and zeta potential of -20 to -30 mV, showing adequate stability. Using an I-optimal design, it was possible to obtain an equation capable of predicting several optimum formulations with defined particle sizes and high process yields.

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COLLAGEN-CHITOSAN SCAFFOLDS CROSSLINKED WITH EDC FOR BIOMEDICAL APPLICATIONS

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Patients with skin injuries and cartilage associated diseases need biomaterials for wound healing [1]. Currently, natural polymers, such as collagen and chitosan, have been widely used in tissue engineering because they promote cell adhesion, growth and differentiation [2,3]. The objective of this work was to develop collagen-chitosan scaffolds improving their physicochemical and mechanical properties by chemical crosslinking with 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC), to be used in biomedical applications. The scaffolds 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 scaffolds. Mechanical tests presented that crosslinked scaffolds have the best mechanical properties. Degradation test indicated that crosslinked scaffolds dissolve more slowly than non-crosslinked scaffolds. Scanning Electron Microscopy showed a rough microstructure that is appropriate for biological applications. Cell attachment and viability tests suggested that crosslinking does not affect the excellent biological characteristics of scaffolds. In conclusion, crosslinking with EDC improves physicochemical and mechanical properties of scaffolds without affecting the biocompatibility.

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SYNTHESIS OF POLYMERS FROM 4-VINYLPYRIDINE AND ACRYLAMIDE BY FREE RADICAL POLYMERIZATION AND THEIR CHARACTERIZATION

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In this study, it is presented the synthesis by free radical polymerization of poly(acrylamide) homopolymer, p(AAm), poly(4-vinylpyridine) homopolymer, and their copolymer, p(4VP)poly(4-vinylpyridine-*co*-acrylamide) p(4VP-*co*-AAm). The stoichiometric ratio between 4VP and AAm was varied. For the synthesized materials, their physicochemical properties were studied, *i.e.* swelling ratio, determination of the critical pH value and their pH-sensibility. Moreover, they were characterized by FTIR spectroscopy, Scanning Electron Microscopy (SEM), Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA).

In the case of the p(4VP-*co*-AAm) copolymer in stoichiometric ratio 1:1, it was found a maximum swelling capacity at 12 h with a value of 190%. Meanwhile, p(AAm) homopolymer reached its equilibrium at 8 h having a maximum swelling percentage of 400%. Finally, p(4VP) homopolymer reached its maximum swelling capacity at 12 h having a maximum swelling percentage of 140%. The critical pH value of the p(4VP-*co*-AAm) copolymer was found around pH=5.5; this value agrees with the one reported by Fuentes (2009) [1]. On the other side, the pH sensibility test showed a very marked response of the homopolymer p(4VP) and copolymer p(4VP-*co*-AAm) to acidic pH (pH=3.3) due to the protonation of the pyridine ring upon passing to a basic pH (pH=9). At the same time, water absorption capacity was diminished because of the deprotonation of the pyridine ring [2]. Finally, from the spectroscopic and thermal characterizations, it was determined the successful incorporation of both monomers into the copolymer structure.

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SYNTHESIS AND CHARACTERIZATION OF POLYBENZIMIDAZOLES WITH APPLICATION IN MEMBRANES FOR GAS SEPARATION

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In the present investigation a serie of polybenzimidazoles (PBIs) were synthesized. These materials are a class of heterocyclic polymers that possess a high thermal, chemical and mechanical stability [1], which are required to form films with application in gas separation [2]. They were synthesized by polycondensation of 3, 3'-diaminobenzidine (DAB) and different aromatic dicarboxylic acids using Eaton reagent as condensing agent and solvent. The reaction times were evaluated in order to optimize the synthesis methodology and the physicochemical and thermal properties analysis of the polymers were obtained. PBIs were characterized by ^{1}H NMR, FTIR, TGA and measurements of inherent viscosity. The ^{1}H NMR spectra in Fig. 1 revealed that the polymers obtained from DAB and terephthalic acid (TPA) at reaction times of 8 hours and 140 °C showed a peak at 13.19 ppm (s, 1H) which is characteristic of the imidazole proton compared to those synthesized at 4 and 6 hours that did not exhibited this displacement. On the other hand, the FTIR spectrum presents bands at 3424.56 cm^{-1} (N-H stretching), 1621.93 cm^{-1} (C=O), 1433.80 cm^{-1} (aromatic), characteristics of a spectrum of polybenzimidazole. The ^{1}H NMR spectrum of the PBI synthesized from DAB and 4,4-oxybis-benzoic acid (OBA) in Fig. 2 revealed the presence of the imidazole proton when polymer was synthesized at 2 hours of reaction, while the FTIR spectrum supports the above.

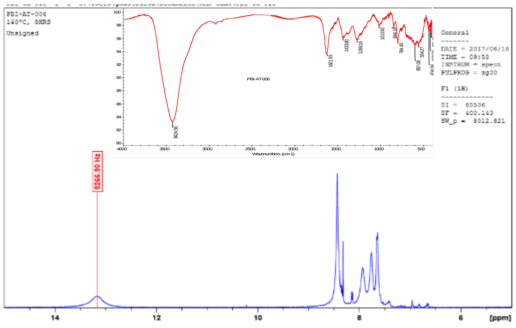

Fig.1 ^{1}H RMN and FTIR spectra of DAB and TPA synthesis.

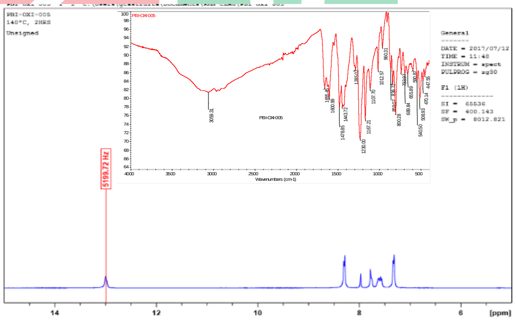

Fig.2 ^{1}H RMN and FTIR spectra of DAB and OBA synthesis.

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Two-step fabrication of micro-sized ZnO: temperature dependence of its electrical resistance

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In this work, micro-sized Zinc Oxide (Mic-ZnO) was deposited in two technological steps: the first consisted in deposition of nanostructured Zn by thermal evaporation method. The second stage was performed to achieve full oxidation and structural stabilization of ZnO. Mic-ZnO was characterized by Hall Effect, Scanning Electron Microscopy, X-ray diffraction, and Photoluminescence measurements. Electrical contacts were deposited to Mic-ZnO samples for their use in characterization of electrical resistance versus temperature. It was found that electrical resistance is decreased when temperature of the Mic-ZnO is increased in the temperature range of 200-500 °C.

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PROCESSING OF DENSE CERAMIC-CARBONATE MEMBRANES FOR CO_2 SEPARATION APPLICATION

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The present research is focused on studying the carbon dioxide permeation properties of a series of perm-selective dual-phase membranes made of a composite ceramic phase of $Ce_{0.9}Pr_{0.1}O_{2-\delta}/Pr_{0.6}Sr_{0.4}Fe_{0.5}Co_{0.5}O_{3-\delta}$ and a molten carbonate phase composed of $Li_2/Na_2/K_2CO_3$ mixture. First, porous membrane supports were produced by uniaxial pressing. Subsequently, dual-phase membranes were prepared by direct infiltration of the sintered supports with molten carbonate. Structural and microstructural characterization of the membranes was carried out by XRD, SEM and gas permeation techniques. CO_2 permeation measurements were conducted at high temperature between 700 and 900ºC.

The experimental conditions for the fabrication of crack free supports and the obtaining of a suitable dual phase membrane microstructure were explored and established. The SDC supports show a microstructure with interconnected porosity through their thickness. Permeation-separation studies using membranes of about 2mm wall thickness show high CO_2 permeation flux and stability. Moreover, prepared membranes exhibit high carbon dioxide perm-selectivity for CO_2/H_2 and CO_2/N_2 gas mixtures. This investigation demonstrates the potential design of highly perm-selective membranes for application on gas separation as well as membrane reactors.

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Study of Polyester Synthesis using Glycerol as Building Block

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The raw materials used to obtain the polymers come from different sources: these can be renewable (from living beings) and non-renewable (fossil resources). But fossil resources are the most common. Of these, petroleum is the basic raw material for the production of plastics, as a consequence of its ease of extraction and the development achieved by the technology to transform it into derivatives. [1] In this context, the use of raw materials from biomass is a more sustainable alternative. The glycerol is the by-product from the transesterification of vegetal oils, which is also obtained during the preparation of bio-diesel. This alcohol can be synthesized through fermentation or other chemical processes. Although many uses have been described for the glycerol (cosmetics, pharmaceutical applications, manufacturing of resins, among others), the demand is still increasing mostly in dental care (tooth paste) and food industries. [2]

This contribution describes the use of glycerol as a building block in polyesters.

Results

The synthesis of glycerol-based polyesters was explored, carrying out condensation reactions of glycerol with adipoyl chloride and glycerol with terephthaloyl chloride. In both cases the formation of a white precipitate was observed which was characterized by FTIR and 1H NMR spectroscopies.

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