

# **3<sup>RD</sup> BRAZIL MRS MEETING**

# October 10-13, 2004

# <u>SYMPOSIUM</u> C: SUPRAMOLECULAR MATERIALS AND DEVICES

Symposium Organizers:

Giovanni Marletta (Universitá di Catania, Italy) Rodrigo Martins (Universidade Nova de Lisboa) Osvaldo Novais Oliveira Jr. (IF-USP São Carlos)

### SYMPOSIUM C

### SUPRAMOLECULAR MATERIALS AND DEVICES

### Monday, 11 October, 2004

### Morning Session I – M1 – Chairperson – Ivo A. Hummelgen

8.00 - 8.40Celso P. Melo (UFPe - Brazil) - Properties of conducting polymer nanostructures obtained by emulsion polymerization 8.40 - 855Ivan H. Bechtold (IF-USP - Brazil) - Liquid crystal alignment on microtextured substrates 8.55 - 9.10 Valtencir Zucolotto (IFSC - USP - Brazil) - Enzyme immobilization in layer-by-layer films and its application in biosensing 9.10 - 9.25Younes Messaddeq (Unesp - Araraquara) - Structural characterizations of tungstate fluorophosphate glasses 9.25 - 9.40Elizabete Zaniquelli (DQ-USP, Rib. Preto) - Sulphated polysaccharide gels containing europium ions linked to two different binding sites. 9.40 – 9.55 Mário J. Politi (IQ –USP) - Naphthalimide Functionalized Calix[4]arene a

hydrophilic host cavity for apolar media.

### Coffee Break – 9.55 – 10.30

### Morning Session II – M2 – Chairperson – Rodrigo Martins

- 10.30 11.10 D. Martin Taylor (Bangor, UK) Interfaces, Traps and Related Effects in Polymer Electronics
- 11.10 11.25 Rodrigo F. Bianchi, (Poli USP) Complex impedance of polyaniline films studied by transfer-matrix technique and Cole-Cole dielectric function approach

- 11.25 11.40 Antonio Riul Jr. (Unesp Pres. Prudente) Layer-by-layer chitosan films for sensing applications
- 11.40 11.55 Ronaldo Giro (IF-USP) New Optoeletronic Multiblock Copolymer: Experimental and Theoretical Study

### Afternoon Session – T1 – Chairperson: Luiz H.C. Mattoso

- 14.00 14.40 John F. Wager (Oregon, USA) Transparent Thin-Film Transistors
- 14.40 14.55 M. N. P. Carreño (Poli USP) Plasma polymerisation of a fluorinated polymer for waveguide devices
- 14.55 15.10 Lucas F. Santos (IFSC USP) Transient photocurrent measurements in conjugated polymers
- 15.10 15.25 Paulo S.P. Herrmann (Embrapa São Carlos) Polyanilines-based sensors obtained using line patterning technique of graphite
- 15.25 15.40 W. M. de Azevedo (UFPe) Conducting polymer composite preparation catalyzed by Kaolinite clay
- 15.40 16.10 Rodrigo Martins (Lisbon, Portugal) Single Electron Thin Film Transistor

### **Poster Session**

### Tuesday, 12 October, 2004

### Morning Session I – M1 – Chairperson – José A. Giacometti

- 8.00 8.40 Frank Karasz (Amherst, USA) Efficiency in Polymer light emitting diodes
- 8.40 855 Laura H. de Carvalho (UFCG Campina Grande) Plasma modification effects on UHMWPE Membranes

- 8.55 9.10 José P. Donoso (IFSC USP) Influence of the nano-crystals in the ion dynamics of Pb-Cd fluorgermanate glass-ceramics investigated by conductivity and NMR.
- 9.10 9.25 Maurício S. Baptista (IQ USP) Chemical and biochemical applications of surface plasmon resonance on nanostructured films
- 9.25 9.40 Paulo B. Miranda (IFSC USP) Molecular orientation in self-assembled azo-polymer thin films studied by second-harmonic generation

9.40 - 9.55 Leonardo G. Paterno (Embrapa - São Carlos) - Fabrication of polyaniline

films by the self-assembly technique and their utilization in taste sensor systems

### **Coffee Break – 9.55 – 10.30**

### Morning Session II – M2 – Chairperson – Leni Akcelrud

- 10.30 11.10 Elvira Fortunato (Lisbon, Portugal) Recent Advances in ZnO Transparent Thin Film Transistors
- 11.10 11.25 Teodósio Del Caño (Valladolid, Spain) Photoelectrical conversion of twolayer and three-layer tytanyl phthalocyanine-perylene pigment organic solar cells.
- 11.25 11.40 Carla Rubinger (UFMG) Adhesion measurements by AFM on poly(5amino-1-naphthol) ultrathin films
- 11.40 11.55 Michelle Meruvia (UFPR) Pseudo-metal-base Transistor
- 11.55 12.10 David S. dos Santos Jr. (IFSC-USP) On the Surface-Enhanced Raman Scattering (SERS) effects in LBL films of silver nanoparticles

# Tuesday Afternoon – Free

# Wednesday, 13 October, 2004

### Morning Session I – M1 – Chairperson: Marília J. Caldas

8.00 - 8.40	Alessandro Gandini (IQSC - USP) - Furan chemistry at the service of
	functional macromolecules
8.40 - 8.55	Paulo T.C. Freire (UFC) - High temperature vibrational properties of L-
	isoleucine and L-histidine.HCl.H2O crystals
8.55 - 9.10	Victor Garcia Rivera (IFGW – Unicamp) – Ion-exchange planar waveguide
	of tellurite glasses, doped with Er3+ ions, for optic amplifiers
9.10 - 9.25	Tarik D. S. Mohallem (UFMG) - Characterization of nanocryslalline TiO2
9.25 - 9.55	Carlos J.L. Constantino (Unesp - Pres. Prudente) - Surface-enhanced Raman
	Scattering Applied to Thin Film Molecular Structure Investigation

### **Coffee Break – 9.55 – 10.30**

### Morning Session II – M2 – Chairperson: Carlos J.L. Constantino

10.30 - 11.10 Douglas S. Galvão (IF - Unicamp) - Computer simulation of nanostructures

- 11.10 11.25 L. P. Masiero (PUC Rio) Design of New Conducting Polymers
- 11.25 11.40 L. F. Roncaratti (UnB) Dynamics of polarons propagation on molecular circuits
- 11.40 12.10 Leni Akcelrud (UFPR) Macromolecular thermal transitions of PMMA probed by chemically bound anthryl chromophores

### Afternoon Session – T1 – Chairperson: Younes Messaddeq

- 14.00 14.40 M. Elizabete D. Zaniquelli Enzymatic catalysis in organized films
- 14.40 14.55 Sérgio Brochsztain (UMC) Characterization of self-assembled thin films of zirconium phosphonate/aromatic imides
- 14:55 15.10 Cléber R. Mendonça (IFSC USP) Possible applications of two-photon absorption phenomena
- 15.10 15.40 S. O. Vásquez (Santiago Chile) Theoretical study of energy transfer between oligothiophenes included in nanochannels.

#### **ORAL PRESENTATION**

#### C-0001 PROPERTIES OF CONDUCTING POLYMER NANOSTRUCTURES OBTAINED BY EMULSION POLYMERIZATION C.P. de Melo, UFPE, 50670-901 Recife, PE, Brazil

We report the principal results of an on-going systematic study on the preparation of different conducting polymers (CP), such as polyaniline, polypyrrole and polythiophene derivatives, organized as nanostructures enclosed in aqueous surfactant micelles and on their characterization by electrical impedance spectroscopy (EIS), and by ultravioletvisible and fluorescence techniques. Emulsion polymerization permits to control the synthesis of the CPs of interest, since the interior of the surfactant micelles provides an adequate ambient for the selective growth of the polymeric chains. EIS techniques allow us to follow the process of micelle formation at different surfactants/CP relative concentrations, and the dielectric characteristics (such as charge transfer and polarization effects) of the dispersed aggregates provide relevant information on their physical properties, both for the nanostructures in solution as for those embedded in a dielectric polymer film. The samples have been investigated by use of scanning electron microscopy and differential scanning calorimetry, as appropriate. We also discuss how the incorporation of metallic (like Fe and Au) nanoparticles can affect the dielectric and spectroscopic properties of these systems. Surfactant-CP nanostructures can find application in different fields such as anti-corrosive paints, environmental remediation, magnetic memories, fluorescent probes and contrasting agents for medical diagnosis.

LIQUID CRYSTAL ALIGNMENT ON MICTROTEXTURED SUBSTRATES I.H. Bechtold, L.T. Thiegui, F. Batalioto, E.A. Oliveira, USP-SP, Dpto. Física Experimental -IF/USP, São Paulo, SP, Brazil, Caixa Postal 66318, CEP 05315-970

C-O002 Surface treatments are used to obtain liquid crystal alignment, which is essential for technological applications. The competition between two aligning mechanisms open the possibility of new orientational states induced to liquid crystals. The use of azo-polymers allow the orientation of a periodic texture, with easy axis of orientation in different directions, by means of photo-alignment by polarized light. Periodic patterns have been recorded on polymers containing azo-groups covalent attached to the main chain, illuminating the film with a periodic pattern of constructive and destructive interference fringes, in the micro-size domain. The microtextured substrate is used to prepare cells, where the second surface is treated to induce a planar orientation, and the cells are filled with a nematic liquid crystal (5CB). The orientation of the liquid crystal molecules is determined by optical observations in a polarizing microscope. Using patterned substrates in the micro-size domain, planar configurations have been observed, however varying the direction of the photoalignment or the periodicity new orientational states are expected.

# C-0003 ENZYME IMMOBILIZATION IN LAYER-BY-LAYER FILMS AND ITS APPLICATION IN BIOSENSING

V. Zucolotto, A.P.A. Pinto, M.L. Moraes, A.P.U. Araújo, O.N. Oliveira Jr., IFSC, Grupo de Polímeros, IFSC, Av. Trabalhador Sao Carlense, 400, São Carlos, SP, Brazil CP 369

The enzyme Cl-catechol 1,2 dioxygenase (CCD) was successfully immobilized in ultrathin films obtained with the electrostatic layer-by-layer (LBL) technique, in which CCD was alternated with layers of poly(amidoamine) generation 4 (PAMAM G4) dendrimers. The fabrication of LBL films from PAMAM and CCD solutions onto quartz substrates was monitored with UV-VIS spectroscopy. An almost linear increase in absorption at 280 nm with the number of bilayers indicated homogeneous growth of the films up to 40 PAMAM/CCD bilayers. Atomic force microscopy (AFM) data showed smooth adsorption onto the substrate, with an average roughness of only 0.5 nm, which is significantly lower than for other polymeric LBL films. The thickness per PAMAM/CCD bilayer was 14 nm. The conformation of the CCD macromolecules was the same either in solution or in the LBL film, as revealed by circular dichroism (CD) spectroscopy. The enzymes showed activity for periods longer than a week after immobilization, thus allowing the LBL films to be used as biosensors for halogenated organic compounds, viz. catechol or Cl-catechol. More specifically, catechol detection was carried out by observing the formation of cis-cis muconic acid when the LBL film was immersed in a catechol solution. The acid is a product from the reaction between CCD and catechol, which displays absorption at 260 nm. Films with 10 PAMAM/CCD bilayers were employed to detect catechol in very dilute solutions, with concentrations as low as 10-11 mol/L

# C-0004 STRUCTURAL CHARACTERIZATIONS OF TUNGSTATE FLUOROPHOSPHATE GLASSES

Y. Messaddeq, G. Poirier, S.J.L Ribeiro, UNESP, Rua Francisco Degni s/n

Tungsten based glasses have shown to be very promising materials because of their specific properties such as high thermal and chemical stability, non linear optical behavior or photosensitivity. Transparent glasses were synthesized in the NaPO3 – BaF2 – WO3 ternary system and several structural characterizations were performed by X-ray absorption spectroscopy (XANES) at the tungsten LI and LIII absorption edges and by Raman spectroscopy. Special attention was paid to the coordination state of tungsten atoms in the vitreous network. XANES investigations showed that tungsten atoms are only six-fold coordinated (octahedra WO6) and are free of tungsten oxide tetrahedra (WO4). In addition, Raman spectroscopy allowed to identify a break in the linear phosphate chains as the amount of WO3 increases and the formation of P-O-W bonds in the vitreous network indicating the modifier behavior of WO6 octahedra in the glass network. Based on XANES data, we suggested a new attribution of several Raman absorption bands witch allowed to identify the presence of W-O- and W=O terminal bonds and a progressive apparition of W-O-W bridging bonds for the most WO3 concentrated samples (330% molar) due to the formation WO6 clusters. Investigations by 31P MAS-NMR confirmed the progressive break of linear phosphate chains by WO3 incorporation and showed that the three bonding oxygens of each phosphate tetrahedron PO4 are bonded to a tungsten atom.

# C-PO005 SULPHATED POLYSACCHARIDE GELS CONTAINING EUROPIUM IONS LINKED TO TWO DIFFERENT BINDING SITES

M.E.D. Zaniquelli, A.P. Ramos, R.R. Gonçalves, O.A. Serra, E.L. Crepaldi, D.Quimica, Fac.Filosof.Cienc.Letras Rib.Preto, Univ.S.Paulo, Av.Bandeirantes, 3900, 14040-901, Ribeirao Preto, SP, Brazil

Applications of carbohydrate-metal complexes are mainly related to analytical chemistry. extraction of heavy metal ions and support materials for solid electrolytes. Furthermore, polysaccharides have been used as gelling or thickening agents. Carrageenans, a sulphated polysaccharide, can produce different kinds of gels. Properties as hardness and syneresis of the gel depend on the supramolecular arrange of carrageenan helices related to the polysaccharide structure and on their aggregation, usually promoted by mono and divalent metal cations. However, gels of trivalent ions are poorly studied. Interesting, Ln(III) ions and Ca(II) are particularly alike in terms of size, nature of bond formation and coordination geometry. In this work we describe the preparation and characterization of kappa, iota and kappa-2 carrageenan gels formed in the presence of different europium ion concentration. The produced gels were analyzed by UV-vis absorption spectroscopy and time resolved emission spectroscopy. Two different binding sites could be distinguished from the emission decay lifetimes (t). At very low Eu(III) concentration the emission decay data can be fitted by a mono-exponential curve (t1 = 0.40 ms). Increasing the Eu(III) concentration, an additional faster decay is identified (t2 = 0.14 ms), associated to a higher symmetry for the Eu(III) binding site, as revealed by the intensity ratio of the bands (I0-2/I0-1) related to the transitions (5D0-7F2) and (5D0-7F1).

# C-0006 NAPHTHALIMIDE FUNCTIONALIZED CALIX[4]ARENE A HYDROPHILIC HOST CAVITY FOR APOLAR MEDIA.

Mario José Politi, I.A. Bagatin, G.J.-F. Demets, H.E. Toma, A.T. Cruz, Departmento de Bioquímica Instituto de Química B12 sala 1258, Universidade de São Paulo, Caixa Postal 26077, 05508-000 São Paulo, Brasil. IQ/USP

The synthesis and the inclusion properties of the title compound are presented. The conepinched calix[4]arene was functionalized with a naphthalimide fluorophore for the development of an optical sensor. Spectroscopic properties of the host (UV/Vis and fluorscence) were determined. Inclusion complex formation with the especially designed N ethanol-1,8-naphthalimide guest was studied and the association constant determined. Laser flash photolysis studies allowed the assignment of the pi-electron interaction character between the imide rings in the inclusion complex.

#### C-0007 INTERFACES, TRAPS AND RELATED EFFECTS IN POLYMER ELECTRONICS D. M. Taylor, University of Wales, School of Informatics, Dean Street, Bangor, Gwynedd LL57 1UT, UK

Interfaces control the performance of most electronic devices. They are no less important in polymer electronics. In this presentation results will be presented on polymer MISFETs based on poly(3-hexylthiophene) as the active semiconductor and either polyimide or polysilsesquioxane as the gate insulator, which suggest that interface states at the semiconducting polymer/insulator interface play a role in the turn-off behaviour of polymer transistors in much the same way as in silicon-based device. We will also show that time-resolved Scanning Kelvin Probe Microscopy coupled with Raman microscopy can be used successfully to investigate the charge-injection and charge charge-blocking nature of electrodes used in polymer electronics.

C-0008 COMPLEX IMPEDANCE OF POLYANILINE FILMS STUDIED BY TRANSFER-MATRIX TECHNIQUE AND COLE-COLE DIELECTRIC FUNCTION APPROACH R.F. Bianchi, A.C. Maciel, W.S. Sousa, J. Mariz G. Neto, J.P. de Lima, H.N. da Cunha, H.N. Nagashima, R.M. Faria, IFSC-USP / LME-EPUSP, Av. Prof. Luciano Gualberto, trav. 3, n 158, 05580-970, São Paulo - SP, Brazil.

The electrical properties of polyaniline films have been examined using a statistical model based on a resistor-capacitor network and on the Cole-Cole dieletric function approach to describe the polymer structure, the carrier relaxation time and also to simulate the real and imaginary components of its complex impedance. The developed statistical model takes into account the intrachain and interchain charge transport processes, as well as the polydispersiveness of the material. By the application of a transfer-matrix technique, it reproduces the complex impedance measurements carried out with polyaniline films in different doping degrees and at different temperatures. The results indicate that interchain processes govern the impedance behavior in low-frequency range, while for higher frequencies, intrachain mechanisms are dominant.

C-0009 THE EFFECTS OF POSITIONAL DISORDER IN EXCITON DISSOCIATION AT THE INTERFACE BETWEEN A CONJUGATED POLYMER AND AN ELECTRON ACCEPTOR

M. Koehler, M.G.E. da Luz, UFPR, Departamento de Engenharia Elétrica, Universidade Federal do Paraná, 81531-990 Curitiba, Brasil

The fabrication of organic photovoltaic devices is possible thanks to the efficient charge transfer across a conjugated polymer/fullerene (C60) interface. The first step of the charge transfer is the electron trapped in the C60 and the hole in the polymer, forming a short geminate pair of carriers. Due to the low dielectric constant of conjugated polymers, such short pairs must be strongly bound by the electrostatic interaction. However, the experimental activation energy of carrier photogeneration (less than 0.1 eV at room temperature) and the observed intrinsic dissociation yields ( in some cases above 50%) indicate that Coulomb attraction between carries within the pair is effectively counter balanced. Assuming the presence of a dipolar layer at the polymer/C60 interface, Arhipov et al. showed that the zeropoint oscillations of the on-chain hole can create a repulsive potential barrier at the heterojunction. Using Monte Carlo simulations, we extend Arhipov\'s model to calculate the potential barrier produced by an array of many dipole moments randomly distributed around an average position at the polymer/C60 interface. It is generally believed that the positional disorder decreases the efficiency of pair separation. We show, however, that the disorder in the position of the dipoles along the interface axis increases the repulsive potential barrier, favoring pair dissociation. This result have important consequences on the design of efficient organic photovoltaic devices.

# C-0010 NEW OPTOELETRONIC MULTIBLOCK COPOLYMER: EXPERIMENTAL AND THEORETICAL STUDY R. Giro, L.Y.A. Davila, A.M.M. Paredes, M.J. Caldas, L. Akcelrud, USP, Instituto de Fisica - DFMT - Rua do Matao, Travessa R, 187, São Paulo - SP - Brazil - Caixa Postal 66318 CEP

In the last decade conjugated polymers have been object of great scientific interest and large technological investments. Of particular interest are aromatic compounds of azomethyne, or Schiff-base type polymers. Polyazomethynes with thienylene and phenylene segments in an alternating form reached the electrical conductivity of 10-2 Scm-1. The low solubility of polyazomethyne is a limitation for technological applications. In this work we exploit a strategy used previosly for solubilizing PPV-type polymers (polyphenylene vinylene), that at same time confines the conjugated (cromophore) segments. To do this, we introduce nonconjugated spacers, forming a multiblock copolymer in a conjugated-non-conjugated form. We have synthetized in this way a new material, poly[oxyoctyleneoxy-(2,6-dimethoxy-1,4phenylene-1,2-ethinylene-phenanthrene-2,4diyl) named as LaPPS19. We performed also a theoretical study using a variety of methods from Molecular Mechanics (MM) to quantum semi-empirical techniques (AM1, ZINDO/S-CI). Our results show that isolated LaPPS19 chains are as expected non-conducting, with relevant electron localization over the phenanthrene group. We found that LaPPS19 could assemble in a pistacked form, leading to impressive inter-chain interaction that allows for electronic delocalization between neighbor chains and an expressive red shift of the phenanthrene-related absorption edge, in good agreement with the experimental results.

#### C-0011 TRANSPARENT THIN-FILM TRANSISTORS

05315-970

J.F. Wager, School of EECS, Oregon State University, USA

ZnO transparent thin-film transistors (TTFTs) are a recent and important development in the emerging field of transparent electronics. The purpose of this presentation is to present an overview of ZnO TTFT fabrication, performance, characterization, and possible applications. Particular emphasis will be devoted to elucidating TTFT device physics issues involving channel mobility and output conductance. Additionally, a new type of TTFT with a novel channel layer material will be reported and discussed in terms of possible future applications.

# C-0012 PLASMA POLYMERISATION OF A FLUORINATED POLYMER FOR WAVEGUIDE DEVICES

M.N.P. Carreño, J.R. Bartoli, E. Arashiro, J. Vatavuk, J.R. Soares, V.M. Giacon, USP, Grupo de Novos Materiais e Dispositivos LME - Laboratório de Microeletrônica,Departamento de Engenharia de Sistemas Eletrônicos,Escola Politécnica da Universidade de São Paulo, Av. Prof. Luciano Gualberto, trav. 3, 158, Sala C2-66 ,CP 61548, CEP: 05424-970, São Paulo, SP, Brasil

Polymer waveguide devices have attracted much attention and investigations in communication and interconnection optics due to the easy fabrication process or patterning capability and the versatile molecular design of polymers structure, allowing refractive index modelling for core and cladding. Polymethylmetacrylate (PMMA) shows the best optical properties among transparent polymers, being a very common core material for optical devices. Fluorinated polymers, with low refractive index, are generally used for cladding. Previous works showed the feasibility to use the plasma fluorination process to produce partially fluorinated polymers on PMMA films, reducing the refractive index of PMMA surface. Plasma of fluorocarbons is frequently used in microelectronic technologies either for etching of substrates or for deposition of polymerised fluorinated films. In this work, PMMA spin coated films (5 to 10 mm) were exposed to the CHF3 plasma (13.56 MHz). The plasma process variables: gas pressure and time were investigated to improve the thickness of the fluorinated polymer deposited on the PMMA. XPS analysis indicated that the surface of the fluorinated polymer has one fluorine atom for each carbon (F/C=1.2). The contact angle of wetting was around 100°. FTIR-ATR analyses showed high absorption intensities relative to CFx species. A thickness of approximately 0.3 mm was determined for the fluorinated layer; that should be adequate for cladding a PMMA waveguide of 10 mm core.

#### C-PO013 TRANSIENT PHOTOCURRENT MEASUREMENTS IN CONJUGATED POLYMERS L.F. Santos, G.C. Faria, A.R. de Andrade, S. Mergulhão, R.M. Faria, IFSC/USP, Av. Trab. S. Carlense, 400, C.P. 369, São Carlos, SP, Brazil

The study of charge-carrier transport phenomena in conjugated polymers has attracted much attention due to their semiconducting properties and potential applications in electronic and opto-electronic devices. In this work, time-of-flight technique has been used to study the transport behavior of both type charge-carriers (electrons and holes) in thin films of poly(2methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene) (MEH-PPV) deposited onto n-type Gallium Arsenide (n-GaAs) and indium-tin oxide (ITO) covered glass substrates, with semitransparent metallic electrodes on top. The technique is based on the measurement of current transients due to the drift by an external electric field of photogenerated charge-carriers produced by a short (in the order of ns) nitrogen laser pulse. Since the optical density of the films is usually high for the excitation wavelength, the photogeneration of electron-hole pairs occurs mainly near the incident surface and the transient photocurrent through the polymer bulk is practically dominated by single-type carriers (depending on the polarity of the applied bias). The transit times and the carrier mobility dependence on the electric field and temperature have been examined in the framework of dispersive transport model, characterized by the energetic and spatial disorder inherent to polymeric systems. Different metallic top electrodes and substrates were used in order to determine the energy barriers at the polymer/electrode interfaces.

C-PO014 POLY-ANILINES-BASED SENSORS OBTAINED USING LINE PATTERNING TECHNIQUE OF GRAPHITE P.S. de P. Herrmann, E.C. Venancio, A.G. MacDiarmid, L.H.C. Mattoso, Embrapa Instr. Agropec., Rua XV de novembro n.1452, São Carlos, SP, 13560 Brazil

> The development of a novel type of electrical sensor based on the line patterning technique of graphite, to the fabrication of inexpensive, disposable and highly sensitive sensors for volatile organic compounds (VOC) and water vapor, using poly-anilines as sensing layers was evaluate. Line patterning (LPT) of graphite was used to produce electrodes of graphite on commercial tracing paper and cloth, which were used as substrates to chemical sensors (VOCs) and water vapor. The electrical resistance [ohms] of the sensors were measured with ohmmeter, in the presence of tolueno and water vapor. The sensors were obtained by coating the electrodes with poly-anilines. The results have shown that the oligomer phenyl/-NH2 end capped tetraaniline emeraldine salt, as active layer of the sensor (sensor A) prepared with tracing paper, and 16-Finger interdigitated electrode, has presented the highest sensitivity to the presence of toluene (sensitivity to 5,000 ppm of ~11.0 %) and the Emeraldine.HCL obtained by in-situ deposition (1M HCl aqueous solution) was used as sensing layer of the sensor (sensor B) on cloth, showing through the results of the electric response that the device is sensitive and reversible to water vapor in dynamic mode. The both results are showing the potentiality of the LPT to developed disposable sensor. Preliminary results, using PET as substrate, are showing that the LPT can be applied to used as sensing units in electronic tongue device.

# C-PO015 CONDUCTING POLYMER COMPOSITE PREPARATION CATALYZED BY KAOLINITE CLAY

W.M. de Azevedo, G. Nascimento, E.F. da Silva Jr., UFPE, Departamento de Química Fundamental, CCEN, Universidade federal de pernambuco 50740-540, Recife, PE, Brazil

It is widely known that Al-silicates supports such as K10 montmorillonite clay behaves like a heterogeneous catalyst for the oxidation selected alcohol, benzylamine, and thiophenol in hydrocarbon solvents at room temperature with potassium ferrate (VI). Despite of excellent results, the role of the K10 solid support is not fully understood. In order to better understand the oxidation properties of Al-silicates, we investigate the oxidation properties of kaolinite clay, on the polymerization of aniline and pyrrole monomer in aqueous medium, the inorganic host serves as a template for a guest molecule to be assembled. The confined environment induces a high anisotropy of electric conductivity. Due to the complexity of this system, interesting questions related to the structure and properties of the nanocomposite remain unanswered. In this work we present an unusual route to synthesize conducting polymer /clay nanocomposites, using the oxidation properties of the Itapuama clay (a mineral clay found in the Pernambuco seaboard), to polymerize the aniline or pyrrole monomer instead of using conventional oxidizing agents. The nanocomposites are characterized by elemental analysis, Xray diffraction, FTIR, NMR and conductivity measurements. The insertion of polyaniline was confirmed by X-ray diffraction analysis, which shows a significantly larger d spacing expansion from 7.01 to 13,6 Å, thus indicating that the conducting polymer chain was aligned with layers of the clay.

#### C-0016 SINGLE ELECTRON THIN FILM TRANSISTOR

R. Martins, E. Fortunato, G. Gonçalves, P. Barquinha, UNINOVA/CEMOP, Campus de caparica, Portugal

The large advances in thin film technology lead today to the production of highly nanostructured thin films where there optoelectronic performances were highly enhanced. Most of the work until now performed aims to relate the performances of inorganic devices. The same happens when nanoscale devices are concerned.

In this paper we present a simulation model that tries to exploit the performances of using single electron devices based on hybrid structures. By doing so, we aim to produce devices exhibiting mobility as high as  $500 \text{ cm}^2/(\text{Vs})$  mare than 2 orders of magnitude larger than the actual values shown by the bulky material and with dynamic resistances above 30 Kohms. The theory and the model that supports all this assumptions will be present and discussed.

#### C-0017 INFLUENCE OF THE COLLECTIVE TRANSPORT IN THE ELECTRICAL PROPERTIES OF DOPED POLY(3-METHYLTHIOPHENE)

E.C. Pereira, L.A.G. Báring, L.C.M. Walmsley, A.A. Correa, UFSCar, Endereço: CMCDM-LIEC, Departamento de Química, Universidade Federal de São Carlos, C.P. 676, CEP 13565-905, São Carlos, SP, Rod. Washington Luís, km. 235

In conjugated polymers, quasi-one dimensional systems, the modulation due to the shorter distance of the atoms taking part in the double bond, compared with that of the single bond, which is called dimerization, is an example of a charge-density wave (CDW) modulation. Conjugated polymers can be considered as correlated insulators that upon doping can show semiconducting or metallic behavior depending on the doping level. The existence of a CDW modulation imply that the electrical transport will take place with two type of carriers: Free carriers and carriers taking part of the CDW condensate. The free carriers are responsible for an ohmic contribution to the conductivity (assuming ohmic contacts) and the collective transport is characterized by an increase of the conductivity with the applied electric field above a very small threshold electric field. In this work we apply Grüner et al phenomenological model of a CDW conductor to the voltage dependent 1kHz impedance (Z) and phase angle (d) room temperature data of doped pellets of poly(3-methylthiophene). The model supposes that the CDW condutor is represented by a resistive-capacitive network: a resistor Rc and a capacitor C in series (CDW branch) in parallel with a resistor Rn (the free carriers branch). The model allows two solutions for the capacitive reactance. Assuming  $Rc \ll Z/sen(d)$  two equations are obtained, one for cos(d)/Z versus V and other for Xc versus V. These equations allowed a good fitting of our data.

### C-0019 CHEMICAL AND BIOCHEMICAL APPLICATIONS OF SURFACE PLASMON RESONANCE ON NANOSTRUCTURED FILMS M.S. Baptista, IQ-USP, Departamento de Bioquímica, AV. Prof. Lineu Prestes, 748. São Paulo, SP

The surface plasmon resonance (SPR) technique, based on the measurements of small changes (10-5-10-6) in refraction index at a solid-liquid interface, has been used in several areas of science and technology, including biosensors, new materials and biochemistry1,2. In this work we describe the development of an on-line detector for determining the index of refraction coefficient of molecules and polymer solutions using SPR3, which is then used in various applications. The latter include work from our group and collaborators on the estimation of the thickness of layer-by-layer films adsorbed on solid substrates from polyelectrolytes, dendrimers, quantum dots and enzymes. SPR is also used to characterize interactions between membrane mimetic surfaces (thiol/lipid bilayer) and proteins (cytochrome C). Finally, strategies will be presented aimed at controlling adsorption of vesicles through the specific modification of the gold surface.

#### C-0020 MOLECULAR ORIENTATION IN SELF-ASSEMBLED AZO-POLYMER THIN FILMS STUDIED BY SECOND-HARMONIC GENERATION

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Ultrathin films of polymers containing azo chromophores are important for many applications such as optical data storage, formation of surface relief gratings, liquid crystal alignment layers and non-linear optical devices. Here we use optical second-harmonic generation (SHG) to study the molecular orientation of Layer-by-Layer self-assembled films of a polymer with azo side groups on a glass substrate. In the SHG technique, a high-intensity laser illuminates the sample and the intensity of the reflected light with twice the incoming frequency is measured. This SHG signal is proportional to the second-order nonlinear susceptibility of the film, which in turn depends on the orientational distribution of the azo chromophores in the film. Analyzing the SHG signal as a function of the input and output polarizations, a few parameters of this orientational distribution can be deduced. The results indicate that there is a preferential orientation of the azo chromophores in the film, leading to a significant optical nonlinearity. The films were found to be anisotropic on the surface plane due to the self-assembly procedure used for their fabrication. Such detailed structural characterization is important for understanding and optimizing the self-assembly technique to yield samples with the desired microscopic arrangement.

#### C-0021 FABRICATION OF POLYANILINE FILMS BY THE SELF-ASSEMBLY TECHNIQUE AND THEIR UTILIZATION IN TASTE SENSOR SYSTEMS L.G. Paterno, E.S. Medeiros, N.K Wiziack, F.H. Kanno, F.J. Fonseca, L.H.C. Mattoso, Embrapa Instrumentação Agropecuária, C.P.741, 13560-970, São Carlos – SP, Brazil

The Self-Assembly technique represents an attractive and simple way to produce ultrathin films of different kinds of materials, including proteins, polyssacarides, conducting polymers. The resulting nanostructured films have been used on the development of different kinds of molecular electronic devices, such as light emmitting diodes, odour and taste sensors and biosensors. Multilayer films can be built by the repetitive dipping of the suport into solutions of different materials. The way those layers are assembled depends on the kind of material deposited what can involve different types of physical and chemical interactions. In this sense, ultrathin films of conducting polymers, such as polyanilines derivatives have been fabricated by the self-assembly technique in our laboratory aiming their utilization as sensitive layers in odour and taste sensors. Different experimental conditions for the fabrication of these films have been investigated in order to understand the mechanisms involved on the polymer adsorption and for optimization of the film fabrication. In a second step, self-assembled films of polyaniline derivatives have been deposited onto gold interdigitated microelectrodes and employed as sensit units in a taste sensor system. A sensor containing 9 sensit units has been developed for beverage taste analysis and has shown to be able to distinguish different brands of commercial orange juice, by means of electrical impedance measurements and computational analysis.

#### C-0022 RECENT ADVANCES IN ZNO TRANSPARENT THIN FILM TRANSISTORS

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Zinc oxide is a well known wide band gap semiconductor material (3.4 ev at room temperature, in the crystalline form) which has many applications, such as transparent conductors, varistors, surface acoustic waves, gas sensors, piezoelectric transducers, UV detectors and more recently is attracting considerable attention for its possible application to thin film transistors. In this paper we present some of the recent results already obtained as well as the ones that are being developed in our laboratory. The main advantage presented by these new thin film transistors is the combination of high channel mobility and transparency produced at room temperature which makes these thin film transistors a very promising low cost device for the next generation of invisible and flexible electronics. Moreover, the processing technology used to fabricate this device is relatively simple and it is compatible with inexpensive plastic/flexible substrate technology

#### C-0023 PHOTOELECTRICAL CONVERSION OF TWO-LAYER AND THREE-LAYER TYTANYL PHTAHLOCYANINE- PERYLENE PIGMENT ORGANIC SOLAR CELLS. T. Del Caño, J. A De Saja, R.Aroca, H. Kageyama, Y. Shirota, Dpto. Física de la Materia Condensada, Facultad de Ciencias, Universidad deValladolid, Spain

In the present work, the performance of organic solar cells based on tytanyl phthalocyanine (TiOPc) and pervlene pigment, N,N'-Bis(propyl)-3,4,9,10а perylenebis(dicarboximide) (PTCDIPr) was investigated. TiOPc was chosen as donor material due to its excellent photocarrier generation ability. PTCDIPr was selected as acceptor due to the strong n-type character of perylene diimides The photoelectric conversion of the original ITO/PTCDIPr/TiOPc/Au bilayer cell was considerable increased by the implementation of two different approaches. First, by incorporating a thin mixed layer of both species between the donor and acceptor. This strategy improved the cell performance by increasing the opencircuit voltage (Voc) and the photocarrier efficiency at the TiOPc absorption region. Further, morphological changes on the three-layer cell were induced by ethanol vapor exposure provoking the TiOPc phase transition form amorphous to alpha-TiOPc. This treatment leads to an increase in the short-circuit photocurrent (Jsc) of the system since the photogeneration of charges carriers of the nanocrystallyne form is considerably higher than that of amorphous. This final three-layer EtOH treated cell shows a conversion efficiency of 0.57% under white light irradiance of 113 mW.cm-2.

# C-0024 ADHESION MEASUREMENTS BY AFM ON POLY(5-AMINO–1-NAPHTHOL) ULTRATHIN FILMS

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Poly(5-amino-1-naphthol) (PAN) is a conjugated polymer with good electrical conductivity and chemical anti-corrosive properties. This material is obtained by electrochemical polymerization of 5-amino-1-naphthol on metallic electrodes via the oxidation of the amine group. The structure of PAN is very similar to the emeraldine form of polyaniline, which is well known for its good passivating property with respect to iron. PAN films have proved to be useful for molecular electronic applications, owing to their semiconducting response and high chemical stability. In view of any of these applications, well adhered smooth films of controlled thickness and high substrate coverage are desirable. Atomic force microscopy (AFM) was used to investigate ultrathin films of PAN deposited by Langmuir-Schaefer (LS) onto silicon substrates. The AFM probe was also used to perform nano-indentation and nanodelamination of the polymeric film. We apply the Matthewson theory developed for studying micro-indentation and micro-delamination of polymers to describe our nano-delamination results. By measuring the applied vertical force at the beginning of the delamination process and by using an appropriated model for micro-indentation of elastic continuous systems, we estimate the critical interfacial shear strength for the PAN/Si interface as being approximately 160 MPa, which indicates that the polymer is well adhered to the substrate.

#### C-0025 PSEUDO-METAL-BASE TRANSISTOR

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A metal-base transistor is a three-terminal device, similar to the bipolar transistor, proposed as high-speed

device. The base is usually composed by a metallic thin film, and emitter and collector by inorganic semiconductors. Due to technically difficult steps involved in the fabrication processes, being the most challenging the deposition of the emitter, simpler and cheaper processes are desirable for wider use of these devices. Recently, we fabricated a very efficient hybrid metal-base transistor substituting the commonly used inorganic semiconductor as emitter for an organic one, showing that the use of organic semiconductors instead of inorganic ones, is not only possible but can also be very efficient. In this work, we present the results obtained by substituting not only the inorganic emitter but also the metallic base by an organic material. The pseudo-metal-base transistors, produced in a vertical structure (C60/Polymer/nSi), are significantly easier to fabricate and retain large values of current gain in the common base configuration.

# C-0026 ON THE SURFACE-ENHANCED RAMAN SCATTERING (SERS) EFFECTS IN LBL FILMS OF SILVER NANOPARTICLES

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The search for substrates for ultra sensitive spectroscopic analysis is a challenge facing surface science today. Substrates with controlled surfaces allow one to explore enhanced signals at metallic surfaces and therefore employ analytes that cannot be studied directly onto metallic surfaces. In order to obtain such systems we employed the layer-by-layer (LBL) technique to produce multilayer nanostructured films containing silver nanoparticles. We have found that dendrimers are suitable template materials that can be alternated with the layers of silver nanoparticles. Upon varying the generation of the dendrimer and the concentration of the solutions, we could alter the contents of silver nanoparticles, in addition to the surface-enhanced Raman scattering (SERS) effect. For the SERS analysis, the 785 nm laser line was employed with 2-naphalenethiol as analyte. The SERS effect was still significant with the analyte in contact with the inert polymer atop the LBL film. This opens up the possibility of ultra sensitive spectroscopy with analytes that cannot be deposited onto the silver surface.

#### C-0027 FURAN CHEMISTRY AT THE SERVICE OF FUNCTIONAL MACROMOLECULES Alessandro Gandini, USP-SC, Av. Trabalhador São Carlense, 400, 13566-590 São Carlos - SP

The specific features of the furan heterocycle were exploited to prepare a series of value-added functional polymers with potential applications in different technologies.

The synthesis of conjugated oligomeric precursors incorporating the furan ring led to the development of macromolecular materials which include luminescent, liquid crystal, mixed conductivity (electronic and ionic) and photosensitive devices. The application of the Diels-Alder reaction to furan/maleimide couplings provided means to prepare polymers with thermally reversible properties, including: -linear and dendritic structures displaying temperature dependent monomer/polymer equilibria; - self-mending cross-linked materials; - recyclable networks, particularly in the field of elastomers (tyres). The purpose of this communication is to illustrate the different approaches in terms of chemical principles (syntheses, mechanisms,...), structural characterisation, specific properties and potential applications. Apart from the intrinsic interest of these strategies, it is important to emphasise that furan derivatives are obtained from ubiquitous renewable resources (agricultural anf forestry by-products) and represent therefore a promising alternative to petroleum-based counterparts. In other words, the biomass can be rationally utilised as a source of advanced materials through farly simple procedures.

#### C-0028 SURFACE-ENHANCED RAMAN SCATTERING APPLIED TO THIN FILM MOLECULAR STRUCTURE INVESTIGATION C.J.L. Constantino, R.F. Aroca, DFQB, FCT-UNESP, CP 467, 19060-900 Presidente Prudente/SP, Brazil

Raman scattering is a powerful vibrational spectroscopy technique for the investigation of molecular structure, molecular organization and interfaces. However, the cross section for Raman scattering is extremely small, approximately 10-29 cm2 per molecule, reducing the scope of applications as an ultra-sensitive analytical technique. Recently, the high sensitivity of dispersive Raman equipment and the enhancement of the optical signal provided by surfaceenhanced Raman scattering (SERS) have allowed detection of the spectrum from monolayers to single molecules. Experimentally, a laser line in resonance with the dipolar plasmon absorption of metal nanostructures is chosen, leading to an amplification of the electric field around the metal. On top of that, surface-enhanced resonance Raman scattering (SERRS) has been used as a complementary technique. The latter is the result of a double-resonance, as both the surface plasmon of the metal and the electronic absorption of the material investigated are in resonance with the incident laser line. In this work we shall describe the use of SERS and SERRS to study molecular structure of Langmuir-Blodgett (LB) and layer-by-layer (LBL) films of several materials, including conducting, luminescent or azo polymers, dyes and target molecules for single molecule detection. Micro-Raman spectroscopy (including mapping and global imaging) contributes with an important addition of micrometer spatial resolution making it a suitable tool for surface analysis.

### C-0029 HIGH TEMPERATURE VIBRATIONAL PROPERTIES OF L-ISOLEUCINE AND L-HISTIDINE.HCL.H20 CRYSTALS

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The vibrational, structural and optical properties of amino acid and amino acid-inorganic complex crystals have received much attention in many laboratories around the world. In the last years we have investigated several crystals of this family under extreme conditions - low temperature or high pressure - and we have begun to study the effect of metal impurities on the growth kinetics and habit of some of them. In the present work we show results of one amino acid crystal, L-isoleucine, and one amino acid - inorganic complex, L-histidine hydrochloride monohydrate (LHICL), under ligh temperature conditions. L-isoleucine is a simple aliphatic amino acid, which crystallizes in a monoclinic structure with two crystallographically independent molecules with trans and gauche I conformations. We have studied the Raman spectra of L-isoleucine from 300 to 420 K, analyzing both the lattice modes and internal modes of molecular units in order to search anharmonic effects and eventual evidences of structural phase transitions. From our results we are lead to conclude that the structure is stable up to the highest temperature observed. The other material analyzed was LHICL which crystallizes in an orthorhombic structure with four molecules per unit cell. From the evolution of the Raman bands associated with the lattice modes we concluded that LHICL undergoes a structural phase transition between 380 and 400 K. Discussion related with the hydrogen bonds in LHICL crystal is also given.

 C-0030 ION-EXCHANGE PLANAR WAVEGUIDE OF TELLURITE GLASSES, DOPED WITH Er3+ IONS, FOR OPTIC AMPLIFIERS
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13083-970

The tellurite glasses doped with ions Er+3 have great importance in the manufacture of several devices in the optic integrated (IO). These glasses offer a great bandwidth in the window of the communications (1,55 um). Glass tellurite are attractive material, must that the optic amplifiers of these materials add greater capacity of transmission in the optical telecommunications systems, Dense Wavelength Division Multiplexer (DWDM), for presenting greater number channels. Detailed investigations into the characteristics silver-diffusion planar waveguides in the glasses tellurite oxides, relating the mode-propagation characteristics to the parameters of the diffusion process and deriving the refractive-index profile. Due this fact, in this work we report the manufacture and characterization of waveguides, whose matrix: 75TeO2-2GeO2-(10+X)Na2O-(12-X)ZnO-1Er2O3 (%mol), (X=0, 2, 5). The stability of the glass samples have been evaluated, using the Hruby criterion and differentiation Tx-Tg. Furthermore, had been made the measures of density, refractive index, Raman, absorption, luminescence and lifetime. After this, the best samples had been submitted to the process of ion-exchange in furnace at the temperature near Tg in a quartz container crucible with molten salt in the ratios 49KNO3-49NaNO3–2AgNO3. The process of ion exchange of ions of Ag+- Na+ is carried through in Tg±60, different time. Trough the method of prism copupling, measure the index and depth of the guides.

C-0031 CHARACTERIZATION OF NANOCRYSTALLINE TIO2 THIN FILMS PREPARED BY SOL-GEL PROCESS

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TiO2 is a very important material due to its multifunctional applications such as photocatalyst, gas sensors, and corrosion protector. Thin films of pure titanium oxide have prepared by the sol-gel process from titanium alkoxide mixed with isopropanol. The films were prepared and deposited on glass and quartz plates using the dip-coating process and they were adherent, transparent, homogeneous and free of microcracks. The influence of various parameters such as chemical concentration, viscosity, withdrawal speed and temperature of densification on film thickness is described. The structure was studied by low angle X-ray diffraction and infrared spectroscopy. Porosity and refraction index were estimated by spectroscopy UV/visible.

#### C-0033 COMPUTER SIMULATION OF NANOSTRUCTURES D.S. Galvão, UNICAMP, CP 6165 IFGW-UNICAMP CEP 13983-970

The study of nanostructures has been object of intense experimental and theoretical investigations in the last years. The advent of sophisticated experimental tools such as atomic force, scanning tunneling, and transmission electron microscopes has opened new and exciting fields of investigations, leading to the discovery of rew physical phenomena at the nanoscale such as new allotrope forms of carbon, quantized conductance, atomic suspended chains, etc..From a theoretical point of view classical and quantum molecular dynamics (MD) simulations have been proved to be a very efficient tool to address structural, mechanical and electronic properties of nanostructures. Classical molecular dynamics is a technique to compute the equilibrium and transport properties of classical many-body systems. A large class of materials can be described in this approach. Especially for nanostructures MD simulations are in many aspects very close to real experiments. Recently, although very limited due to its high computational cost, ab initio MD techniques have been developed and implemented, largely increasing the kind of properties addressable by MD simulations. In this presentation we will review and discuss some applications of these methodologies. We will focus on recent results obtained by our group for carbon nanostructures, metallic nanowires, and supramolecular structures.

#### C-0034 DESIGN OF NEW CONDUCTING POLYMERS L.P. Masiero, M.A.C. Pacheco, PUC-Rio, RUA JARDIM BOTANICO, 616 - AP 203 - BL A -CEP 22461-000

In the last years the possibility of creating new conducting polymers exploring the concept of copolymerization (different structural monomeric units) has attracted much attention from experimental and theoretical points of view. Due to the rich carbon reactivity an almost infinite number of new structures is possible and the procedure of search these new structures until now is the exhausting search. In this work, we have used a Genetic Algorithm (GA) to generate new structures with pre-specified properties. GAs are stochastic algorithms whose search methods model some natural phenomena: genetic inheritance and Darwinian strife for survival. The metaphor underlying GAs is that of natural evolution. In evolution, the problem each specie faces is one of searching for beneficial adaptations to a complicated and changing environment. The \"knowledge\" that each specie has gained is embodied in the makeup of the chromosomes of its members. Each polymer is represented by a chromosome that is evaluated using the LCAO (Linear Combination of atomic Orbitals) method. This way, evaluating each chromosome becomes a computational intensive task. Therefore, a distributed GA was employed and a cluster of computers, evaluating chromosomes in parallel. In this work, we have searched for one single structure of polymer. The results obtained suggest that the search for new complex structures of polymers is promising.

C-0035 NETWORKS AND BLENDS OF POLYANILINE AND POLYURETHANE: STRUCTURAL AND MORPHOLOGICAL CHARACTERIZATION BY CYCLIC VOLTAMMETRY, XPS AND EPR

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The interconnection of polyaniline (Pani) chains through polyurethane (PU) blocks of the same length but with different spacing has originated a series of new semi-conducting networks of varying crosslinking density, with good mechanical properties. Cyclic voltammetry, XPS and EPR were used to probe the molecular features of the conducting species, and to test a morphological model proposed previously, where a continuous Pani phase percolates a PU matrix, linked together by a mixed interphase. Blends with the same composition of the networks and a model structure of crosslinked Pani were also prepared for comparison purposes. The linkage between the two polymers, a urea type group, as well as hydrogen bonds was demonstrated by XPS. The degree of protonation for the pure components, crosslinked Pani and the networks, determined by XPS for CSA doped materials, showed that the networks are easier to protonate than the corresponding blends. The electrochemical behavior of the Pani/PU networks is similar to that of pure Pani showing somewhat broader peaks in the second redox process. EPR parameters demonstrated that the paramagnetic species was the same for pure Pani and the networks (cation-radical with g=2.0028) and the existence of a pure Pani phase for compositions richer in the conducting polymer, as indicated by AHpp values.

# C-0036 CHARACTERIZATION OF SELF-ASSEMBLED THIN FILMS OF ZIRCONIUM PHOSPHONATE/AROMATIC IMIDES

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The zirconium phosphonate echnique developed by Mallouk et al. is one of the most versatile methods for the construction of self-assembled thin films. The method allows the incorporation into the films of organic compounds containing phosphonic acid functionalities on opposite ends of the molecule (a,w-bis-phosphonates). Our group has been employing Mallouk's method to grow multilayered films incorporating phosphonate-substituted aromatic imides, which are organic compounds with outstanding photophysical, photochemical and electrochemical properties. The imides employed in the present work were N,N-bis-(2phosphonoethyl)-1,4,5,8-naphthalenediimide (NDI), N,N'-bis-(2-phosphonoethyl)-3,4,9,10perylenediimide (PDI) and N,N'-bis-(2-phosphonoethyl)-1,2,4,5-benzenetetracarboxymide (PMI). The films were grown on silicon and quartz substrates, which were primed using 3aminopropyltriethoxysilane (APTS), followed by phosphorylation with POCl3. The surfaces were then exposed alternately to aqueous solutions of a zirconium salt and the aromatic imide. Film growth was monitored by ellipsometry (silicon), UV/Visible absorption (quartz) and contact angle (both substrates), and was found to be linear (the same amount of material was incorporated at each deposition cycle). Comparison of the absorption spectra of the imides on the films and in solution revealed that the chromophoric groups (the aromatic rings) were stacked in the films, suggesting that compact layers were formed.

#### C-0037 PLASMA MODIFICATION EFFECTS ON UHMWPE MEMBRANES L.H. de Carvalho, H.L. Lira, T.L. Leal, K.M. Souto, C. Alves Júnior, UFCG, DEMa/CCT/UFCG, Caixa postal 10034, Campina Grande, PB. CEP 58109-970

The pore size and porosity of filtration membranes are essential for selectivity. It was shown that the pore size of UHMWPE membranes needed to be reduced if these membranes were to be used for water/oil separation. In this work, plasma surface modification effects on the pore size of sintered UHMWPE were investigated. Two different UHMWPE samples, having the same particle size (180 m) and different molecular weights (3x108 and 7x108 g/mol) were used to make the membranes. Sintering conditions were: 200°C for 60, 75 and 90 minutes. Surface modification was performed by methane plasma for 60 min; 419-423V; 0,01-0,02 A and 46-58°C. Membranes were characterized by SEM, contact angle and permeated water flow rate. Our results indicate that, for the unmodified membranes, increased sintering times led to flow reduction and that this decrease was more significant for the membrane manufactured with the lower molecular weight polymer. These results were associated with pore size reduction and better compactation. Plasma surface modification led to significant water flow reduction of the membranes. A 90% flow reduction was achieved for the membrane manufactured with the higher molecular weight polymer, sintered for 60 minutes. This behaviour was attributed to higher surface tension of the walls, lowering the flow. SEM analysis and contact angle measurements showed that plasma modification successfully modified the membranes surface characteristics and led to pore size reduction

#### C-0038 LAYER-BY-LAYER CHITOSAN FILMS FOR SENSING APPLICATIONS A. Riul Jr, B.A. Stracçalano, D.S. dos Santos Jr, C.J.L. Constantino, O.N. Oliveira Jr, UNESP, DFQB, Rua Roberto Simonsen 305, Presidente Prudente, SP, Brazil, CP 457, CEP 19060-900

The control of molecular architecture provided by the layer-by-layer (LbL) deposition method has been exploited in nanostructured films of chitosan and poly(styrenesulfonate, sodium salt) (PSS) to be used as sensing units in an "electronic tongue". Positively charged chitosan was obtained according to [1] while the commercially available PSS was used as the negatively charged polyelectrolyte. All solutions employed had pH = 3 and were prepared with ultrapure water supplied by a Milli-Q system. Three bilayers of (PSS/chitosan), (chitosan/PSS) and (chitosan/chitosan) films were adsorbed onto quartz plates. The rationale is to obtain distinct electrical properties for the LbL films with different architectures, though using the same materials. A further degree of control in film properties was the use of two acids to process chitosan, namely hydrochloric and acetic acid. In all cases studied a higher material adsorption occurred for chitosan processed with acetic acid. Strong hydrolysis of chitosan was observed in a short period of time (~ a week), altering significantly the film assembly. In order to check the suitability of the chitosan LbL films for sensing applications, stability studies were carried out in which the films were extensively washed with distilled water. Ongoing studies are being taken to look into possible interactions of chitosan LbL films with trace levels of heavy metal ions in aqueous solutions.

[1] D.S. dos Santos Jr et al, Macromol. Biosc. 3 (2003) 591.

# C-0039 OPTICAL AND ELECTROCHEMICAL PROPERTIES OF ELECTROCHROMIC SMART WINDOWS

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Electrochromic smart windows are of considerable technological and commercial interest because of their controllable transmission absorption and or reflectance. We have investigated the optical and electrochemical properties of an all-solid electrochromic. The electrochromic layers were WO3 and WO3:Ta films and CeO2-TiO2 film as counter-electrode, polymeric films based on natural polymers like starch or cellulose was used as electrolyte. Transmission spectra were recorded in the wavelength range 350–2200nm at different intercalation levels. The results show that transmittance of the device decreases upon intercalation in the devices and the insertion/extraction processes are reversible. The transmission difference between transparent and blue color states was about 40 %.

# C-0040 THEORETICAL STUDY OF ENERGY TRANSFER BETWEEN OLIGOTHIOPHENES INCLUDED IN NANOCHANNELS

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Energy transfer processes between guest chromophores in host-guest organic systems show interesting properties for optoelectronic applications. Recent experimental data of energy transfer processes between thiophene oligomers included in self-assembled nanochannels of perhydrotriphenylene (G. Bongiovanni et al.) are studied from a microscopic quantum chemical viewpoint. Ground state and excited states calculations for Terthiophene and Quinquethiophene molecules at different ab-initio levels are in good agreement to reported data on geometry and energy levels. Orientational and distortive effects due to inclusion of chromophores in the nanochannels are studied at a semi-empirical level and allows to determine in more detail mechanistic aspects and calculation of energy transfer rates between these oligomers. Macroscopic observables such as temporal resolved decays from the singlet excited states are obtained using statistical averages over the entire optical center\'s population.

C-0041 DYNAMICS OF POLARONS PROPAGATION ON MOLECULAR CIRCUITS L.F. Roncaratti, G.M. e Silva, UnB, Intituto de Física, Universidade de Brasília, 70910-900 Brasília, DF, Brazil

The branching of polyene chains has important consequences on the dynamics of nonlinear exitations like solitons and polarons. We concentrate ourselves to the scattering problems of a polaron caused by a branching in the polymer chain.

In the current work we study the charge propagation on conjugated polymers with bifurcation in order to model a molecular circuit. We report molecular dynamics results of charge propagation in molecular circuits build from branching off conjugated polymers. A 2-D tightbinding Hamiltonian is used to model the conjugated polymers with a bifurcation.

#### **POSTER PRESENTATION**

C-P001 POLARIZATION OF A SILICA SURFACE BY ELECTRIC FIELD: A STUDY BY SCANNING ELECTRIC POTENTIAL MICROSCOPY
R. F. Gouveia, A. R. Costa, M. C. V. M. Silva, F. Galembeck, UNICAMP, Bloco D sala 218. Caixa Postal 6154 - Campinas, SP - CEP 13083-970

Silica thin films grown on silicon wafers are electrostatically nanopatterned by DC polarization of gold stripe electrodes deposited on silica. The patterns are detected by concurrent AFM and scanning electric potential imaging. Samples used are 500 nm thick silica films formed by wafer oxidation and partially coated with sets of interdigitated parallel electrode stripes, using microlithography techniques. One set of electrodes was biased at voltages in the 1-10 V range while the other set was grounded. The images were acquired while electrodes were biased and also after they were all grounded, by scanning 10 nm above the surface. Potentials change while the electrodes are biased producing patterns that disappear slowly when the electrodes are short-circuited. These results are interpreted considering the following model: the silica surface contains OH groups from silanol or adsorbed water, that are reduced by electron injection from the electrodes and discharged as H2, leaving behind -SiO- negative ions firmly bound to the silica, that cannot be oxidized. The excess negative charges thus produced are slowly dissipated following adsorption of water vapor and O2 release. Surface charge concentrations were calculated and they reach 2.2 electron charge units per square micron. These results point towards the clear possibility for silica surface electrostatic nanopatterning by stamping with patterned electrodes.

#### <u>C-P002</u> NANOSTRUCTURED ORGANIC-INORGANIC HYBRID POLYANILINE FILMS FOR DOPAMINE SENSING

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Nanostructured polyaniline (PANI) films were employed in the fabrication of modified electrodes for dopamine (DA) sensing using either the Langmuir-Blodgett (LB) or the electrostatic layer-by-layer technique (LBL). The PANI used in the LB films was chemically synthesized in the emeraldine base form and then functionalized with CSA and mcresol prior to the dissolution in CHCl3. LB hybrid films (31 layers) were deposited onto ITO substrates in conjunction with a ruthenium complex Rupy 10 mol%. The water-soluble PANI used in the fabrication of the LBL films was prepared via the functionalization of the PANI emeraldine form with DMAc. LBL films were deposited using PANI as polycation in conjunction with FeTsPc. The LB or LBL films were subjected to DA detection using cyclic voltammetry experiments. In the presence of DA in the electrolytic solution (HCl), the PANI modified electrodes showed additional redox peaks at 0.27 and -0.09 V, and 0.23 and 0 V for LBL and LB films, respectively. The detection limit of concentration of DA was 4 x 10-5 and 2 x 10-4 mol/L for PANI-Rupy LB films and for PANI-FeTsPc LBL films, respectively. Of special interest in modified electrodes used in DA detection is the ability to distinguish between DA and ascorbic acid (AA) since these substances coexist in vivo. Both LBL and LB electrodes were able to distinguish between AA and DA.

#### <u>C-P003</u> POLYMER LIGHT-EMITTING DIODES BASED ON LANGMUIR-BLODGETT (LB) FILMS PRINCIPAL

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Among the several types of conjugated polymers used in recent investigations, PPV derivatives are prominent for being able to combine a reasonably good environmental stability with good optoelectronic properties. In this context, LB films may be an interesting alternative, once may be obtained with high degree of thickness control, low number of defects, and some degree of organization at the molecular scale. In this work, we report the use of a OC1OC6-PPV (poly(2metoxy-5-hexyloxi) p-phenylenevinylene), in the form of LB films for the fabrication of devices. We report the optical and electrical characterization of the device, which was fabricated in a sandwich configuration (ITO/OC1OC6-PPV/Al). UV-vis absorption measurements were used to probe the structural anisotropy of the LB films. For the sake of comparison, cast films also were fabricated and also deposited onto ITO to obtain the same device structure described above. The current vs. voltage measurements reveal that the device presents a classical behavior of a rectifying diode. The threshold value is about 1 V, and the onset of visible light occurs at around 8 V. The current for this LB-based device is 2 orders of magnitude higher than in a similar device, but with a cast film of OC1OC6-PPV as active layer. In addition, the LB device appears brighter than its cast-film counterpart, probably due to the anisotropy of the LB films.

#### <u>C-P004</u> TREATMENTS WITH OXYGEN PLASMA ON THE ITO FILMS FOR CONSTRUCTION OF ELECTROLUMINESCENT DEVICES

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Indium Tin Oxide (ITO) films are called Transparent Conductive Oxides (TCOs) has been a very used in electroluminescent devices as: Polymer or Organic Light Emitting Diodes (P/O PLEDs) devices due present good electrical and optical characteristics as: with wide-bandgap 4,5-4,8 eV, low resistivity, adherence on polymer and gl ass substrates and transparency (90 % at 550 nm), fundamental factors for construction of devices. Treatments with oxygen plasma on the ITO films surface improve the performance increasing the shine and decreasing voltage operation. In our experiment we carry out treatments on the ITO surface using Oxygen Plasma in Reactive Ion Etch (RIE) reactor type. The samples used in this work are commercial and deposited on Polyethylene Terephthalate (PET). The parameters condition were the exposition time from 5 to 80 minutes and 100 and 200 mtorr pressure, maintaining the constant temperature in 293 K inside the chamber. For analyses we used the sheet resistance measures with four point probe equipment, the thickness by profilometer technique and transmittance with UV-Vis spectroscopy. All techniques were measured in room temperature.

# <u>C-P005</u> MOLECULAR BLENDS WITH APPLICATION TO ORGANIC LIGHT EMMITING DEVICES

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Since the first report of an organic-light emmiting device (OLED), much research has been done aiming understanding the charge injection and recombination mechanisms in these devices. The simplest OLED wich can be done is constituded by a single emmiting organic layer. But these devices are not efficient enough. Adding some organic layers or blending materials with specific properties can enhance the luminescence and efficency of the devices. In this work, we investigate the electrical characteristics of devices made from blends of two molecules, one hole transporting (HTM Tri) and the other electron transporting and light emmiter (ETM Alq3). A band diagram of the HTM based on absorption spectrum and cyclic voltamogram is proposed. The devices are constructed in sandwich structure, the hole injection electrode being FTO (fluorine doped tin-oxide) and the electron injection electrode Ca:Al. The molecular layer is evaporated under vacuum. Devices made with different relative concentration of the molecules show different transport mechanisms, as revealed by the current density versus voltage cuves. At same voltage, the better device is that one in wich the current density is the highest one, increasing the recombination probability. The major current at 2 V is achieved by device with a concentration of 0.75 ETM. The morfology of the devices was studied using AFM, demonstrating a strong concentration dependence with the device with 0.8ETM showing a comparable smoother surface.

<u>C-P006</u> OPTICAL AND ELECTRICAL CHARACTERIZATION OF A NEW BIPHENYLENEVINYLENE DERIVATIVE

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In this work we determine the optical and electrical characteristics of a poly(pphenylenevinylene) derivative, poly(2,2'-bromo-5,5'-hexyloxy-biphenylenevinylene) or BHBPV. We determinate the positive charge carrier mobility of this polymer using currentvoltage measurements in F-TO/BHBPV/Al devices, applying the space-charge limited current model (F-TO:fluorine doped thin oxide). The F-TO substrates are conducting, showing low sheet resistivity (10 -15 ohm/). We determine the optical gap using UV-visible absorption spectrum and the ionization potential from the oxidation onset in cyclic voltammetry experiments, where BHBPV was deposited onto gold substrate. We use the photoluminescence spectrum to determine CIE chromaticity coordinates. Another important aspect in this work is a comparison with a previous work with another PPV derivative, poly(2bromo-5-hexyloxy-p-phenylenevinylene) (BHPPV), correlating changes in electrical and optical behavior with changes in the polymer backbone.

#### <u>C-P007</u> SYNTHESIS AND OPTICAL CHARACTERIZATION OF PSS-ND FILMS A. Marletta, M.C. Silva, F.H. Cristovan, W.O. Cruz, UFU, Faculdade de Física, Universidade Federal de Uberlândia, CP 593, 38400-902, Uberlândia-MG, Brasil.

The physic-chemistry phenomena present in the study of new materials are scientific important due to their relation with the development of technological products. In the case of Rare-Eaten (TR), this application is now present in optical components, glasses, phuorescence lights, nuclear energy equipments and others. Moreover, the optical properties of lantanideous are independent of the host matrix and, consequentially, the electronic structure is not affected considerable. For that reason, the solid-state materials, amorphous or crystalline, can be used to study the electronic structure of these elements. In this work, we present the synthesis route and the photo-physic study of polystyrene sulphonate (PSS) films doped with Neodymium ions (Nd3+). Films are available using conventional chemical characterization and the chemiometic methods were used to optimization the synthesis process. In best experimental condition, the incorporation of Nd3+ in the matrix is 13.92% without decrease the optical characteristic. In comparison of the literature, the spectroscopy data present similar results for this ion. The UV-Vis-IR spectrum presents an intense characteristic electronic transition 4I9/2 ® 4F5/2 + 2H9/2 at 800 nm and the infrared spectrum presents an enlargement as a result of Nd3+ coordination with PSS molecule. Nd-PSS films emission at 1061 nm (transition 4F3/2®4I11/2) was observed

#### <u>C-P008</u> THE METAL/POLYMER INTERFACE OF LAYER-BY-LAYER PPV FILMS

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Electronic properties of conjugated polymers in the interface electrode/polymer depend, generally, on the polymer chemical syntheses and the film processing. In this work we investigate the influence of the thermal conversion process of poly(p-phenylene vinylene) (PPV) films on hole injector electrode (indium-tin oxide - ITO). The thermal reaction elimination of the non-conjugated PPV precursor polymer introduces chemical sub-products (HCl) that react with ITO forming InCl3. These products diffuse in the polymer film and act as an oxidative agent, changing the polymer electronic structure in ITO/PPV interface. To minimize this effect, we used a new PPV precursor route with less aggressive chemical leaving groups deposited via layer-by-layer technique (LBL) in non-self-limited process. In this case, the LBL ITO/PPV films on a non-metal substrate. With this analysis we indirectly observe the decrease in the ITO-electrode degradation on metal/semiconductor interface. Atomic force microscopy technique was used to analyze quantitatively the microscopic proprieties of the film surface.

#### <u>C-P009</u> EFFECT OF ANNEALING ON RHODIUM PHTHALOCYANINE LANGMUIR-BLODGETT FILMS L. Gaffo, M.J.S.P. Brasil, F. Cerdeira, M.A. Cotta, W.C. Moreira, UNICAMP, Instituto de Física Gleb Wataghin, Cidade Universitária Zeferino Vaz, Campinas, Brazil, Caixa Postal

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Metallic phthalocyanines (MPc) are highly conjugated molecules with a wide range of applications due to their interesting optical and transport properties as well as their high thermal and chemical stability. Possible applications of MPcs include dyes, light-emitting diodes (LEDs), solar cells, gas sensors, electrochromic devices, electrochemical microsensors, optical sensors and high-speed printers. These compounds can be deposited as thin films using several techniques, such as the Langmuir-Blodgett (LB), vacuum-deposition, casting and others. We have studied the annealing effect over rhodium phthalocyanine (RhPc) LB films using ultraviolet-visible (Uv-vis.) spectroscopy and atomic force microscopy (AFM). The annealing was performed at temperatures between 100 and 200°C under a helium (He) or air atmospheres. Significant changes in the Uv-vis. spectra were only observed when the samples were annealed at 200°C. The changes depend on the presence or absence of oxygen in the atmosphere. The oxygen presence can be responsible for destroying bonds at high temperatures resulting in a markedly decrease of the Uv-vis. absorption bands. Annealing at 100°C resulted in a significant decrease of the film roughness. When the LB films are transferred to the substrate, water molecules are trapped with the RhPc molecules. Heating these films, water molecules are released from the film, while RhPc molecules are reorganized on the substrate.

C-P010 SELF-ASSEMBLING LITHIUM CLUSTERS STABILIZED BY AMINE LIGAND IN MOS2 - DIALKYLAMINE INTERCALATION COMPOUNDS, INVESTIGATED BY NMR SPECTROSCOPY

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Intercalation compounds of the group 4-6 transition metal dichalcogenides have been a subject of considerable interest during the last two decades mainly due to their potential importance as materials for electrodes in solid-state batteries. In this work we investigate the lithium mobility in a series of molybdenum disulfide-dialkylamine intercalation compounds. NMR experiments were carried out in the nanocomposites Li0.1MoS2[X]0.1-0.2, where X represents the organic species C4H10NH (diethylamine), C8H18NH (dibutylamine) and C10H22NH (dipentylamine). The temperature dependence of the NMR line shape and relaxation times of both Li-7 and H-1 resonances indicated the formation of self-assembling clusters stabilized by amine ligands within the interlaminar space of the intercalation compounds. The temperature dependence of the Li-7 spin-lattice time relaxation rates was attributed to fast exchange motion of the lithium ions between sites of this cluster. The NMR results shown that the lithium motional correlation time scale with the amine size of the nanocomposite, suggesting that the lithium exchange rate became smaller in the nanocomposites with greatest amine sizes. The alteration in the lithium dynamics (the gradual decrease in exchange rate) seems to be related to confinement effects in these systems, which can be ascribed to the geometrical restriction and packing effects resulting from the intercalation of the molecules.

C-P011 NEW POLYMER GEL ELECTROLYTES BASED ON HYDROXYETHILCELLULOSE STUDIED BY CONDUCTIVITY AND NMR J.P. Donoso, L.V.S. Lopes, G.O. Machado, A. Pawlicka, IFSC-USP, C.P. 369, CEP 13560-970 São Carlos, SP

The polymer gel electrolytes formed by hydroxyethylcellulose plasticized with glycerol and containing lithium perchlorate are investigated by complex impedance spectroscopy and Nuclear Magnetic Resonance (NMR). Solid polymer electrolytes have been extensively studied because of their potential use in technological applications, as solid state batteries and electrochromic devices. The characterization of the film samples was performed by thermal analysis (DSC), X-ray diffraction, scaning electron microscopy, and UV – Vis - NIR spectroscopy. The results shown that the addition of solvent enhances the conductivity, which reaches 6'10-5 S/cm at room temperature in heavily plasticized samples. The Li-7 NMR results indicate that this enhancement is associated with a decoupling of the lithium ion dynamics from the local motion of the polymer host, the increase in the mobility of the ionic species, and the increase of the charge carrier concentration resulting from the salt dissiociation after the addition of the solvent. The temperature dependence of the lithium NMR spin-lattice relaxation are interpreted assuming that there are two lithium ion dynamics. The potential applications of these gel electrolytes in electrochromic devices are discussed in consideration of the conductivity, NMR and optical spectrosopy results.

#### <u>C-P012</u> CHARGE MOBILITIES VALUES OF ORGANIC MATERIALS IN THIN FIELD EFFECT TRANSISTORS

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The development of organic electronics is growing fast due to the potential advantages of using organic materials as the semiconducting layer in electronic devices. In this work we have investigated the electrical characteristics of polymers and molecules using thin field effect transistors. The FET charge mobility could be obtained measuring current-voltage characteristics of the transistor with known channel length, operating in depletion mode under different gate voltages. Current – voltage characteristics of FET devices of organic materials will be presented and their FET mobility values compared with conventional mobility values obtained form sandwich diodes previously published. The FET-transistors were constructed using gold as the gate electrode, poly methyl-metacrilate as the insulator and nickel electrodes as the source and drain electrodes. The channels length are lower than 40  $\mu$ m. We would like to thank RENAMI/CNPq for financial support

#### <u>C-P013</u> EFFICIENT LUMINESCENCE POLARIZATION IN CONJUGATED POLYMERS UNDER LOW STRETCHING LEVELS

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This work reports a detailed characterization of the absorption and luminescence polarization properties of poly-(phenylenevinylene), PPV, thin films under very low deformation levels. The samples were prepared by casting the PPV precursor on Teflon tape, followed by a thermal conversion step at 230°C. Continuous axial stretch was applied at room temperature to the PPV/Teflon films inside the cryostat under vacuum (10-5 torr) which enabled simultaneous luminescence and absorbance measurements. Unlike the usual methods that use high draw ratios (L/Lo 2) to obtain highly ordered films, we demonstrate that low levels of deformation (1<L/Lo<2) are enough to obtain high luminescence polarizations (P// P^ =9). We suggest that the weak stretching is more effective in the disordered emissive regions, forcing a stacking not usually found in pure PPV, favoring polarization conversion.

#### <u>C-P014</u> ELECTRICALLY DETECTED MAGNETIC RESONANCE APPLIED TO ALQ3 BASED LIGHT EMITTING DIODES G.B. Silva, C.F.O. Graeff, F. Nüesch, L. Zuppiroli, FFCLRP-USP, Av. Bandeirantes 3900,

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In this work, we use electrically detected magnetic resonance (EDMR) to provide microscopic insight in processes such as charge injection, transport and recombination. We demonstrate that this sensitive technique can be used to study processes such as carrier transport and recombination in real devices. For this study we used homopolar and bipolar device architectures based on tris(8-hydroxy-quinolate) aluminum (Alq3), such as ITO/CuPc/alpha-NPD/Alq3/LiF/Al (bipolar), ITO/Alq3/alpha-NPD/Ag (hole-only) and Al/LiF/Alq3/LiF/Al (electron-only). In an EDMR experiment, microwave-induced changes in the conductivity are measured as the sample is subjected to a swept DC magnetic field. The measurements were done using an X-Band (9 GHz) and a K-Band (24 GHz) spectrometer at room temperature. In the case of bipolar devices, the EDMR signal is only observed in forward bias and when the diodes start to emit light. This signal is attributed to the spin dependent exciton formation and is composed of two lines. The first component has a linewidth of 16 G and a gfactor that decreases from 2.0046 to 2.0041, as the forward bias increases from 3 to 8 V. The second one is attributed to anions, and has a gfactor of 2.0035 and linewidth that increases from 20 to 35 G. The first component is attributed to cations, while the second one to anions. These signatures are corroborated by measurements in hole-only and electron-only devices where spin dependent hopping processes were observed.

 <u>C-P015</u> PHOTOPHYSICAL STUDY OF A CONJUGATED-NONCONJUGATED PPV-TYPE ELECTROLUMINESCENT COPOLYMER
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This work reports photo and electroluminescence studies of emitting species of one the first reported blue emitters, the conjugated-non conjugated multi-block copolymer, poly[1,8-octanedioxy-2,6-dimethoxy-1,4-phenylene-1,2-ethenylene-1,4-phenylene-1,2-ethenylene-3,5-dimethoxy-1,4-phenylene]. The steady-sate fluorescence spectroscopy of the polymer in solution at several concentrations as well as in film form, showed that in concentrated solutions and solid state, the spectra are characteristic of associated forms, such as ground-state dimers and/or excimers. Time-resolved fluorescence on the nanosecond time scale recorded at lem = 415 nm (24096 cm-1) showed a monoexponential decay of 1.20 ns, which is compatible with rigid forms of stilbene derivatives. It was demonstrated that only the aggregated forms are the emitting species in electroluminescence. The interplanar distance between the associated chains estimated by the Davidov splitting and theoretically calculated, was 3-5 Å.

C-P016 INFLUENCE OF CARBON NANOTUBES IN THE PERFORMANCE OF ORGANIC PHOTOVOLTAIC DEVICES

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Studies have been demonstred that the eficiency of photovoltaic systems is increased when the photoinduced charge transfer occur in interfaces conjugated polymer/fulerenes. Similar behavior can be obtained with mixtures of conjugated polymers and carbon nanotubes. In this work, we have used poly(3-hexyl thiophene) (P3HT) and different concentrations of multi walled carbon nanotubes (MWNTs) filled with iron oxide as active layer. The devices were made in sandwich structure with tin oxide doped with fluorine (FTO)/Baytron-P (Bayer) and aluminun as electrodes. The optical and electrical properties were studied by action spectra and J x V characteristics. The morfological aspects of films were analysed by SFM and TEM. Photovoltaic devices based on these composites demonstrated being more eficiency in exciton dissociation and charge transport until an certain concentration of MWNTs in the mixture. Above the specific concentration the J x V characteristics are MWNTs property. In order to improve some engineering aspects of the devices, a bilayer geometry was proposed and it was possible to modify the J x V characteristics obtaing rectifying curves with open circuit current.

#### <u>C-P017</u> CHALCOGENIDE FILMS FOR HOLOGRAPHIC RECORDING

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Because the density of information storage in optical media can be up to orders of magnitude better than in magnetic discs, there has been extensive researche into materials capable of optical recording. Chalcogenide films have potencial in this area and have been investigated as optical recording media for mass-memory applications such as data disc for video recording. In this paper we used the photoexpansion to record diffraction grating on a surface of photosensitive Ga10Ge25S65 thin films by means of interference of two UV laser beams at 351 nm.The diffraction efficiency (η) of first diffracted order were measured. Atomicforce-microscope (AFM) was used to perform a 3D imaging analysis of the sample surface topography that shows the superposition of an imprinted grating over the topography of the glass. The change in the absorption edge and the refractive index has been evaluated and a structural approach of the relief grating on the film surface has been discussed.

CHARACTERIZATION AND OPTICAL PROPERTIES OF A POLYQUINOLINE WITH C-P018 ETHER LINKAGES

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The interesting photophysical properties, high thermooxidative stability and high electron affinity of polyquinolines have attracted attention due to their potential application in electronic and optoelectronic devices. This work describes the synthesis and characterization of a polyquinoline where the quinoline rings alternate with phenyl ether, namely  $poly{[(2,2'-bis-$ (4-phenylquinoline)-1,4-phenylene]-alt-phenoxy. The monomers were 2,2'-bis-(6-bromo-4phenylquinoline)and 1,4-hydroquinone. The phenylquinoline was obtained through the Friedlander reaction that involves the condensation of an aminoketone and a diketone.Hydroquinone was used as received. The polymer was prepared by the aromatic nucleophilic substitution polymerization technique. The structural characterization was performed using FTIR. Good films were cast from NMP solutions. The absorption spectrum showed peaks at 290 and 360nm. The fluorescence spectrum exhibited emission maximum at 425nm and is red shifted 20nm in relation to the quinoline moiety. The absorption spectrum of protonated solutions showed a shoulder at 440nm in addition to the spectrum of non-protonated solutions. The fluorescence spectrum presented a large band centered at 464nm. The observed red shift of 40nm in relation to the non-protonated form suggests the presence of charge transfer from a non-protonated to a protonated part via an intra and/or intermolecular pathways.

# <u>C-P019</u> PECVD SILICON OXYNITRIDE FILMS FOR APPLICATION IN OPTICAL WAVEGUIDES

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In recent years, the interest for silicon oxynitride (SiOxNy) films in integrated optoelectronic devices applications has received great attention mainly motivated by their promising optical properties such as: low absorption losses in the visible and near infrared range, low mechanical stress and mostly because these materials would permit an integration with microelectronic devices making possible a larger packing density. Besides this, SiOxNy films, obtained by plasma enhanced chemical vapor (PECVD), can be easily deposited with different composition ranging from SiO2 to Si3N4 by simply varying the deposition parameters, such as it has already been demonstrated in previous works. These results lead to a high flexibility in choosing the refractive index of the films allowing the fabrication of waveguides structures with favorable characteristics and tunable properties. In this work, SiOxNy films with different chemical compositions were deposited by PECVD technique and used as core and cladding layer in optical waveguides. In order to obtain high optical quality and low attenuation levels the nitrogen composition of the core and cladding was varied from 3% up to 34% and the index contrast from 1% up to 12%. The optical characterization showed that depending on the chemical composition of the core and cladding layers it is possible to obtain low optical loss. Finally, these results are correlated with the physical and chemical characteristics of the constituent materials.

#### <u>C-P020</u> ORGANIC SWITCHING DEVICE FOR MEMORY APPLICATIONS R. Toniolo, M. Lepienski, A. Hümmelgen, UFPR, Departamento de Física

Organic switching devices are able to abruptly decrease its electrical resistance when the applied voltage reaches a critical value (Vcrit). This phenomenon is particularly useful for applications in data storage devices. In this work we present some results obtained with switches made of poly(5-amino-1-naphthol) between silver contacts. The device structure consists of a silver stripe formed onto a glass substrate. Perpendicular to the stripe length a gap is made thought a controlled scratch (using a nanoindenter) that cutes the stripe. In the gap, PAN is deposited and the device is ready to operate. When the applied voltage reaches Vcrit the device reduces its resistance by a factor between three and four orders of magnitude. This condition remains until the applied voltage is lowered to a limit value (Vhold < Vcrit). Thus, the high resistance (ON) and low resistance (OFF) states can be achieved adjusting the applied voltage. An important parameter for designing memory devices is the switching time, i. e., how fast the device can switch between OFF and ON states. In the present device, switching times of about 30 ms were observed. The controlled change between OFF and ON states and the fast switching time achieved for this device are suitable in applications where a volatile memory (RAM: random access memory) is required. The authors acknowledge CNPq and CAPES for financial support.

C-P021 FABRICATION AND ELECTRICAL CHARACTERIZATION OF POLYANILINE/SILICON CARBIDE HETEROJUNCTIONS M.L.L. Tashiro, E.A. de Vasconcelos, E.F. da Silva Jr., W.M. de Azevedo, UFPE, Grupo de Física de Semicondutores e Novos Materiais, UFPE- Departamento de Física, Recife, PE, Brazil, 50670-901

> Polyaniline (PANI) is a promising material for organic-semiconductor systems and devices. In the past few years, we demonstrated the fabrication of high quality PANI/Si diodes with high reliability and rectification ratio and its use in gas detection and ionizing radiation monitoring [1]. In this work, we present new developments in PANI/semiconductor applications with the successful fabrication of PANI/silicon carbide heterojunctions. We discuss the technique to obtain rectifying heterojunctions and the basic electrical characterization of the devices. The heterojunctions were formed by spin-coating of polyemeraldine base onto a silicon carbide (SiC) substrate (epitaxial layer, n-type 6H SiC, Si face). A gold top contact and a large area aluminum backside contact were deposited onto the PANI and SiC surfaces, respectively, to complete the device structure. The current-voltage (I x V) measurements were taken with a HP4155A Semiconductor Parameter Analyzer in a shielded dark box. At low biases (below  $\pm 1.0$  V) the I x V characteristics are approximately linear. At higher forward biases, they follow a power law dependence typical of space charge limited current in poor conducting materials with traps. Further investigation is under way to clarify the details of current transport and evaluate potential applications for this newly developed device structure.

<u>C-P022</u> PEO-BASED COMPOSITE POLYMER ELECTROLYTES STUDIED BY NMR AND CONDUCTIVITY

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Composite polymer electrolytes formed by poly(ethylene oxide) PEO, lithium salt and inorganic oxides have been the object of a great deal of research in the last decade because of their potential importance in the development of solid state batteries. The addition of nanoparticles of inorganic materials to polymer electrolytes materials has been found to improve ionic conduction and in some cases enhance film mechanical properties. In this work we investigated the influence of the space charge created by the presence of TiO2 nanoparticles on the lithium and polymer chain mobility in PEO LiClO4, by using complex impedance spectroscopy and nuclear magnetic resonance (NMR). The purpose of our investigation was to establish new reliable criteria for the composite preparation, in which the effect of the different parameters affecting the conductivity, as the space charge created by the presence of TiO2 nanoparticles, can be evaluated separately. Conductivity and H-1 and Li-7 spin-lattice relaxation NMR measurements were undertaken in composite samples prepared with PEO8LiClO4 and TiO2 nanoparticles of different sizes. Special care was taken with the synthesis and the characterization of the TiO2 particles and with the composite preparation. The NMR and conductivuty results shows that total surface area of the nano-particles is a important parameter in the definition of the electric properties of the composite and its control is necessary to achieve reproducible results.

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# <u>C-P023</u> A PHOTOPHYSICAL STUDY OF POLY(METHYL METHACRYLATE-CO-9-ANTHRYL METHYL METHACRYLATE)

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A series of poly(methyl methacrylate-co-9-anthryl methyl methacrylate) was prepared in which the anthryl groups were interspersed between each 2, 4, 10, 25 and 35 methyl methacrylate mers. The effect of the proximity of the chromophores in the photophysical properties was studied in dilute and concentrated conditions, showing that the association of anthryl groups giving rise to aggregates or excimers is strongly dependent of the chain conformations. The photophysical properties of cast-films of largely spaced copolymers are characterized by two decays: one of the isolated chromophore (longer decay rate and vibronically structured emission) and another of aggregated species (faster decay with some broadening of the rededge of the emission band). Copolymers having the chromophores separated by two or four methyl methacrylate units presented the highest degree of association and were the only electroluminescent materials. The proximity of anthryl moieties and the conformation of the polymer chains are important factors governing excimeric-like emission and film properties of anthracene containing polymers used in technological applications.

#### <u>C-P024</u> INFRARED-TO-VISIBLE CW FREQUENCY UPCONVERSION IN ER+3/YB+3 DOPED PHOSPHATE GLASSES WAVEGUIDES

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Glasses with nominal composition of xEr+3/yYb+3 doped 0.75NaPO3- 0.25Nb2O3 were prepared using conventional melting process, with y of 1 mol % and x ranging from 0.1 to 1.0 mol %. The optical properties of the glasses were measured by prism coupling technique at 632.8 nm, 543.5 nm and 1550 nm. Absorption spectra have been obtained at room temperature and Er3+ emission at 1.5 mm was evaluated as a function of the Er3+ concentration. Infraredto-visible upconversion emission, upon excitation at 980 nm, has been observed for all the samples. The upconversion results in green and red emissions. The investigation of the upconversion dynamic as a function of the Er3+ concentration and excitation power, show that processes such as excited state absorption and energy transfer upconversion are effective.

#### <u>C-P025</u> ELECTRICAL CHARACTERIZATION OF FLEXIBLE POLYANILINE FILMS FOR STRAIN GAUGE APPLICATIONS

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This work describes the design and the operation of thin polyaniline films used to produce a conducting polymer base-strain gauge sensor. Polymer strain gauges are of great interest due to their large recoverable strains, low cost, and potential for integration with other polymer devices, including diodes, transistors and batteries. Thin polyaniline films were prepared by insitu polymerization method on an interdigited chromium-gold microelectrodes previously deposited on poly(ethylene terephthalate) - PET substrates. The electrical characteristics of the polymer device were carried out as function of the polyaniline doping level using a typical Wheatstone bridge circuit in order to improve the device performance and efficiency. This circuitry allows the measurement of small strains characteristics of the polymer system deformation around 0.1 % and gauge factor higher than 5, which is typical of inorganic solids material under tension. The excellent adherence of the PANI films on PET, as well as the recoverable strain of greater than 1 % may be useful in the design of future devices. This work was sponsored by Fapesp, CNPq and IMMP/MCT.

# <u>C-P026</u> ENCAPSULATION OF FLEXIBLE ORGANIC LIGHT-EMITTING DIODES USING PHOTOCURABLE COATINGS AND POLYVINYLIDENE CHLORIDE (PVDC) C.S.B. Ruiz, R.F. Bianchi, E.A.T. Dirani, F.J. Fonseca, A.M. de Andrade, LME-EPUSP, Av. Prof. Luciano Gualberto, trav. 3, n 158, CEP 05508-970 São Paulo - SP, Brazil

One of the most promissing display technology to come along the last decades are the organic light-emitting diodes (OLEDs). They have potential to be produced on large flexible substrate which would enable processing in a roll-to-roll manner. However, as the organic material is very susceptible to water vapor and oxygen, thorough encapsulation is indispensable, which is crucial to performance and lifetime of the polymer display. Moreover, the barriers coatings requirements for such flexible devices must exhibit good adhesion to the display surface, as well as it must not damage their actives components. In this work we have investigated the use of photocurable coatings (urethane aliphatic diacrylate resin, 1,6 hexanodiol diacrylate monomer, photoinitiator, light stabilizer HALS and UV absorber) and polyvinylidene chloride (PVDC) films as protective layers of flexible light-emitting diodes based on poly (2-methoxy-5- (2'ethyl-hexyloxy) p-phenylene vinylene) - MEH-PPV. The material coatings were applied onto the botton and top of a typical device structure (PET/ITO/MEH-PPV/Al), and the electrical and optical characterisitcs of the OLEDs were carried out as function of light exposure time in air. The improving of the lifetime, as well as the excellent adherence of the coatings on the flexible sustrate, on the cathode and on polymer emissive layer shows the potential for such class of barrier materials to be used in OLEDs. This work was sponsored by Fapesp, CNPq and IMMP/MCT.

#### <u>C-P027</u> WRITING WITH CONDUCTING POLYMER

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One of the promises of this century will be the development of extremely low cost disposable plastic/paper electronic, which will be found in intelligent material devices, the requirement will be the use of standard office equipment instead of multiple etching and lithographic steps used in semiconductor technology. In this meeting we present a straightforward route to prepare conducting polymer patterns in subtract such as, plastic, transparence, paper, any material, using mostly standard office equipment, e.g. an office deskjet printer. Different of the process developed by MacDiarmid our proposal involve the polymer printing instead of use the printer ink to produce the patterns and afterwards proceed the polymerization on the blanc space left in the printing polymer images and ready only memory ROM devices using polyvinyl alcohol as a solid support doped with aniline monomer and transition metals. This method uses photons and transition metals instead of conventional oxidants to promote polymerization of aniline monomer deposited on a surface medium. The photo induced polymerization methods yields a composite patterns composed of conducting polymer and reduced metals.

<u>C-P028</u> OPTIMIZATION OF SYNTHESIS OF POLYSTYRENE WITH END-FUNCTIONALITY FOR CONSTRUCTION OF WELL-DEFINED BLOCK COPOLYMER WITH OPTICAL PROPERTIES

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The synthesis of well defined block copolymer by living free radical polymerization, have been studied in our research group be used in optical data storage materials. The synthesis strategy employed use a polymer chain end-capping with a nitroxide who acts as macroinitiator during copolymerization step. To obtain useful yielding in copolymer is necessary a good chain-end fidelity of nitroxide groups in macroinitiator b permit the re-initiation of chains with other comonomer. The literature points that the fidelity of chain-ends in case of polystyrene decreases as molecular mass increase, committing like this its employment in copolymerization step. In this study we use a factorial design[3] to plan the synthesis of polystyrene by living free radical polymerization mediated by 2,2,6,6-tetramethyl-piperidynoxy (TEMPO) to better understanding the factors that in reality affect the fidelity of nitroxyl groups in chains. The bulk reactions were design using a factorial planning 3x3 where the temperature, reaction time and molar ratio TEMPO/initiator (AIBN) were investigated. Three level of each factor were evaluated to better understand the possible interactions of these factors and how theses affect the yield. Until now the experimental results shows for low reaction time that high conversion can be reached in low and high temperature but good polymer yielding just is reached when temperatures in range of 122 at 130 oC is used.

<u>C-P029</u> COMPARISON OF THE STRUCTURAL PROPERTIES OF THE PECVD SIOXNY DIELECTRIC LAYER WITH THE INTERFACE ELECTRICAL PROPERTIES IN SI/SIOXNY/AL CAPACITORS

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Plasma enhanced chemical vapor deposition technique is considered an excellent candidate for fabricating SiOxNy dielectric materials due to the low temperatures utilized and to the ease of tuning the films dielectric properties with the deposition conditions. In previous works we demonstrated the possibility of producing higher dielectric constant SiOxNy films, allowing thicker insulating layers, minimizing tunneling current problems. However the interface state and effective charge density is worst than the obtained with standard SiO2 thermally grown films. This was attributed to a certain extent to the low deposition pressure of these films, which causes a high ion-bombardment of the growing surface. In this work we produce and characterize SiOxNy films deposited from SiH4/N2O/He gaseous mixtures at different deposition pressures in order to analyze the effect of this parameter on the films structural properties and on the SiOxNy/Si interface quality. The inert gas He is added to the gaseous mixture in order to prevent phase gas reactions when the deposition pressure is increased. In order to compare the film structural properties with the interface (SiOxNy/Si) quality, MOS capacitors were fabricated using these films as dielectric layer. The results show that for a deposition pressure of 120 mtorr, films with lowest interface state densities are obtained. A correlation between interface state density and concentration of nitrogen in oxygen-like sites is observed.

#### <u>C-P030</u> VERY WIDE BAND GAP DIAMOND LIKE A-SIC:H OBTAINED BY PECVD K.F.Albertin, A. Abe, M.N.P. Carreño, EPUSP, Laboratório de Microeletrônica, Av.Prof. Luciano Gualberto, 158, Travessa 3, CEP 5424-970, CP 61548, São Paulo, SP, Brazil

Hydrogenated amorphous SiC alloys (a-Si1-xCx:H) obtained by PECVD technique are of great interest due to the possibility of control the carbon content of the films by varying the relative concentration of the carbon gas precursor. In previous works we have studied the production of high quality stoichiometric a Si0,5C0,5:H semiconductor films, however the production of a high quality dielectric for future applications in opto-electronic devices is also important. So, in this work we focus on the production and properties of carbon rich material, with wide optical band gap and with the higher possible electrical resistivity. The a-SiC:H films are deposited from methane (CH4) and silane (SiH4) gas mixtures and two series off samples are studied : in the first series was varied the CH4 concentration in the chamber (90 to 99%) and in the second one was varied the substrate temperature (50° to 250°C). The films are characterized through electrical measurements and by infrared, Raman, UV-Visible and RBS spectroscopy to study the Si and C chemical bonding, optical band gap and carbon content of the films. Preliminary results show that the samples with the highest carbon content exhibit a very high optical band gap (3,6 eV) and very low electrical conductivity. This suggest that the excess of carbon in the films is incorporated in a diamond like form (sp3 C-C bonding). However, it is still not clear whether it is incorporated in a random bonding network or in diamond nano-clusters.

#### <u>C-P031</u> AN ALGEBRAIC SOLUTION FOR THE PREISACH FUNCTION V.B. Nunes, S.I. Zanette, A.O. Caride, Pontifícia Universidade Católica do Rio de Janeiro, Departamento de Física - Laboratório Van de Graaff - Caixa Postal : 38071 - Cep : 22452-970 - Rio de Janeiro - Brazil

In this work the Preisach function for the hysteretic behavior of a ferroelectric material is assumed to be approximated, as usual, by the product of two one-dimensional distributions with different mean values. We show that when the distributions are in bell shape, positive defined and they can be normalized, an algebraic expression for these functions is obtained using only the polarization data of the maximum loop and its derivative.

#### C-P032 CORRELATIONS BETWEEN MORPHOLOGY AND AGEING PROCESSES IN XLPE L. Akcelrud, J.V. Gulmine, UFPR, Departamento de Química, Centro Politécnico da UFPR, Caixa Postal 19081, CEP 81531-990, Curitiba/PR, Brazil

Crosslinked polyethylene (XLPE) is progressively replacing other types of polyethylene in electric cable insulation due the combination of better mechanical and thermal performance with good dielectric properties. An important issue related to this particular application is the resistance to outdoor conditions, since the replacement of damaged parts is onerous and requires the interruption of electric supply. In this regard morphology plays a very important role and was approached in terms of crosslinking density and crystallinity. The changes in the structure and properties of series of XLPE samples wth systematic variation in the extent of crosslinking were evaluated by SEM, DMA, XRD and tensile tests. A morphological model was proposed for these materials, in terms of the mechanisms and rate of the processes involved. Depending on time and temperature, gel content and average molecular weight between crosslinks can reach a plateau where further increments in peroxide concentration are detrimental since they only lead to more degradation products, without any consequence in structural parameters. The major part of the crosslinking process occurs at the first minutes of cure, therefore it is also of no use to extend the reaction for longer times. It seemed that the crystallization mode is more likely the Flory crystallization lamellar model than the "folded chain" structure, based on the differences found for crosslinking density for molten and crystalline samples.

#### <u>C-P033</u> EFFECT OF DOPANTS ON NANOSTRUCTURED POLY(O-ETHOXYANILINE) FILMS E.D. Brugnollo, D.S.Izidoro, H.H. Takeda1, F.J. Fonseca, L.G. Paterno, L.H.C.Mattoso, Interunidades em Ciências e Engenharia de Materiais

Nanostructured films containing layers of conducting poly(o-ethoxyaniline) POEA alternated with sulfonated poly(styrene) PSS were fabricated by the layer-by-layer method and the effect of different dopant acids on the film properties was evaluated by UV-Vis spectroscopy and AC impedance measurements. Different films were deposited onto gold interdigitated microelectrodes to test their sensing ability. UV-Vis data have shown that the amount of POEA on the POEA/PSS films increases linearly with the number of layers deposited independently on the type of dopant acid used in the polymeric solution. As a consequence, each layer deposited has contributed with the same amount of polymeric material but this amount was found to be strongly dependent on the type of dopant used. From the impedance measurements it has been observed that films containing different dopants have exhibited distinct electrical responses when immersed in a same kind of liquid leading to a characteristic finger print of the liquid analysed. Preliminary data have demonstrated the possibility of using such different POEA/PSS films as sensing units in a gustatory sensor system.

## <u>C-P034</u> EFFECTS OF ADDITIVES ON THE WEATHERING OF POLYETHYLENE FILMS WITH VARYING THICKNESS

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The rate of ageing polymeric materials used in outdoor conditions, in particular cables and assemblies for the electric industry are of prime importance, since they determine the lifetime of these items. The main parameters that govern weathering effects are solar radiation, temperature and thermal cycles, humidity, atmospheric pollutants, incidence of rain, oxygen content in the air. The resistance to ageing is determined by intrinsic factors as chemical structure and morphology and extrinsic factors as well, such as shape and dimensions. The incorporation of stabilizers to prevent photo- and thermal oxidation to weathering and to protect the material during processing is a widespread practice. This communication reports the results obtained with exposing polyethylene films to natural ageing in the city of Cuiabá, which is located in Mato Grosso State, having a warm weather with rain and dry periods. The polyethylene samples built with four polymer layers, were submitted to exposure during six months, with regular times of inspection. The ageing effects on the chemical structure were evaluated by the carbonyl absorption in ATR - FTIR. The attenuated total reflectance (ATR) was the most appropriate technique to probe the modifications, due to the films' lack of transparency in most of the cases. The performance of polyethylene was followed in samples with and without antioxidants, and with and without carbon black and correlated with the depth reached by the radiation.

#### <u>C-P035</u> DEPOSITION AND CHARACTERIZATION OF CONJUGATED POLYMERS ON TEFLON FOR POLARIZED AND FLEXIBLE LIGHT-EMITTING DISPLAYS F.C.B. Maia, F.E.G. Guimarães, R.M. Faria, IFSC/USP, Rua Trabalhador.

In display technology, flexible organic light emitting device (FOLED) is an organic light emitting device (OLED) built on a flexible base material, such as clear plastic film, instead of the usual glass base. The combination of flexibility and transparency raises new possibilities for displays. FOLED displays can be rolled up, folded, or worn as part of a wearable computer. The combination of flexibility and transparency raises new possibilities for displays. This work reports on absorption and luminescence properties of poly-(phenylenevinylene), PPV, films on Teflon. A thin PPV precursor (poly-(xylylidene tetrahydro-thiophenium chloride) was deposited by spin-cast and Layer-by-Layer methods on a Teflon tape (Dielectrix, 250 m thick) and thermally converted at 110 and 220 oC under vacuum during 30 minutes. Optical measurements, such as absorbance, could be easily carried out with Teflon which has a wavelength window that is almost transparent for the emitted visible light. In addition, the use of a Teflon tape as substrate for PPV allows the application of a cold stretching on very thin PPV films with an isotropic lateral contraction. It is particularly interesting, however, to study the optical properties of polymeric films under very low deformation levels. Unlike the usual methods that use high draw ratios (L/Lo 2) to obtain highly ordered films, we demonstrate that low levels of deformation (1 < L/Lo < 2) are enough to obtain high luminescence polarizations.

<u>C-P036</u> POLYMER/FULLERENE PHOTOVOLTAIC DEVICES: OPTIMIZATION AND CARACTERIZATION

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In this work we investigated the opto-electrical properties of organic photovoltaic devices formed by a heterojunction of a semiconducting polymer and fullerene. This combination has attracted significant attention after the discovery of the ultrafast photoinduced electron transfer from conjugated polymer to C60, wich is an excellent electron acceptor. Our photovoltaic bilayer devices were fabricated in a sandwich structure, using FTO(Tin Oxide doped with Fluorine)/PEDOT(PSS) as hole collecting electrode and aluminum as electron collecting electrode. The photoactive layers are the poly(3-hexylthiophenewith a sublimed layer of C60. The P3HT layer has different thicknesses, and the C60 layer has a fixed thickness. We present dependence of photocurrent with photoactive thickness layer. The electrical properties were investigated by measuring the action spectra and the current versus voltage characteristics in dark and under illumination in several wavelengths. The understanding of the process of charge generation and transport of these charges is indeed important for obtaining improved efficiency. The authors acknowledgements CT-ENERG/CNPq and RENAMI for financial support.

<u>C-P037</u> AL-SI MATRIX PREPARED NON-HYDROLYTIC SOL-GEL ROUTE USED IN IONOMER GLASS

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In this work we investigate the preparation of the ionomers glasses by non-hydrolytic sol-gel route as an alternative methodology to obtain aluminum-silicon matrices. The preparations of the gels were carried out in oven dried glassware in two ways. In the first one, the AlCl3, SiCl4, CaF2, AlF3, NaF, AlPO4 and ethanol were reacted in reflux under argon atmosphere. In the second one, only AlCl3, SiCl4 and ethanol were initially mixed, and the other components were added at the end of the reaction. Europium III chloride was added as a structural probe. The powders mixtures were dried and -heated-treated at 1000oC during 4 hours. The formation process and structure of the powders were studied by means of thermal analysis (TGA/DTA/DSC), photoluminescence (PL) and nuclear magnetic resonance (NMR 27Al-29Si). The TGA/DTA/DSC show a constant loss of mass in the first methodology and this can be ascribed to a structural change during heat. In the second methodology only one loss of mass occur until 300oC, indicating that the matrix stabilized after this temperature. The excitation spectra present maximum in 392 nm corresponding to 5L6 level and emission spectra of Eu III ion present bands characteristic transitions arising from the 5D0 - 7FJ (J = 0, 1, 2, 3, 4) monifolds excited at their maximum. The magnetic dipole 5D0 - 7F1 and electric dipole 5D0 - 7F2 transition present more band than allow, this indicated different Eu III site in matrix.

<u>C-P038</u> MICROWAVE SYNTHESIS OF YAG:EU BY SOL-GEL METHODOLOGY

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With this work we investigated the preparation of YAG by non-hydrolytic sol-gel route as an alternative methodology to obtain yttrium-aluminum matrix from inorganic precursors (yttrium and aluminum chloride). The preparation of the gel was carried out in oven dried glassware. The AlCl3, YCl3 and ethanol were reacted in reflux under argon atmosphere. Europium III chloride was added as a structural probe. The powder was dried and heat-treated in modified microwaves. The samples were pre-treated at 50 and 800oC during 1 hour and then heated in microwaves for 30 seconds, 2 and 4 minutes. The formation process and structure of the powders were studied by means of X-rays diffraction (XRD) and photoluminescence (PL). XRD presents only picks corresponding to the YAG phase. PL date showed that the YAG phase was formed in 2 minutes with the samples pre-treated at 50oC. For the samples pretreated at 800oC, the YAG phase appears in 30 seconds. The excitation spectra present a maximum of 394 nm corresponding to the 5L6 level and emission spectra of Eu III ion present bands characteristic transitions arising from the 5D0 - 7FJ (J = 0, 1, 2, 3, 4) monifolds excited at their maximum. The magnetic dipole 5D0 - 7F1 transition presents more intensity than the electric dipole 5D0 - 7F2 transition. This methodology showed efficiency in obtaining YAG phase.

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<u>C-P039</u> REVERSIBLE COLOUR CHANGES IN PHOSPHONIOBATE GLASSES A.J. BARBOSA, R.R. GONÇALVES, F.A. DIAS FILHO, R.H. SHIBUYA, J.P. DONOSO, C. MAGON, Y. MESSADDEQ, S.J.L. RIBEIRO, 1: UNESP-IQAr Endereço: Laboratory of Photonic Materials, PoBox 355, Araraquara-SP, 14801-970, Brazil

Glasses were prepared by using conventional melting process with nominal composition (molar fraction) of 1-x NaPO3- x Nb2O5, with x varying from 0.15 to 0.30. Stable glasses have been obtained with refractive index varying from 1.58 to 1.75 with the increase in the Niobium content. The optical and structural properties were analysed as a function of experimental parameters, such as melting temperature ranging from 1100 to 1400C and nominal composition. Changing the melting temperature distinct coloured vitreous systems were obtained with reversible behaviour. Absorption spectra and Electron Paramagnetic Resonance results clearly show that the colour transition could be assigned to the Nb5+DNb4+ equilibrium. Structural properties were analysed by Raman, FT-IR, UV-VIS and 31P NMR. The introduction of the Nb2O5 promotes a strong modification in the phosphate chains evidenced by 31P NMR and Raman analysis. This changes together with the observed increase in Tg with the increase in the niobium content allowed suggesting that niobate groups are incorporated in the vitreous network by P-O-Nb-O-P bonds.

<u>C-P040</u> LAYER-BY-LAYER NANOFILMS INCORPORATING HUMIC ACIDS AND POLYELECTROLYTES

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We report on the preparation and characterization of nanostructured layer-by-layer films incorporating poly(allylamine hydrochloride) (PAH) and humic acids (HAs). HAs are organic macromolecules with polydisperse colloidal and polyelectrolyte characteristics. The functional groups in HAs are mainly carboxylic and phenolic hydroxylic groups. Based on the effective charge reversion (PAH-HA), many PAH/AH bilayers were deposited onto different substrates, namely glass, quartz, and ITO and Au-covered glass substrates. Film growth was monitored layer by layer via UV-VIS spectroscopy. The films presented well-defined globular morphology comprising grains of ca. 10 nm, as revealed by atomic force microscopy (AFM). The thickness of a PAH/AH bilayer was estimated with AFM to be ca. 0.8 nm. The HA-incorporating LbL films were further analyzed using cyclic voltammetry, showing a reduction peak at ca. 0.67 V (vs Ag/AgCl). A linear increase o the reduction peak as a function of number of bilayer was observed. Furthermore, the influence of the scan rate on the peak current of ITO/PAH-HA is indicative of charge transport involving the HAs layers and PAH. FTIR-ATR measurements confirmed the presence of specific interactions between the carboxylic groups from HAs and the amine groups from PAH.

<u>C-P041</u> CAPACITANCE SPECTROSCOPY APPLIED TO OPTOELECTRONIC POLYMERIC DEVICES

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In this work, we apply capacitance spectroscopy in a broad frequency range (10-1 to 106 Hz) to study photocarrier generation, transport and recombination processes in semiconducting polymeric devices using monochromatic light excitation (photon energy  $\sim 1.5 - 4$  eV). It is observed that the illumination increases the device overall dc conductivity as well as the equivalent capacitance for photon energies above the optical absorption band edge. The dc photocurrent action spectra as well as the photocurrent-voltage curves (I-V) of the devices are used in the interpretation of the capacitance spectra obtained at different photon energies. The increase of the capacitance in the low-frequency regime is attributed to the formation of a thin depletion layer close to the polymer/electrodes interfaces. The temperature dependence of the capacitance-frequency curves presents activation energies in the order of few tenths of eV, indicating the presence of shallow carrier trapping levels. In addition, the bias dependence of the junction capacitance, extrapolated from dielectric response functions, allows the determination of the acceptor concentration as well as the width of the space charge region.

<u>C-P042</u> SULFONATED POLYANILINE/POLY(3-METHILTHIOPHENE) - BASED PHOTOVOLTAIC DEVICES F Muchenski R M O Mello L Micaroni L S Roman · LA Hümmelgen UEPR

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We investigate the influence of sulfonated polyaniline (SPAN) film as intermediate layer between electrode, tin oxide (TO), and the active layer of photovoltaic devices based on poly(3-methilthiophene), PMeT. Both, PMeT and SPAN are prepared by eletrochemical methods. TO fims are produced by chemical vapor deposition onto glass substrates. The TO films had a thickness of ~ 470 nm, roughness of ~ 6 nm and electrical resistivity of ~ 7x10-5 ohm.m. In TO/SPAN/PMet/Al devices the IPCE reaches 12.1 % and power conversion efficiency 0.8 % under monochromatic irradiation (wavelenght = 580 nm; 0.8W/m2). When submitted to AM 1.5 irradiation these devices present power conversion efficiency of 0.04 % at 1,000 W/m2. As the morphology of the films produced by eletrochemical methods has strong thickness dependence, it is reasonable to expect that it largely influences the present results. For larger thickness we have an increase in the roughness in the PMeT surface and as a consequence, an expected improvement in the electron-hole pair dissociation rate at the PMeT/Al interfacedue to increase in effective interface area and existance paths for exiton diffusion up to dissociation sites shorter than those of homogeneously thick films. The authors thank CNPq and CT-ENERG/CNPq for financial support.

<u>C-P043</u> PHYSICAL AND THERMOCHROMIC PROPERTIES OF WO3 BASED THIN FILMS B. Montanari, G. Poirier, M. Siu Li, S.J.L. Ribeiro, Y. Messaddeq, UNESP – IQA Laboratory of Photonic Materials, Araraquara, São Paulo, Brazil, PoBox 355

Tungsten oxide films have been studied intensively during the last decades, due to their interesting properties such as electrochromism, photochromism, thermochromism and catalysis. Many applications have been envisaged for WO3 films, such as switchable windows, displays and mirrors, gas sensors and others. Many systems were investigated but the properties of these films are largely influenced by many experimental parameters witch are difficult to control. This behavior is due to the facility of tungsten atoms to adopt various oxidation states.

In this work, vitreous samples were prepared in the NaPO3 – BaF2 – WO3 ternary and in the NaPO3 – WO3 binary systems. These glasses present high thermal stability, large chemical and mechanical resistance and good optical quality. Samples containing high amount of WO3 (concentrations above 40% molar) have been used as target to prepare thin and thick films. Such films were deposited by electron beam evaporation method. The evaporation rate has shown to be a fundamental parameter for the final chemical composition. The films were characterized by X-ray diffraction, perfilometry, UV-visible transmittance, infrared reflectance spectroscopy. The optical properties of these films are very dependent of the room atmosphere. In fact, their thermochromic properties are related with the oxidation states of tungsten atoms witch are influenced by the atmospheric humidity.

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#### <u>C-P044</u> A THIENYLENE-PHENYLENE COPOLYMER AND OLIGOMER WITH DI (ETHYLENE OXIDE) SIDE CHAINS AND ITS USE IN LIGHT EMITTING DIODES R.A. Silva, L.A. Cury, F.M. Matinaga, P.S.S. Guimarães, M. Bouachrine, J.-P. Lère-Porte, S. Löis, J. Moreau, F. Serein-Spirau, UFU, Faculdade de Física, Bloco X, Campus Santa Mônica, CEP:38400-902, Uberlândia, Minas Gerais, Brazil

An entirely new copolymer, thienylene-dialkoxyphenylene, was prepared by condensation between a bis-stannyl thiophene reagent and a substituted dibromobenzene derivate in the presence of a palladium catalyst. Owing to the presence of 2-(2-butoxy-ethoxy)-ethoxy polar side chains the polymer is soluble in most organic solvents and exhibits excellent glass adhesion properties. The optical properties of the copolymer can be controlled by adjusting the size and nature of the side chains, making it a promising material for the fabrication of light emitting diodes (LED) and light electrochemical cells (LEC). In this work we report a study of the electrochemical and optical of thin films of thienylene-dialkoxyphenylene. The calculated bandgap derived from cyclic voltammetry data (2.21eV) is in good agreement with the one calculated from the UV-VIS spectrum edge (2.15eV). The films for the optical measurements were prepared by spin casting on glass and silicon substrates. Photoluminescence and absorption spectra were recorded in the temperature range from 279 K to 18 K. The evolution of the optical spectra with temperature allows the determination of the variation of the bandgap with temperature. The analysis of the relative intensity of the zero-phonon, 0-1 phonon and 0-2 phonon bands indicates a change in the conjugation length with temperature.

<u>C-P045</u> STRUCTURAL CHARACTERIZATION OF BLENDS CONTAINING PVDF AND NATURAL RUBBER LATEX R.D. Simões, A.E. Job, N. Alves, J.C.S. Camargo Filho, O.N. Oliveira Jr., C.J.L. Constantino, UNESP, Faculdade de Ciências e Tecnologia, Rua Roberto Simonsen, 305, 19060-900, Presidente Prudente, SP, Brazil

> We report on the investigation of blends made with PVDF and natural rubber latex, whose biocompatibility could be explored in bone tissue growth. The choice of these materials was based on the piezoelectric activity of PVDF, which is crucial for growing bone tissue, while using latex allows one to produce blends with no solvents to dissolve PVDF. Different volumes of latex (0.3, 0.5, 0.7 and 1.0 mL) were added to 2.0 g of PVDF. The mixture was submitted to high pressure under 180oC during ca. 5 minutes. Thermomechanical properties were investigated through thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and dynamic-mechanic analysis (DMA). The blends are thermally stable up to ca. 300oC, the phase transitions found were Tg at ca. -60oC and the crystalline melting point at ca. 167oC. The elasticity modulus was in the range of the bone (MPa) and could be varied by altering the amount of latex in the blend. Spectroscopic characterization of the blends, using micro-Raman scattering and Fourier transform infrared absorption (FTIR) techniques, indicated that the blends become more homogeneous as the amount of latex is increased. However, no chemical interaction was noted between the latex and PVDF. These results suggest that the PVDF/latex blends are suitable for the intended applications, particularly because of their thermomechanical properties. The implantation of blends in rabbits is being carried out.

<u>C-P046</u> INVESTIGATION OF THE MOLECULAR STRUCTURE IN LANGMUIR AND LANGMUIR-BLODGETT (LB) FILMS OF A POLYMER CONTAINING AN AZO DYE D. Volpati, P.A. Antunes, F. Pavinatto, A. Riul Jr., O.N. Oliveira Jr., C.J.L. Constantino, J.A. Giacometti, UNESP, Faculdade de Ciências e Tecnologia, Rua Roberto Simonsen, 305, Presidente Prudente, SP, Brazil, 19060-900

> Langmuir and Langmuir-Blodgett (LB) films of a polymer containing an azo dye (DR19Cl-IPDI) mixed with stearic acid have been produced, aimed at future applications in optical storage and surface-relief gratings. The -A isotherms showed that the Langmuir films can support high collapse pressure indicating a good molecular packing on the water surface. Only a slight aggregation was observed during the compression-decompression cycle (hysteresis). However, the molecular structure of the Langmuir film is restored after each cycle, which is indicated by the superposition of the isotherms. The slight aggregation is maintained in the LB films as confirmed by the similarity between the UV-VIS. Absorption spectra for the LB film and the polymer solution. The spectrum for the mixed LB films containing 1, 11, 24, 33 and 51 layers showed also that absorption increased linearly with the number of deposited layers. Polarized UV-VIS. absorption spectra did not indicate any preferential molecular organization parallel or perpendicularly to the dipping direction in the plane of the substrate. The vibrational spectroscopy characterization using micro-Raman and surface-enhanced Raman techniques of the LB films has not revealed any chemical interaction between the azopolymer and the stearic acid. With enhancement of the Raman signal it was possible to investigate even the LB monolayer. This surface-sensitive method indicated that all LB films investigated here have the same molecular structure.

<u>C-P047</u> STUDIES ON THE INTERACTION BETWEEN HUMIC SUBSTANCES AND CONDUCTING POLYMERS FOR SENSOR APPLICATION E.C. Venancio, N. Consolin Filho, C.J.L. Constantino, L. Martin Neto, L.H.C. Mattoso, EMBRAPA-CNPDIA, Rua XV de Novembro, 1452, São Carlos,

The interaction between humic substances and poly(o-ethoxyaniline) (POEA), a conducting polymer, was investigated for both solution and self-assembled films. The results have shown that the humic substances induce doping of POEA by protonation, as indicated by UV-vis and Raman spectroscopies. The atomic force microscopy studies on the self-assembled films have shown that the average roughness of the polymer film has increased after exposing it to humic substances (fulvic and humic acids), consistent with the interaction between POEA and the humic substances. However, this change in morphology is reversible by washing the sensing units with water, in agreement with the electrical data, allowing using this system in sensor applications. Here, the sensor formed by an array of different sensing units has distinguished between two humic substances (fulvic and humic acids) as shown by multivariate analysis (principal component analysis). The motivation to detect humic substance comes from its importance in terms of quality control of water or soil.

#### <u>C-P048</u> PHOTOLUMINESCENCE IN LANGMUIR BLODGETT (LB) FILMS OF A POLYFLUORENE DERIVATIVE M. Ferreira, A.M. Machado, L. Akcelrud, O.N. Oliveira Jr, UNESP/PP, Rua Roberto Simonsen, 305, CP 467. 19060-900

The Langmuir and Langmuir-Blodgett (LB) properties of a PPV type polyfluorene derivative, namely poly(9,9-di-hexylfluorenediyl vinylene-alt-1,4-phenylenevinylene)(LaPPS16) are reported. Langmuir films of LaPPS16 were formed rom chloroform solutions spread on an ultrapure water subphase. The area per monomer in the condensed phase in surface pressure (p-A) isotherms was ca. 75 Å2, indicating the formation of true monolayers. The maximum surface potential was approximately 320 mV. Y-type LB films were transferred onto quartz and ZnSe substrates at a constant surface pressure of 35 mN m-1 and with dipping speed of 6 mm min-1. UV-VIS. absorption and FTIR spectroscopy measurements on 21-layer LB films confirmed the transfer of LAPPS16, with an absorption peak centered at 320 nm and FTIR bands assigned to uC-H (hexyl) at 2954-2844cm-1, uC-H (olefinic) at 3054cm-1 and uC=C (olefinic) 957cm-1. The absorption at 1687cm-1 corresponds to the di-substituted trans C=C olefinic bonds. The photoluminescence (PL) of the film can be readily seen by naked eyes upon shining UV light onto the sample. The PL spectrum displays an emission peak at approximately 500 nm.

# <u>C-P049</u> AZOBENZENE POLYMER FILMS AS COMMAND SURFACE FOR ALIGNING LIQUID CRYSTALS

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The use of azo-dye molecules attached to polymers allows manipulating the liquid crystal alignment by trans-cis-trans isomerization cycles. When a polymer film containing azo-dye moieties randomly oriented is irradiated with linearly polarised visible light, a selective reorientation of the azo-dye groups takes place perpendicular to the polarisation direction. This linear photoisomerization gives a certain anisotropy to the polymer film that can be used to align the liquid crystal molecules once in physical contact with the irradiated polymer surface. In this work a systematic study of the orientation induced to a thermotropic nematic liquid crystal, 5CB, by polymeric films containing different concentrations of azo-dye groups in the side chain, p(MMA-DR13), was performed. The investigated aspects are the kinetics of orienting the azo-dye polymer film, the influence of the irradiation energy and of the azo-dye concentration on the polymer alignment, the thermal and temporary stability of the alignment induced to the liquid crystal, and the azimuthal anchoring strength. The photopolymerization was performed using a Nd:YAG laser operating at 532 nm. The sample transmittance was measured as function of the incident laser power and of the exposure time, for different azodye concentration. We expect to find experimental parameters that allow us to make a theoretical description between the azo-dye concentration and the induced liquid crystal orientation.

### <u>C-P050</u> HIGHLY SENSITIVE SENSOR ARRAYS OF CHROME ELECTRODES FOR TASTE SENSORS

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A novel sensor array with inexpensive electrochemically chrome-deposited electrodes is employed as taste sensors, which show high sensitivity, using impedance spectroscopy measurements and a different electrode geometry [1]. With data analysis based on principal components analysis (PCA), the array was capable of distinguishing among solutions containing trace amounts of basic taste substances, namely NaCl (salt), HCl (sour) and sucrose (sweet). The high sensitivity allowed detection of these substances and of CuSO4 at a concentration of 10E-12 mol/L. This sensitivity was achieved at low frequencies (i.e. 200 Hz), where double-layer effects become important, whereas with frequencies above 800 Hz the array was considerably less sensitive. In addition to detecting trace amounts of substances, the array was used to distinguish samples of wine, thus demonstrating that it also works with complex liquids. In order to further test the new electrodes, we observed that a reasonable distinguishing ability can be obtained when only one electrode is employed, but the electrical response computed contains signal from different measuring conditions. This feature also lowers the cost of the taste sensor, which extends the possible applications of taste sensors.

#### <u>C-P051</u> CHARACTERIZATION OF BLENDS OF MEH-PPV AND COMMERCIAL POLYMER V.C. Gonçalves, K.C. Teixeira, D.T. Balogh, IFSC/USP, Grupo de Polimeros - IFSC-USP, Av. Trabalador Sao Carlense, 400 - C.P. 369 - 13560-250, São Carlos- SP - Brasil

In this work polymer blends of poly[(2-methoxy-5-(2-ethyl-hexyloxy))-p-phenylenevinylene] (MEH-PPV) and polycarbonate (PC) were studied. Blend films onto glass substrate were prepared in appropriate proportions of MEH-PPV from chloroform solutions. The blends were characterized by FTIR and UV-Vis absorption and photoluminescence and the photodegradation was followed by exposing the films to a white light (25 mW/cm2) and recording their absorption spectra in visible region. FTIR showed that there is no interaction between MEH-PPV and PC in molecular level. The thermal transitions of the MEH-PPV could not be visualized clearly by the DSC technique and the thermal transitions of PC were not significantly changed by the presence of MEH-PPV. The photoluminescence spectrum of MEH-PPV was not affected by the presence of PC in the blends. The blend degradation kinetics in solid state are monoexponential, first-order, for all film thickness. However for the pure MEH-PPV, the photodegradation kinetics is biexponential (slow and fast stage) for higher thickness. These results indicate that MEH-PPV can be dispersed in PC forming immiscible blends but with no phase separation could be clealy observed by optical microscopy. The presence of PC presence changed the MEH-PPV photodegradation mechanism probably by changing the oxygen diffusion, the blend films showing photodegradation rates similar to the slower stage of pure MEH-PPV films. Acknowledgements: FAPESP, CNPq, IMMP/MCT.

C-P052 THERMALLY STIMULATED DISCHARGE CURRENT OF SULFONATED POLYSTYRENE IONOMERS FOR APLICATION IN POLYMERIC ELECTROLUMINESCENT DEVICES

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Ionomers are íon-containing polimers that have a relatively small amount ionic group along polymer backbone chains. Recently research reported the effect of ion concentration in the ionomers used as an electron injecting layer in polymer light-emitting devices. Interactions between the ionic groups attached to the polymer backbone changes dramatically the properties of ionomers and are responsible for the electron injection properties of these materials. These interactions are dependent on the number of ionic groups and on its chemical nature. This paper describes the use of thermally stimulated discharge current (TSDC) technique to investigate structural transition of potassium sulfonated polystyrene ionomers, with sulfonation level ranging from 1 to 15 mol% as a function of ionic conduction in the temperature interval of 273 to 500 K. The TSDC spectra exhibit three discharge features in order of increasing temperature with two main transition around 120-160 °C and above 180 oC. A region of diffusion is observed above of Tg material. The results were interpreted in order to explain the effect of the number of charges in ionomers on the discharge current of depolarization. These results were discussed in order to use these ionomers as electron injection material in polymer EL devices.

<u>C-P053</u> POLY-(AMIDE-IMIDE) AND AZOPOLYMER MIXTURES. I. EFFECTS ON POLYAZOURETHANE PROPERTIES

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An important challenge in the production of polymers containing azo chromophores is that the azopolymers are generally brittle, with poor mechanical properties. This difficulty may be overcome if mixtures of azopolymers are made with commercial polymers. In this work mixtures of poly-(amide-imide) with a polyurethane synthesized by polymerization of 4,4'methylene- diphenylisocyanate and the azo dye 4-[N-bis-(2-hydroxy-ethyl)]-amino-2'chloro-4'-nitroazobenzene (MDI-DR19Cl) were prepared in order to obtain self-standing and flexible films with optical storage properties. Films with 5% of azopolymer were obtained, showing good optical properties and high coloration degree and flexibility after a curing process. The mixture presented a glass transition temperature 10 oC lower than the values obtained for the glass transition of the pure PAI and no phase separation could be visualized by optical microscopy. The films of the mixture showed better mechanical stability showing no degradation after several weeks, whereas films of the pure azopolymer were brittle. The self standing films used in optical storage experiments showed remanent optical storage values after relaxation slightly lower than the value obtained for a film of the pure azopolymer cast on glass slides. But the values obtained are sufficient high to show the viability of the use of these mixtures in optical storage applications that require flexible films.

#### <u>C-P054</u> SYNTHESIS AND CHARACTERIZATION OF A PPV ORTHOGONALLY SUBSTITUTED WITH FLUORENE UNITS A.M.Assaka, P.C. de Souza, A.R.M. Oliveira, L. Akcelrud, UFPR/LACTEC, Centro Politécnico - Curitiba - PR – Brasil

Despite its good opto-electronic characteristics, PPV lacks processibility and various approaches have been tried to overcome this drawback, like the insertion of alkyl and /or alkoxy substituents. This strategy also provides a means to tune the emission color, and good film forming ability as well. In the present contribution, we propose a new type of substituent: orthogonally placed fluorene units in the 3,6 positions of the aromatic ring of PPV, which apart from solubilizing the main PPV chain, contributes to a better thermal and oxidative stability in relation to the usual aliphatic substituents. Another interesting feature of the new structure is the emissive character of the ramification. The synthesis was performed through the Wittig condensation between 1,4-difluorenyl-3,6-dicarboxaldehyde-benzene(1) and p-xylylenebis(triphenylphosphonium bromide)(2).(1) was prepared by reacting p-xylene with bromine resulting in 1,4-dibromo-p-xylene (3), which was reacted with acetic acid in acetic acetate to form 1,4-dibromo-3,6-dicarboxaldehyde-benzene(4) and then lithiated to form 1,4-diboronic acid-3,6- dicarboxaldehyde-benzene(5).Finally, 2,7-dibromofluorene was reacted with (5) to form (1).All structural characterizations were performed using FTIR, 1H and 13C NMR.The photophysical behavior of polymeric structure was characterized by UV absorption and fluorescence emission spectroscopy, in solution and in the solid state. The molar weight was determined by GPC technique with PS standards.

#### <u>C-P055</u> CARRIER INJECTION AND TRANSPORT OF IN-SITU POLYMERIZED POLYANILINE FILMS

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The electrical properties of in-situ polymerized polyaniline (PANi) thin films have been examined upon different doping levels, temperature and metals used as electrode (Au and Al). The polymer was prepared using the chemical synthesis and deposited in-situ onto glass substrate having on its surface gold or aluminum lines arrays as electrodes. Electrical measurements were performed using a Solartron Impedance/Gain-Phase analyzer, in the frequency range from 0.1 Hz to 10 MHz (AC measurements) and a Keithley current-source measuring unit, in the -10 to 10 V range (DC measurements) in the dark and under vacuum, to avoid photocurrent and photoxidation processes, respectively. A model is presented for describing the DC and AC measurements characteristics of the PANi systems that encompass: (i) the charge injection from metal to the polymer bulk through the metal-PANi interfaces, and (ii) the Cole-Cole dielectric function and the the random free energy barrier model for accounting the conduction process. Fittings of DC and AC electrical characteristics are in good agreement with experimental data. The dependence of the zero-field contact barrier (PANi-Al and PANi-Au interfaces) for carrier-injection, as well the carrier mobility on the electrical field and the influence of doping level on the polymer permittivity are obtained.

#### <u>C-P056</u> SYNTHESIS AND SPECTROSCOPIC STUDY OF EU(B-DIKETONATE):A-CYCLODEXTRIN INCLUSION COMPOUND A.O. RIBEIRO, O.A. SERRA, FFCLRP-USP, Ribeirao Preto, Brasil - 14040901

Cyclodextrins (CD) are cyclic oligosacharides compounds that can incorporate molecules of appropriate size in your hydrophobic cavity, forming of the so-called inclusion compound. In this work we describe a study of the photophysical properties of the Eu(b-diketonate)3:a-CD inclusion compounds in aqueous solution and in a solid state. The complexes [Eu(tta)3.2H20] and [Eu(bta)3.2H20] (tta=thenoyltrifluoroacetone, bta=benzoyltrifluoroacetone) were synthesized, characterized and included in a alpha-cyclodextrin aqueous solution by stirring the suspension for one week. Part of the solution was dried to obtain the inclusion complexes in a solid state. The study of the properties of the materials was done through luminescence spectroscopy, ultraviolet-visible absorption (UV-Vis), 1H NMR, infrared (FTIR), MALDI and thermal analysis (TGA/DTA). The excitation spectra of Eu(tta)3:a-CD and Eu(bta)3:a-CD inclusion compounds in aqueous presented the maximum shifted approximately 15 nm relatively to the non a-CD complexes. Infrared absorption and 1H NMR confirmed the interaction of the complexes with the a-CD. The emission spectra of compounds show the bands characteristics of the Eu3+ in all environments. The stoichiometry of the inclusion compounds was calculated by absorption in aqueous solution by Job's method of continuous variation and was confirmed by MALDI and thermal analysis of solid compounds.

#### <u>C-P057</u> SURFACE TENSION STUDIES ON DIMER AND TRIMER LIQUID CRYSTALS

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In this work, the surface tension of a,w-bis[(4,4'-cyanobiphenyl)oxy] alkane dimer liquid crystals (CBA-n) and trimer liquid crystals (CBA-Tn) having -O(CH2)nO- flexible spacers (n = 9, 10) between the 4,4'- cyanobiphenyl ends was evaluated for ranges of temperatures corresponding to the nematic and isotropic phases of the materials, using the pendant drop method. Pressure Volume Temperature (PVT) data of dimer and trimer liquid crystals were used to predict the influence of temperature on the surface tension of materials studied. For all the LMMLCs studied it was observed that the surface tension suffers a discontinuity near the transition temperature nematic to isotropic, TNI. The results of surface tension discussed in light of the ordering of the molecules.

## <u>C-P058</u> INFLUENCE OF THE SOLVENT IN THE OPTICAL STORAGE FEATURES OF AN AZO DOPED CHITOSAN FILMS

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Chitosan can sequestrate azodyes, in a process that depends on the chemical structure of the dye and on pH. It opens up new possibilities to combine optical properties from the azo compounds with chitosan in biological applications in order to produce sensors and probes. Systems containing azoaromatic chromophores has been exploited for optical storage and formation of surface-relief gratings. In this paper we report on the optical storage properties of chitosan films doped with azo dye Ponceau-S (PS). Particular emphasis is given to the increase in the optically induced birefringence signal and rate, when the samples are immersed into different solvents prior to the optical storage measurements. Our results indicate that the solvent is entrapped in the samples affecting the electrostatic interactions between the molecules in the film, in such a way that the preclusion effect brought about by such interactions on the writing processes could be diminished.

#### <u>C-P059</u> MORPHOLOGICAL AND OPTICAL CHARACTERIZATION OF SILICA HYBRID FILMS PREPARED BY SOL-GEL PROCESS

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The sol-gel process have been used to prepare inorganic-organic glasslike films, providing unique possibilities to tailor the mechanical, electrical and optical properties with respect to numerous applications. In this work, thin silica hybrid films were prepared on glass plates using the dip-coating process, from starting solutions of silicon alkoxide (TEOS) dissolved in ethyl alcohol and methacrylic acid or TMPS. The influence of parameters such as concentration, pH, dipping velocity and temperature of thermal treatment were determined with the purpose of obtaining hybrid films. The films are adherent, transparent and free of cracks. The morphology of the obtained films was studied by atomic force microscopy and the optical properties were determined by UV-Vis spectroscopy. Hydrophobic tests were made with the aim of study application in ophthalmic lens supplies.

<u>C-P060</u> CHIRAL 3-SUBSTITUED POLYTHIOPHENES AND N-SUSTITUED POLYPYRROLES J.C. Ramos, R.M. Souto Maior, M. Navarro, UFPE, Departamento de Química Fundamental -CCEN-laboratório de eletrossíntese orgânica-Cidade Universitária- CEP 50.670.901- Recife – PE

> 3-Substitued thiophenes and N-substitued pyrroles monomers with R(-) or S(+) 3,5dinitrobenzoyl-alfa-phenylglycine has been chemically polymerized in chloroform using FeCl3 as oxidant agent for 48 h under N2 flux at room temperature. FTIR spectra were taken to analyze the structural properties of polymers, indicating alfa-alfa coupling of monomers. Surface analyses of polymers powder were clarified by scanning electron microscopy. Thermal analyses were done by thermogravimetric analysis and showed a typical three step weight loss behavior. The first step started at about 150 °C for polypyrroles and 140 °C for polythiophenes. Polarimetry measures showed that chiral properties of monomers were maintained in the polymers. Electropolymeric synthesis, determinmation of electrochromic properties and evaluation as polymeric chiral stationary phases are carrying out.

### <u>C-P061</u> OPTICAL PROPERTIES OF LINB1-XTAXO3 THIN FILMS PREPARED FROM POLYMERIC PRECURSORS

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Lithium niobate-tantalate (LiNb1-xTaxO3) thin films were deposited on sapphire (0001) substrates by dip coating process using polymeric organic solution. The coated substrates were thermally treated at 600°C for 3 h under oxygen atmosphere. In order to study the influence of tantalum composition (x) on the crystallinity, morphology and optical properties, films with x = 0, 0.5 and 1 were deposited. X-ray diffraction results showed that preferentially (006)-oriented LiNb1-xTaxO3 films were obtained. Atomic force microscopy (AFM) analyses revealed that the surfaces are not only crack-free but also appear relatively dense. The multilayer LiNb1-xTaxO3 films displayed spherical grain structures with a superficial roughness of approximately 1-3 nm. Modified envelope method was used for obtaining optical properties and the thickness of the films by using the transmission spectra. The packing density for the LiTaO3 film was 0,9337, indicating that this film presented a best morphologic quality.

C-P062 INTERACTION OF SMALL AMOUNTS OF BOVINE SERUM ALBUMIN WITH PHOSPHOLIPID SURFACE MONOLAYERS INVESTIGATED BY SURFACE TECHNIQUES AND ATOMIC FORCE MICROSCOPY W. Caetano, M. Ferreira, R. Itri, O.N. Oliveira Jr, USP/IF/SP, CP 66318, 05315-970, São Paulo-SP, Brazil.

> Surface pressure and surface potential isotherms have been used to investigate the dynamic adsorption and penetration of small amounts (nanomolar) of bovine serum albumin (BSA) into the Langmuir monolayers of zwitterionic dimethyl-DPPE and anionic DMPA at the air-water interface. Emphasis is placed on the monolayer stability under successive compressiondecompression cycles. The surface pressure isotherms are shifted to larger molecular areas when a waiting time elapses between spreading and compression. This indicates adsorption and penetration of BSA, causing the phospholipid monolayer to reorganize, especially in the anionic DMPA. The morphology and stability of supported phospholipid monolayers transferred as Langmuir-Blodgett films onto mica substrates were investigated using atomic force microscopy. The AFM images of one-layer LB films from DPPE and DMPA, transferred from the condensed phase, displayed a non-uniform morphology with defects and regions with different heights. On the other hand, the LB films transferred from phospholipid/protein monolayers were uniform with defect-free areas, indicating the presence of lipid domains modified by interaction with BSA. Taken together with the results from the surface pressure and surface potential isotherms, the effects from such small amounts of protein mean that the phospholipid responds cooperatively to BSA.

<u>C-P063</u> LANGMUIR-BLODGETT FILMS OF MIXED MONOLAYERS OF PORPHYRIN (TPYP)/DMPA

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Langmuir monolayers and Langmuir-Blodgett (LB) films have been produced from neat tetrapyridyl porphyrin (TPyP) and metalated Ni(II)-TpyP or mixed with dipalmitoyl phosphatidic acid (DMPA). The increase in the area per lipid molecule confirms incorporation of the porphyrins. In anionic DMPA a stronger effect was observed for Ni(II)-TPyP, with the appearance of a liquid-expanded to liquid condensed phase transition at approximately 10 mN/m. This phase transition is probably due to reordering of the zwitterionic, anionic lipid molecules within free spaces between the bound pure and mettalated Ni(II)-TpyP. In this case, reordering may be enhanced by interaction of metallic center with the negatively charged phosphate groups of DMPA. Y-type LB films were transferred onto quartz and Au substrates at a constant surface pressure of 45 mN m-1 and with dipping speed of 7 mm min-1. UV-VIS. absorption and FTIR spectroscopy measurements on 21-layer LB films confirmed the transfer of neat porphyrin and porphyrin/DMPA 25% in weight of porphyrin. The electronic spectra show absorption peaks centered at ca. 410 nm (soret band) and 540 nm, 560 nm and 600 nm (Q bands) and FTIR bands at ca 3000 cm-1 (CH), 1275 cm-1 (CN). The spectroscopy data are consistent with a stronger interaction between the porphyrin and the lipid, in comparison with neat porphyrin.

#### <u>C-P064</u> HARDNESS OF ACETYLENE PLASMA POLYMERS TREATED BY PIII D.C.R. dos Santos, R.P. Mota, R.Y. Honda, E.C. Rangel, UNESP, Laboratório de Plasmas, Guaratinguetá, SP - Brazil, 12516-410

Plasma-polymerized thin films have many applications in electronic, optical and biomaterial industries, among others, due to their interesting physical and chemical characteristics. Plasma polymer application, however, can be limited because of some surface properties. These properties can be improved by post-treatments, such as plasma immersion ion implantation (PIII). In this technique, the target immersed in a plasma environment is polarized by high voltage negative pulses. Consequently, the energetic ions from the plasma are accelerated and implanted into the exposed areas of the target, inducing modifications in the chemical structure and atomic composition of the near-surface region of the sample. The degree of such changes is highly dependent on the plasma conditions (composition, frequency, power, pressure), pulse parameters (form, magnitude, frequency, duty cycle) and implantation time. In this work, amorphous a–C:H films deposited from radiofrequency (RF) plasmas of acetylene (13.56 MHz, 100 W, 9.3 Pa, 90 min) were treated by nitrogen PIII (13.56 MHz, 70 W, 1.87 Pa). In order to do that, triangular pulses (10 kV, 2.3X10-3 s) were applied to substrate-holder, at two different frequencies, 30 and 100 Hz. For each frequency, implantation time varied from 15 to 120 min. Polymer film hardness was availed by indentation technique, using an automated Hysitron Triboindenter®.

#### <u>C-P066</u> STUDY OF GEOMETRIC PROPERTIES OF PHENYLENE SYSTEMS THROUGH DIFFERENT AB INITIO METHODS

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There is urgent need to describe accurately the structure of

open systems, dependent on interaction between non-bonded atoms, within Density Functional Theory DFT. However, for these systems there are regions with very low electronic density, where errors are amplified. A typical case is the conjugated polymer polyparaphenylene PPP in which the phenylene rings are connected through carbon-carbon bonds in para-position. The torsion angle between rings (a structural parameter that can strongly influence the electronic properties) is affected by the balance between the coulombic repulsion between hydrogen atoms from neighbour rings, van der Waals attraction and pi-delocalization energies coming from the backbone pi-electrons. We compare DFT methods, within the Local-Density LDA and the Generalized Gradient Approximation GGA to calculate the torsion angle between rings of finite and infinite systems of PPP: molecular biphenyl, crystalline biphenyl and 1D PPP. We have chosen three different basis set expansion models: localized functions SIESTA[1], plane waves ABINIT[2] and mixed-basis PAW[3]. For LDA we find a difference in torsion angles between methods of roughly 7 degrees while for the GGA the difference is 12 degrees approximately. We found that the results strongly depend on the XC potential used, and on the convergence criteria.

#### C-P067 TRANSPORT PARAMETERS IN OLIGO-ANILINE CRYSTALS L.Y.A. Dávila, M.M. Garcia, M.J. Caldas, IF-USP, Instituto de Fisica-Universidade de Sao Paulo, R. do Matao, Tr R, Cidade Universitaria, CEP 05508-900 Sao Paulo, SP Brasil

Organic polymers such as polyanilines (PANi) are in evidence due to conducting properties comparable of metals, however, despite the large amount of theoretical and experimental efforts, the mechanism of transport in PANi compounds is still not completely and quantitatively understood, not less because the material is usually disordered, which makes it difficult to model. Recent experiments in crystals of oligomers of aniline have called our attention, since in the case of trimers of pernigraniline the arrangement results in crystalline order, with almost-perfect pi-stacking of the central rings. We thus studied theoretically the geometrical and eletronic properties of this crystal, using ab initio methods within the density functional theory (DFT) with the local density approximation (LDA). To proceed, we need to treat an open, current-driven system: the most successful theoretical approach to transport in confined systems is the formalism of Buttiker-Landauer, that allows to calculate the conductivity from electronic properties. We then extract, from the obtained crystal and isolated molecule wave functions, the energy terms that allows us to calculate the transfer integrals between molecules (via the projection of the coefficients of wave functions of the isolated molecules in the crystal). The transfer integrals are then used as input parameters to the formalism of Buttiker-Landauer, that in turn supplies the conductance of the material.

#### <u>C-P068</u> LIGHT-EMITTING DEVICES BASED ON GREEN-PHOSPHOR/CONDUCTIVE-POLYMER BLEND COMPOSITES

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A new composite based on a conductive polymer blend and a zinc silicate phosphor (ZSP) has been produced for applications in electroluminescent devices (ELD). The polymeric blend was composed by p-Toluene Sulfonic Acid (TSA) doped poly-o-methoxyaniline (POMA) and poly(vinylidenefluoride-co-trifluoroethylene) (PVDF-TrFE copolymer), in different compositions. Manganese-doped zinc silicate (Zn2SiO4:Mn) was used as the green-emitting phosphor. We report on the electroluminescence (EL) of devices formed by a single layer of the active composite deposited by drop-casting onto ITO substrates with vacuum-evaporated Aluminum top electrodes. The distribution of the solid phase (ZSP) was analyzed with Scan Electron Microscopy (SEM) for various relative concentrations. Current density-voltage (J-V) and radiance-voltage (R-V) characteristics were analyzed in order to investigate the nature of the electroluminescence of the active material. The devices presented good stability in time, high luminance in the green and homogeneous bright over effective areas up to 5 cm2. This kind of device represents an attractive alternative for potential low-cost flexible displays applications.

<u>C-P069</u> CHARGE CARRIER MOBILITY INVESTIGATIONS IN MOLECULARLY DOPED POLY(9-VINYL CARBAZOLE)

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A systematic investigation of the charge transport mechanisms in molecularly doped poly(9vinylcarbazole) (PVK) films with Ytterbium bisphthalocyanines (YbPc2) at different doping levels is presented is this work. Devices in a ITO/PVK:YbPc2/Al structure presented a substantial modification in the absorption spectrum, with appearance of bands in the visible range due to the organo-metallic dopant specie. Transient photocurrent technique has been used to determine the transit time of charge carriers in the samples and, consequently, the carrier mobility. The analysis of the experimental results is based on the dispersive transport model proposed previously by Scher and Montrol. . It has been observed that the transit time presents E-1/ dependence, with  а   corroborating the dispersive character of the transport. The variation of the dopant concentration influenced the charge carrier mobility as well as the disorder parameter. Additionally, for high dopant levels, a photocurrent response was observed in the visible region, in contrast to pure PVK films which only respond when excited with shorter wavelengths (in the UV region).

<u>C-P071</u> SURFACE ENERGY CHARACTERIZATION OF LIGHT-EMITTING DIODES BY ATOMIC FORCE MICROSCOPY (AFM): CONTACT ANGLE AND SURFACE ENERGY DETERMINATION

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Polymer light-emitting diodes (PLEDs) devices consist of a thin film (100 to 300 nm) of an electroluminescent (EL) conjugated polymer sandwiched between two electrodes, where at least one is transparent. Intermediate layers between the EL polymer and the electrodes are used as electron/hole injection and/or as hole blocking layer and also as protective coatings over the (ITO) anode to avoid the electroluminescent polymer contamination by ITO. As a consequence these systems are constituted by several interfaces and interfacial properties such as interfacial energy or surface energy are important parameters to be controlled in the development and design of PLEDs. The development of micro and nanometer scaled devices has encourage the development of new characterization tools suitable to monitor these surfaces at micrometric/nanometric scale. In this work we propose the use of AFM to monitor the wetability of the substrate by the polymers used as EL active or as interface materials and a procedure to determine the contact angle and the surface energy of the substrates. As substrates it was used glass, glass substrate coated with indium tin oxide (ITO) (untreated and aquaregia treated). Thin films were deposited by spin coating and than annealed to cause dewetting at temperatures above the glass transition temperature of the polymers (MH-PPV, PS-PMMA ionomer).

<u>C-P072</u> XPS AND AFM SURFACE STUDIES OF PVC/PHB BLENDS C.M. Almeida, G.B. Baptista, R. Prioli, R. Sánchez, M.O. Siqueira, PUC-Rio, Depto. de Fisica, PUC-Rio, Caixa Postal 38071, CEP 22452-970, Rio de Janeiro, Brasil E-Mail: <u>clara@vdg.fis.puc-rio.br</u>

Blends formed by the biodegradable polymer Poly-3-hydroxybutyrate (PHB) and by the conventional polymer Polyvinylchloride (PVC), were prepared in a chloroform solution leading to membranes with different relative concentrations. The blends were chemically analyzed using X-ray photoelectron spectroscopy (XPS) while its surface was observed with atomic force microscopy (AFM). The amount of each polymer in the blend surface was determined by XPS and contact angle measurements. The blend surface analyzed by AFM presents crystalline structures that are characteristic of PHB. The crystalline structure is inserted in an amorphous PVC/PHB phase. The presence of these crystalline structures in the blend was confirmed through the observation of the change of polarization of the incident light. We correlate here the morphology of the surface with the relative concentration of two polymers in the surface of the blend.

<u>C-P073</u> DESIGN OF A NEW SUPRAMOLECULAR COMPOSITE BY THE ELECTRONIC STRUCTURE INVESTIGATION OF RHODAMINES+SOL-GEL MATRIX A. Sampaio-Silva, S.G.C. Moreira, P.A. Alcantara Jr., J. Del Nero, UFPA, Conj. Cidade Nova IV. WE42. n.212. Bairro Coqueiro.Ananindeua. Pará

> Rhodamines are a fascinating class of materials for opto-electronic applications. They form an exciting group of molecular materials and could be compared with several organic materials and presents properties between the monomolecular and polymeric regimes. In a recent study it has been demonstrated that the rhodamines could be used as dye laser. Also, these gels are attractive hosts to new hybrid materials, envisaging temperature sensitive compounds entrapment on the polyphosphate network in mild reaction conditions, thus preventing degradation of the active species. This strategy may lead to new sensors and optical devices. In this work we describe a new material that could be utilized as supramolecular composite resulting from the incorporation of rhodamine dye within this matrix, envisaging the preparation of a new sensor. The aims of this work were to investigate theoretically the optical properties of rhodamine and new possibilities of synthesis of a supramolecular composite based on the incorporation of this dye in a polyphosphate gel network. The theoretical methodology were based on semiempirical (AM1, PM3 and INDO/S-CI) and Density Functional Theory (B3LYP/3-21G). Our results reveal the existence of different electronic patterns for the different forms of these molecules. Our results show that rhodamine could be successfully incorporated in the host matrix, leading to auto-standing films and the gel network differs from its behavior in aqueous solution.

#### <u>C-P074</u> ENERGY TRANSFER FROM ALQ3 TO RH590 IN A THIN FILM COMPOSITE R.D. Fazenda, J. Ramirez-Fernandez, W. J. Salcedo, Laboratório de Microeletrônica da EPUSP, Av. Luciano Gualberto - travessa 3 ,São Paulo, SP, Brazil, C.P.61548, 05424-970

This work report the energy transfer process from tris(8-hydroxyquinouline) aluminum (Alq3) to Rhodamine-590 (Rh590) molecules in the thin solid film composite. The solid thin films were obtained by spin-coated the organic solution of Alq3:Rh590:Polystyrene on glass substrate. The organic solution was obtained through the following process: First it was prepared 1wt% polystyrene (PS) solution in chloromethane, after this was added 30% of Alq3 and 20% of Rh590 relative to weight of PS. The film was characterized by optical absorption and fluorescence spectroscopies. The optical absorption spectrum shows three band features centered at 353nm corresponding to Alq3 absorption and 514nm and 550nm corresponding to Rh590 absorption. The film was excited by light source at 355nm because results obtained by mean of optical absorption spectra; the emission spectra of the film showed a two bands emission centered at 500nm and 580nm which can be corresponded to Alq3 emission and Rh590 emission respectively. The band centered at 580nm showed highest emission intensity. In order to identified the emission mechanism, it was analyzed the emission spectra of thin film containing only the Rh590 moieties; in this case the emission spectra not showed features at 500nm and 580nm. These results showed that the band emission at 580nm, in the Alq3:Rh590:PS film, was due to energy transfer process from Alq3 to Rh590 moieties.

<u>C-P075</u> STRUCTURAL AND MORPHOLOGICAL STUDY OF RUBBER PARTICLES OF ABS POLYMERS BY TRANSMISSION ELECTRON MICROSCOPY (TEM), SMALL ANGLE X-RAY SCATTERING (SAXS) AND SOLID-STATE NMR G.L. Mantovani, E.R. de Azevedo, T.S. Plivelic, I. Torriani, E. Hage Jr, T.J. Bonagamba, IFSC – USP, Laboratório de Espectroscopia de Alta Resolução, Av do Trabalhador Saocarlense, 400, Caixa Postal 369, São Carlos, Brazil.

> Regular morphologies that are routinely observed in multiphasic polymer systems can be suitably probed by small-angle neutron scattering (SANS), small and wide-angle X-ray scattering (SAXS, WAXS), transmission electron microscopy (TEM), and recently by scanning probe microscopy (SPM). The spin diffusion technique in solid-state NMR spectroscopy has been widely used in recent years to simultaneously study phase domains size and interface thickness of multiphasic polymer systems, which provides important information without destructing the samples. In this work, transmission electron microscopy, small-angle X-ray scattering with synchrotron radiation and solid-state NMR spin-diffusion experiments were used to characterize the morphology of the rubber particules and interface structure of ABS polymers. SAXS measurements were performed at the small-angle scattering workstation of the LNLS - National Synchrotron Light Laboratory (Brazil). Spectra were taken for all samples for 15 minutes using a wavelength of ?= 1.608 Å, at a sample-detector distance of 794.1 mm. The SAXS curves were registered using an one dimensional position-sensitive gas detector. The morphologies were examined using a PHILIPS CM 120 transmission electron microscope (TEM) at an accelerating voltage of 120 KV. Ultrathin sections were obtained by cryomicrotoming samples from moulded IZOD bars, using a REICHERT ULTRACUT FC S microtome at -80 oC. Thin sections (20-25 nm) were stained with OsO4 vapour for 15 h.

<u>C-P076</u> SYNTHESIS AND CHARACTERIZATION OF DIPYRIDYL CONTAINING POLYMERS FOR THE PREPARATION OF EU3+RED-EMITTING POLYMERS V.A.F. Deichmann, L. Akcelrud, UFPR/LACTEC, Laboratório de Polímeros Paulo Scarpa, Departamento de Quimica-UFPR, Centro Politécnico, S/N°, Jardim das Américas, Curitiba, PR, Brasil.

> One promising approach for the obtaintion of red-emitting polymers is the complexation of appropriate chain sites with Eu3+(monochromatic fluorescence emission at 613nm). The excitation mechanism of the central metal ion differs widely from that of organic fluorescent compounds; the ions are excited via intramolecular energy transfer from the triplet excited states of the ligands. The excitation energy of the ligand's triplet state, which may be directly generated by carrier recombination, can also be utilized to excite the emitting center. Thus, there is no limitation, up to 100%, of the internal quantum efficiencies for devices using lanthanide ion chelates as emitters. In this work we have used 2,2' dipyridine units as complexing sites alternated with 2,5-dihexyloxy-1,4-phenylene, providing a fully conjugated polymer, namely poly(2,5-dihexyloxy-1,4-phenylene-alt-biyiridil)in which the level of Europium incorporation could be controlled and measured. The synthesis was accomplished via a Suzuki polycondensation, using 5,5'-dibromo-2,2'-dipyridyl(1) and 2,5-dihexyloxy-hidroquinone boronic diacid(2)as starting materials.(1)was obtained from the bromination of bipyridine, in the 5,5'positions,(2)was obtained from the the alkylation of 2,5dibromohydroquinone with hexyl bromide in basic medium, after lithiation and reaction with isopropyl borate. The desired structure was confirmed by NMR and GPC, absorbed at 350nm and emitted 440nm. It will be used as a precursor for Eu3+ red emitting polymers.

<u>C-P077</u> MECHANICAL CHARACTERIZATION OF ACRYLONITRILE-BUTADIENE-STYRENE / POLYANILINE COMPOSITES OBTAINED WITH PREVIOUS SUPERFICIAL ADSORPTION OF ANILINE

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The great potential and the diversity of applications for the polymeric films intrinsically conductive demand a good compatibility with other materials. There is a great interest in application of conductor / conventional polymeric composites in the control of the optical characteristics and mechanical and electric properties. In this work the polymerization of the aniline was promoted on acrylonitrile-butadiene-styrene (ABS) substrate (with previous aniline superficial adsorption from 0 to 10 minutes) resulting in the growth of a superficial layer of polyaniline (PANI). By mean of the four probe superficial conductivity measure system and of the tensile test in the films composites with different times of aniline adsorption was possible correlate the superficial conductivity with the mechanical properties of the composites. It was also possible to analyze by scanning electronic microscopy the interface between the substrate and the superficial layer of polyaniline after cryogenic fracture of the composite. It was observed that a small aniline adsorption degree promoted an increase of the PANI anchorage (in the ABS surface) and of the superficial conductivity about four times higher. It's possible to conclude that the mechanical and electric properties of the composites can be controlled through aniline adsorption degree in ABS matrix surface making possible countless applications.

<u>C-P078</u> ENERGY TRANSFER BETWEEN CONJUGATED POLYMERS AND AZO CHROMOPHORES: EFFECT FROM EXCITON SPECTRAL DIFFUSION BEFORE RECOMBINATION H.R. Favarim, D. Spadacio, V. Zucolotto, O.N. Oliveira Jr, F.E.G. Guimarães, IFSC/USP, São

H.R. Favarim, D. Spadacio, V. Zucolotto, O.N. Oliveira Jr, F.E.G. Guimaraes, IFSC/USP, Sao Carlos-SP, Brazil.

Radiationless energy transfer between an emissive polymer (donor) and a dye molecule (acceptor) has been used to control the emissive properties of polymer films. Generally, a basic prerequisite for energy transfer (Förster type) is the resonance between the emissive states of donors and the acceptor absorption states. Here we demonstrate that this resonance condition is not sufficient to account for the energy transfer process in disordered conjugated polymers when efficient exciton spectral diffusion (donor-to-donor process) occurs prior to the radiative recombination. This was carried out using layer-by-layer (LBL) deposition of poly(pphenylene vinylene), PPV, and an azodye, the Brilliant Yellow (BY), spatially separated by inert bilayers of polyelectrolytes. The novelty lies in the possibility of changing the energetic position of the BY absorption band with respect to the polymer emission by changing the pH of the BY solution during the LBL fabrication. Luminescence results indicate that efficient Förster transfer still occurs even for a small overlap between the polymer emission and the BY absorption spectra. Probably the donor-to-donor exciton relaxation process (spectral diffusion) is affected by BY states, which are controlled by producing BY layers under different pH conditions. The introduction of BY states as non-radiative channels may be important to produce devices employing a polymer-dye system as emissive layer.

<u>C-P079</u> CORRELATION BETWEEN INDIUM TIN OXIDE ELECTRODE AND OPTICAL MODIFICATIONS IN POLYMER LIGHT-EMITTING DEVICES C.A.M. Borges, F.E. Montoro, R.M. Faria, F.E.G. Guimarães, IFSC/USP, Av. Trabalhador São carlense 400, C.P. 369, 13560-970, São Carlos-SP, Brazil.

> Organic light-emitting devices (OLED's) are based on very thin polymeric multilayered structures and have been subject of growing interest. These devices may contain conductive films that act as electrodes for charge injection to an active electroluminescence polymeric layer. As the total multilayer thickness is of the order of 100 nm in OLED's, one expects that electrode material parameters such as diffraction index and reflectance, as well as surface morphology may play an important role. This work reports the dependence of the optical properties of a polymer active emitting layer on the Indium Tin Oxide (ITO) pre-treatment and on the insertion of an inert spacer layer between the ITO electrode and the emissive layer. A very thin poly(p-phenylene vinylene), PPV, probe layer (1.5 nm) was used to map the optical properties of the ITO/polymer interface. We have employed Layer-by-Layer method, which allows control of layer deposition at the monolayer level. The ITO surface modifications were carried out by soft acidic aquaregia treatment. We observe that ITO reflectivity is strongly dependent on the treatment time and on the inert spacer thickness. The effect of the morphology of the ITO surface is discussed. In spite of the constant thickness, the PPV emission and absorption increase with the increasing of the spacer layer thickness. These results can be explained in terms of interference effects produced by the optical cavity formed by ITO, spacer and polymer films.

### <u>C-P080</u> ELECTRICAL CHARACTERISTICS OF MEH-PPV LIGHT-EMITTING DIODES USING ZnO AS ANODE

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Current vs. voltage (I vs. V) and alternating conductivity (AC) measurements were carried out in poly[(2-methoxy- 5-hexyloxy)-p-phenylenevinilene] – MEH-PPV light-emitting diodes having zinc oxide (ZnO) as transparent anode and Al as metallic cathode. MEH-PPV is a PPV derivative, which emits in red spectra; ZnO has work function similar to that of ITO, but is less aggressive to the polymer, less expensive and easily processed. The retificated I vs. V curves shows that the direct current depends on the temperature. Moreover, the real and imaginary components of alternating conductivity (ac) present typical behavior of somewhat disordered material: the imaginary component grows as a function of the frequency and the real component was observed to be frequency-independent for lower frequencies, and follows a power-law above a certain frequency. The Random Free Barrier model approaches and a resistance in series for the interface phenomenon were developed and adjusted for the ac results. This experimental-theoretical fitting we obtained important parameters of the devices as well as, quantitative informations about the MEH-PPV transport phenomenon.

<u>C-P081</u> THERMALLY STIMULATED DISCHARGE CURRENT OF SULFONATED POLYSTYRENE IONOMERS FOR APLICATION IN POLYMERIC ELECTROLUMINESCENT DEVICES

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One of the obstacles for the good performance of polymeric light-emitting diodes is the difficult of finding on appropriate material for electron injection. Recently, an ionomer deposited as electron transport layer in between the Al-cathode and the luminescent active polymer showed a good result, improving the device efficiency. In the sense to understand how the thin layers of potassium sulfonated polystyrene ionomers improve the injection of electron from the anode; we performed several studies of this material by thermal stimulated current technique. We varied the sulfonation level in between 1 a 15 mol% and the measurements were carried out in the 300 to 500 K range. The TSDC spectra of this material exhibit three discharge features in order of increasing temperature with two main transition around 400-440 K and about 500 K. A region of diffusion is observed before of Tg material. The results were interpreted in order to explain the effect of the number of charges in ionomers on the discharge current of depolarization. These results were discussed in order to use these ionomers as electron injection material in polymer EL devices.

#### <u>C-P082</u> ELECTROCHEMICAL PREPARATION AND CHARACTERIZATION OF POLY(P-PHENYLENE) FILMS AND COPOLYMERS

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Conjugated polymers have attracted considerable attention in the last years mainly because the number of applications they find in electronic, opto-eletronic and electrochemical devices. Among a number of electroluminescent polymers, poly(p-phenylene) (PPP) and its derivatives have become potential candidates as active layers in display devices emitting in the visible region. Here, we investigated the optical and electrochemical properties of electrochemically synthesized PPP and copolymers based on poly(3-methylthiophene) (P3MET) and polypyrrole (PPY). The homopolymers PPP, PPY, P3MET, and copolymers poly(p-phenylene-pyrrole) (CPPY), and poly(p-phenylene-3-methylthiophene) (CP3MET) films were electrochemically polymerized on transparent fluorine-tin-oxide glass (FTO) electrodes in a non-aqueous medium by cyclic voltammetry. The electrochemical response of the films in a monomer-free solution and their optical properties were investigated by cyclic voltammetry and in situ spectroelectrochemical measurements, respectively, which allowed us to obtain characteristics of the films such as electrochemical stability and optical transitions under successive cycling and applied potentials. Since the spectra are taken at different states of doping of the films, i.e. at different applied potentials, we estimated the electronic and optical band gap of each polymer from the values of oxidation and reduction potentials of the polymer films and their optical responses in the UV-VIS range

#### <u>C-P083</u> OPTIMIZATION OF THE DEPOSITION PARAMETERS OF POMA OBTANIED BY SPIN COATING USING ARTIFICIAL NEURAL NETWORKS J.P.H. Lima, A.M. de Andrade, E.A.T. Dirani, R.F. Bianchi, F.J. Fonseca, EPUSP, LME, Av. Prof. Luciano Gualberto, tv 3, 158, Sao Paulo, Brazil, PO: 05508-970

Using Artificial Neural Networks it was possible to simulate and optimize deposition parameters of thin films of POMA deposited by spin coating and their morphological characteristics. This new approach allows the prediction of thickness and roughness of films with reasonable accuracy. Changing the concentration of the solution of POMA, the spin velocity and the times of rotation we obtained experimentally different films and fed the Neural Network with this data. We used a multilayer perceptron network because of its simplicity, robustness and ability to represent multivariable functions. The relations of deposition process parameters and the morphology of films was estimated and is shown that the rotational time is not a crucible deposition process factor. This work provides a new method for estimating parameters in spin coating deposition process based in some films obtained previously.

#### <u>C-P084</u> ELECTROMAGNETIC INTERFERENCE SHIELDING EFFICIENCY ON POLYANILINE FILMS

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The number and the variety of the electronic devices are in increasing demand today although the operation of these systems can be affected by the electromagnetic radiation emitted from the electro-electronic equipments. Therefore, it is necessary that these components be protected against interference of electromagnetic radiation. The aim of this work is to evaluate the properties of the polyaniline films synthesized by chemical methods to be used as electromagnetic interference shielding efficiency.

By using the reflectrometry technique on ultra-high microwave frequency region (50MHz-2GHz), it could be applied an electromagnetic radiation on the polyaniline film by mean of the transmission coaxial line with a subsequent measurement of the reflected radiation. Thus, the can be obtained in the whole continuous frequency spectrum, which makes possible to obtain the shielding efficiency in decibels units. The complex dielectric permittivity is directly obtained from the reflection coefficient data, and the frequency dependence of the real and imaginary component of the permittivity can be studied as a function of the temperature.

#### <u>C-P086</u> DIELECTRIC CHARACTERIZATION IN POLYANILINE FILMS

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The electric conduction in polymeric films intrinsically conductive has been object of countless works in the last decade due to the insertion of those materials in electro-electronic applications, such as, sensors, electronic components and in electromagnetic shielding. In order to prepare polyaniline films with the capacity for storing charge the dielectric behavior of self-supporting films of polyaniline was investigated using the dielectric spectroscopy technique. The polyaniline films were obtained in the salt emeraldine form by oxidizing the aniline with ammonium persulphate. The polyaniline in solution was protonated and solved in chloroform with 5% v/v of meta-cresol. The polyaniline in solution was protonated with camphorsulfonic acid and dispersed in aluminum layers, and dried. The dielectric dispersion (frequency dependence of the real and imaginary components of the dielectric permittivity) was obtained as a function of the temperature in the frequency range of 100Hz to 10MHz. With these results, a mechanism was proposed for the electrical conduction along the polymeric chains and a conduction mechanism between the chains.

#### <u>C-P088</u> ELECTRICAL OPTIMIZATION OF SINGLE-LAYER LIGHT-EMITTING DIODES BASED ON BINARY ORGANIC SEMICONDUCTOR BLENDS A.Gusso, I.A. Hummelgen, M.G.E. da Luz, UFPR, Departamento de Física, Universidade Federal do Paraná, CEP 81531-990, Curitiba-PR, Brazil, C.P. 19044

We perform a theoretical analysis of the current-voltage characteristics optimization of singlelayer organic light-emitting diodes (OLEDs) made from binary organic semiconductors blends. Firstly, based on experimental results presented in the literature we propose a phenomenological expression to describe the electron and hole effective mobilites resulting from the mixing of two distinct organic semiconductors at different proportions. Using a simple model for bipolar charge and current distributions in OLEDs we then calculate the different J x V responses as a function of the blend concentration r. Finally, we discuss how a minimum in the power consumption during device operation can be achieved by choosing appropriate values of r. The influence on the optimization process of the quality of the ohmic contacts, assumed throughout our analysis, is also considered.

#### <u>C-P089</u> CHARGE MOBILITIES VALUES OF ORGANIC MATERIALS IN THIN FIELD EFFECT TRANSISTORS

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The development of organic electronics is growing fast due to the potential advantages of using organic materials as the semiconducting layer in electronic devices. In this work we have investigated the electrical characteristics of polymers and molecules using thin field effect transistors. The FET charge mobility could be obtained measuring current-voltage characteristics of the transistor with known channel length, operating in depletion mode under different gate voltages. Current – voltage characteristics of FET devices of organic materials will be presented and their FET mobility values compared with conventional mobility values obtained form sandwich diodes previously published. The FET-transistors were constructed using gold as the gate electrode, poly methyl-metacrilate as the insulator and nickel electrodes as the source and drain electrodes. The channels length are lower than 40  $\mu$ m. We would like to thank RENAMI/CNPq for financial support.

### <u>C-P090</u> ELECTRICAL CHARACTERIZATION OF POST-GROWTH CRYSTALLIZED PECVD SIC FILMS

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SiC based semiconductor electronic devices are developed for use in high-temperature, highpower, and/or high-radiation conditions under which conventional semiconductors cannot adequately perform. Its outstanding physical properties related to its high binding energy (~5 eV) and its large band gap (2.4 eV) makes it a very promising material for applications in aggressive environments. In this context, devices based on SiC electronic devices operating under high temperature are being fabricated with prospective for several industrial applications. However, the high production cost of SiC wafers has stimulated the development of growth of SiC on Si substrates. In previous works we have contributed in this direction, obtaining a-Si0.5C0.5:H films with high chemical and structural order by PECVD technique at low temperatures (~300 °C), and performed the crystallization of this material at temperatures around 1000 °C. However, the knowledge of the substrate doping level and the electrical behavior of the material is a requirement for device fabrication. So, in this present work, we report the electrical properties of unintentionally doped and phosphorus n-type and boron ptype ion implanted doping on crystallized SiC. The electrical properties were studied by Hall effect and electrical dark conductivity measurements. Based on these data, a comparison of the different effects of doping and annealing temperature on the properties of SiC are reported and discussed.

<u>C-P091</u> APPLICATION OF ATOMIC FORCE MICROSCOPY ON ADSORPTION PROCESS: CHARACTERIZATION AND MODELING F.L. Leite, P.S.P. Herrmann, C.E. Borato, O.N. Oliveira, L.H.C. Mattoso, Interunidades em Ciência e Eng. de Materiais - USP/ São Carlos, Embrapa Instrumentação Agropecuária, Rua XV de Novembro 1452, São Carlos

> Atomic force microscopy (AFM) and contact angle measurements are used to investigate the adsorption process of layer-by-layer (LBL) films of poly(o-ethoxyaniline) (POEA) on glass and mica substrates. AFM shows that LBL films of POEA grow via nucleation and growth of large primary islands, followed by the adsorption of secondary, smaller islands until coverage is complete. The shape and size of the islands and the kinetics of growth depend upon the substrate and film preparation conditions. A discussion is made of the effects from pH and number of the layers on the formation of POEA aggregates, as revealed by the images in the contact mode of AFM. The adsorption phenomenon of POEA is described by a theoretical model based on the fractal exponent, roughness and topography data. Surface roughness results provide a quantitative comparison among the different films, whereas the domain distribution and orientation were inferred using the fractal dimension method. Also was studied the effect from changing the polyelectrolyte charge density on the surface topography and adhesive properties. AFM was employed to image individual polymer chains at low adsorption densities and to characterize the layer topography and coverage at higher adsorption densities. The data indicate the formation of electrostatic bridges, particularly when highly charged polyelectrolyte (POEA) was used.

<u>C-P092</u> CHARACTERIZATION OF THE NATURAL RUBBER USING BLANKETS OF COTTON AND JUTE WITH POLYANILINE AS CONDUCTING REINFORCEMENT AGENT G.S. Silva, F.C. Ferreira, N. Alves, A.E. Job, UNESP, Depto. de Física, Química e Biologia, FCT-UNESP, CP 467, CEP 19060-900

> The research on technologies with "ecologically correct" has been a great concern in the last years. In this context, the natural fibers are being explored for applications as reinforcements in polymeric composites. In this work is presented a method of preparation and characterization of composites of natural rubber and conducting reinforcement agent using blankets of cotton and jute, with and without a treatment with polyaniline. It was also investigated the possible advantages by treating the blankets with NaOH that acts as carrier of the polyaniline into the fiber. The characterization of the materials was carried out through optical microscopy (OM), vibrational spectrosocpy (FT-IR) and thermal analysis by differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The results showed that the composite films are uniform and present high storage modules (E') compared with natural rubber films. The glass tansition temperature (Tg) of the samples is between -58oC and -32oC, showing interaction among the compounds since the Tg of the rubber (-67oC). The pre-treatment with NaOH provoked modifications in the thermal behavior of some samples, however it does not seem to have influenced in the dynamic mechanical properties. Samples of blankets treated with polyaniline shown conductivity in the order of 10-4 S/cm. The interation of the compounds was confirmed by FTIR. The application of this material will be tested in in-shoe pressure sensor.

<u>C-P093</u> BIODEGRADATION OF POLY(E-CAPROLACTONE), CELLULOSE ACETATE AND THEIR BLENDS BY STURM TEST AND SELECTED FUNGUS CULTURES M.R. Calil, C.G.F. Guedes, D.S. Rosa, USF, Laboratorio de Polimeros Biodegradaveis e Soluções Ambientais. Rua Alexandre Rodrigues Barbosa, 45, Itatiba, SP, Brazil

> Considering disposal options, biodegradable polymers offer an attractive approach to environmental waste management and contribute to the solution of these disposal problems. Poly(e-caprolactone) is one of the most promising synthetic biodegradable polymers since it is degradable in aqueous medium or in contact with microorganisms and can be used to make compostable polymeric devices. However, the high cost of PCL has prevented the widespread industrial use of this polymer. Natural polymers such as starch and cellulose are good base materials for rapidly degrading plastic, which are easily digested by microorganisms and inexpensive. In this work, the biodegradation of poly(e-caprolactone) (PCL), cellulose acetate (CA) and their blends was assessed based on an aerobic biodegradation technique known as the Sturm test and by a pool of selecting biodegrading fungus strains in solid medium with the plastics samples as sole sources of carbon. In the latter, biodegradation rate was determined though of the mass loss. The polymers were also characterized by melt flow index (MFI), according to ASTM D1238 and by thermal analysis using differential scanning calorimeter (DSC). The results showed that 40PCL//60CA blend present bigger release of CO2 in the aerobic biodegradation. In the test on solid medium the pure PCL suffered a considerable attack from the fungus in relation to the AC, however, it presented less mass reduction, probably because a bigger water absorption. The 60PCL//40CA

<u>C-P094</u> DEWETTING OF POLYMER THIN FILMS APPLIED TO POLYMERIC LIGHT EMITTING DEVICES A.J.F. Carvalho, M.A. Pereira-da-Silva, R.M. Faria, IFSC-USP, Grupo de Polímeros, Av.

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Polymer light-emitting diodes (PLEDs) technology uses thin polymer film structures and its properties are strongly dependent on the thin film processing. These polymeric devices consist of a thin film (100 to 300 nm) of an electroluminescent conjugated polymer sandwiched between two electrodes, where at least one is transparent. Additional layers used as electron or hole injection/blocking layer or to protect the electroluminescent polymer from contamination by ITO are of fundamental importance in PLEDs devices. These additional layers have thickness ranging from 10 to 30 nm and its structure and morphology are of great importance in the device characteristics. These thin polymer films with less than 100 nm are unstable and can goes to a dewetting process given rise to holes and drops affecting the PLED operation. In this work, we studied the application of ionic polymers (ionomers) as electron and hole injection layers for applications in PLEDs, focusing on the dewetting of these films as function of polymer composition and film thickness. The ionic polymers studied were low sulfonated copolymers of styrene and methyl methacrylate. The polymer films were obtained by spin coating deposition with thickness ranging from ~5 and ~100 nm. Films were characterized by AFM in tapping mode and by optical microscopy. The increase in ion content of polymers decrease dewetting in all tested conditions and the most suitable solvent for polymer deposition was methyl ethyl ketone.

<u>C-P095</u> CHARACTERIZATION OF NATURAL RUBBER LATEX (HEVEA BRASILIENSIS) RRIM-600 CLONES FROM INDIANA – SP R.D.Simões, C.J.L. Constantino, N. Alves, A.E. Job, UNESP, Depto. de Física, Química e

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The quality of the Brazilian latex is evaluated by simple methods, such as dried rubber content, alkalinity, plasticity, percentage of ashes, color test and percentage of nitrogen. In this work is presented a characterization of the as-collected and stabilized latex plus the natural rubber prepared from the respective latexes without the traditional vulcanization agents. The object is to explore their physical and chemical properties seeking to the preparation of blends and composites of natural rubber with other types of materials (polyaniline and carbon black). The latex was collected in Indiana, SP, Brazil, of rubber tree clones Hevea brasiliensis RRIM 600. A part of the latex was maintained as-collected while another was stabilized with 2% of ammonia and both were employed to prepare films of natural rubber using the casting method for what the temperature was kept at 65oC during 6 hours. The latexes and the natural rubber films were characterized using techniques such as electrical conductivity, thermal analysis (DSC, TGA, DMA), FTIR coupled with TGA and microscopy (MEV and AFM). The electrical conductivity of the as-collected and stabilized latexes is in the order of 10-3 Scm-1. The latex contains 40% of dried rubber as determined by TGA and films with uniform surface and low roughness were obtained as shown by microscopy. It is concluded that the rubber obtained either from as-collected or stabilized latex can be used in the preparation of blends and composites.

<u>C-P096</u> THE INFLUENCE OF THE CATIONIC POLYELECTROLYTE ON THE PHOTOINDUCED BIREFRINGENCE OF AZOBENZENE-CONTAINING LAYER-BY-LAYER FILMS

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Photoinduced birefringence is exploited in layer-by-layer (LbL) films of polyazobenzene PS 119<sup>®</sup> assembled with three polycations, viz.: poly(allylamine hydrochloride) (PAH), poly(diallyldimethylammonium chloride) (PDAC) and poly(ethyleneimine) (PEI). The LbL films were prepared via the alternate immersion of glass substrates into the polycationic and polyanionic aqueous solutions. A linear increase was observed in the peak at 490 nm (assigned to the pi-pi\* transition of the azobenzene moiety), indicating that the same amount of material is deposited at each deposition step. Birefringence was optically induced in polycations/PS119 films using a 532 nm NdYAG laser. The writing time - corresponding to the time to achieve 50% of maximum birefringence - was estimated as 17 min. for PEI/PS119 films, 6.5 min. for PAH/PS119 films and ca. 3.5 min. for PDAC/PS119 films. These differences in writing times are probably related to the structural differences of the polycations, which determine the degree of interactions between polycation and polyanion. Indeed, interactions between PS119 and PDAC are expected to occur to a lesser extent (in comparison to the other films) due to the hindering promoted by the dimethyl group in the quaternary ammonium salt, minimizing the interaction with sulfonated groups from PS119. With less interaction the azobenzene groups are more mobile, thus causing the writing time to be shorter for PS119/PDAC films.

#### <u>C-P097</u> SYNTHESIS AND CHARACTERIZATION OF BIODEGRADABLE TRIBLOCK COPOLYMER OF POLY(LACTIDE-CO-CAPROLACTONE)-PEG-POLY(LACTIDE-CO-CAPROLACTONE)

L. Zhao, W.S. Hui, D. Yung, Poli, Laboratório Macromoléculas, Departamento

Biodegradable and amphiphilic copolymers material are much searched recently. Polylactides (PLA), poly(e-caprolactone) (PCL) and their copolymers have widespread application in biomedical area as biodegradable sutures, resorbable protheses and containers for sustained drug release. In our recent work, we have successfully synthesized copolymer of PLA-PCL-PEG20K-PCL-PLA by ring opening copolymerization in the presence of the initiatior tin(II) octoate. The difficulty to copolymerize with poly(ethylene glycol) (PEG) of high molar mass was compensated by a long duration of the reaction. The products were characterized by permeation chromatography (GPC), differential scanning calorimetric (DSC), dynamic mechanical thermal analysis (DMTA) and nuclear magnetic resonance spectrometry. The results had been compared with other copolymers PLA-PCL of the same composition. All prepared copolymers presented good elastomeric properties.

<u>C-P099</u> SYNTHESIS AND CHARACTERIZATION OF NANOFIBERS CONDUCTING POLYMERS USING INTERFACIAL POLYMERIZATION E.S. Medeiros, P.S.P. Herrmann, S. Manohar, A.G. MacDiarmid, L.H.C. Mattoso, Embrapa Instrumentação Agropec. e UFSCar, Rua XV de novembro n. 1452, São Carlos, SP, Brazil, C.P. 741, 13560-970

Interfacial polymerizazion has arised as a very simple and promising method to produce nanofibers of conducting polymers. The use of nanofibers of conducting polymers in sensors can open up many possibilities such as the detection of chemical species at low concentration and fast sensor response due to their large surface area. In this sense, we are developing nanofibers of a conducting polymer, namely Polyaniline, to produce nanostructured films for sensor applications. These nanofibers have been characterized by cyclic voltammetry (CV), conductivity measurements, fourier transform infrared (FTIR), ultraviolet-visible spectroscopy (UV-Vis), field emission gun scanning electron microscopy (FEG/SEM) and electron paramagnetic resonance (EPR). The capability of nanostructured films as sensoactive layer in vapor and taste sensors are currently under investigation by electrochemical impedance spesctroscopy (EIS) and atomic force microscopy (AFM) measurements.

<u>C-P100</u> TIME DOMAIN REFLECTOMETRY (TDR) TECHNIQUE FOR MEASUREMENT OF THE ELECTRIC RESPONSE OF THE TASTE SENSOR, BASED ON ULTRA THIN FILM OF CONDUCTIVE POLYMERS, IN SOLUTION M. Carrizo, C.M.P. Vaz, L.H.C. Mattoso, P.S.P. Herrmann, Embrapa Instrumentação

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The electric response (dielectric permittivity and impedance) of the interdigitated electrodes coated with ultra thin film of conductive polymers, developed as a taste sensor, was investigated using time domain reflectometry (TDR) technique. The interaction between the polymer and the substances responsible for the different palate types, imply in the modification of the electric properties of the transducer material, that was measured by TDR. The membranes were obtained by using the self assembly technique through polymeric films adsorption on golden interdigitated electrodes. The devices were exposed to the basic substances, responsible for different palates (sodium chloride, sucrose, hydrochloric acid, quinine) and different beverages such milk, coffee and wine. To characterize the sensors, the Scanning Electron Microscopy (SEM) was used to evaluate the interaction between the polymers and the samples. The performance of the tasting sensors, according to their sensitivity and selectivity, were investigated. And with the use of AC measurements and Principal Component Analysis (PCA), it was possible to evaluate that the electronic tongue was selective.

<u>C-P101</u> ANISOTROPY IN POLY(9,9-DIOCTYLFLUORENYL-2,7-DIYL) SOLUTIONS: THE ROLE OF THE SOLVENT PROPERTIES R.F. Cossiello, H.P.M. de Oliveira, P. Aramendía, T.D.Z. Atvars, UNICAMP, Instituto de Química, Campinas - SP, Caixa Postal 6154 CEP 13083-970

Physicochemical properties of conjugated polymers depend critically on the environment. A great variety of properties of conjugated polymers have been studied by several spectral techniques. Poly(9,9-dioctylfluorenyl-2,7-diyl)-hole transport end capped (PF) shows red shift in both absorption and emission spectra in poor solvents, revealing a compact conformation of the macromolecular chain. This red shift is accompanied by a decrease of extinction molar coefficient at the maximum of absorption spectra. The steady state emission anisotropy correlates the appointed spectral characteristics: in poor solvents the anisotropy is higher than in good solvents. Time-resolved fluorescence shows that PF has excited state lifetime about hundreds of picoseconds range, displaying the shortest lifetime in poor solvents. The compact conformation of polymeric chain in poor solvents can explain the excited state deactivation by interaction with the solvent more probable than deactivation by interchain interaction. Opposite behavior is found in good solvents. In these media, stretched molecular conformation favors excited state deactivation by inter- and intrachain energy transfer.

<u>C-P102</u> ORGANIC MATERIAL AS GAS SENSORS FOR FARM APPLICATION

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Polyaniline and phthalocyanines are organic materials with potential use in \'electronic nose\' sensors and has been shown to be highly sensitive to ammonia. This paper shows results of the characterization of ultra thin films of polyaniline and/or phthalocyanines for applications as gaseous ammonia sensor at NH3 monitoring at chicken farms. A sensitive layer based on such materials deposited on the top of interdigital gold electrodes previously deposited onto a glass substrate, with 100  $\mu$ m. The structure of the films are investigated by ultraviolet-visible (UV-VIS) and of the infrared (FTIR) absorption spectra. The electrical characteristics are obtained through conductivity measurements in continuous and alternate field, DC and AC, respectively, in order to determine its dependence with ammonia concentration, humidity and temperature, the main parameters to be controlled in the chicken's farm. The results show the potential of such class of device to be used as active material in chicken grows applications.

#### <u>C-P103</u> LANGMUIR-SCHAEFER FILMS OF POLY(5-AMINO–1-NAPHTHOL)

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Poly(5-amino–1-naphthol), henceforth PAN, is a conductive organic polymer which has been synthesized by electropolymerization of 5-amino–1-naphthol. PAN is very suitable for protection of metallic surface against corrosion. PAN shows good response as the active element of a voltage-regulator device. In these applications, the characteristics of the polymeric film such as uniformity, roughness, thickness, have strong influence on the final quality and possible applications. Thus, in order to contribute to the understanding of the molecular organization and to the formation of good quality ultrathin solid films of PAN, we started a systematic study of Langmuir-type films of this material. We report on the preparation and characterization of Langmuir and LS-type PAN films. The thermodynamics of the Langmuir films at the air/water interface is investigated at different aqueous subphase pH values and compression speeds. The stability of the Langmuir PAN film is investigated by measuring the film behavior under subsequent compression/decompression cycles. Horizontal lifting procedure allowed the transfer of the Langmuir films to a solid substrate, under optimized transfer ratios. Atomic force microscopy (AFM) and Raman spectroscopy were used to characterize the resulting Langmuir-Schaefer films.

<u>C-P104</u> PHOTO AND THERMAL ISOMERIZATION KINETIC OF FUNCTIONALIZED POLYMERS USING AZO DYE

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Memory optical storage and photo-induced birefringence are some of applications of azo dye in photo reactive organic film, which dependent the kind of the photochromic units are incorporated in the polymeric matrix. These can be gotten by two different ways: doping or functionalizing at different positions in polymer (side-chain or main-chain). The kinetic photo and thermoisomerization of polystyrene (PS) with the dye [4-(N-(2-hidroxiethyl)-N-ethyl)-2\'chlore-4'nitroazobenzene] (DR13) doped (PS/DR13) and functionalized (PS-DR13) differs significantly. The doped polymer shows higher photo and thermoisomerization kinetic rate constant than functionalized polymer due the lower rotational and translational moving of dye in the matrix. It was verified the influence of matrix polarity on kinetic behaviors through the copolymerization of methylmetacrylate (MMA) units and styrene with the copolymers functionalized with DR13, growing the dielectric constants of polymeric matrix, resulting an increase of conversion rate.

<u>C-P105</u> EFFECT OF MICROSTRUCTURE ON THE THERMAL PROPERTIES OF THE PVDF AND P(VDF-TRFE) COPOLYMERS

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The knowledge of the thermal properties (thermal diffusivity, thermal conductivity and specific heat) of polymers is crucial in the description and analysis of the extrusion process and it is also of fundamental importance in many processes and projects in polymer engineering. In this work it was studied the morphology influence of the poly(vinylidene fluoride) (PVDF) and P(VDF-TrFE) copolymers containing 50, 70 and 80 mol% of VDF on the thermal diffusivity, thermal conductivity and specific heat of these materials. Disc shaped samples 1.0 mm diameter and 0.3 mm thickness with different morphologies were obtained through different crystallization conditions. The micrographs of morphologies were obtained by scanning electron microscope (SEM). The laser flash technique was employed in the experimental determination of the thermal diffusivity. Modulated DSC was employed in the specific heat determination. With the knowledge of the thermal diffusivity (a), specific heat (c) and the sample density (d), the thermal conductivity was derived by using the equation k = dca. Experimental results showed a strong influence of the morphology on the thermal diffusivity and specific heat. On the other hand, a week influence of the morphology on the thermal conductivity was observed. These results are then explained considering the different mechanisms of heat propagation throughout those materials.

<u>C-P106</u> Pt3Co/C AND Pt3Ni/C ALLOYS AS ANODE AND CATHODE ELECTROCATALYSTS FOR DIRECT METHANOL FUEL CELLS J.R.C. Salgado, E. Antolini, E.R. Gonzalez, IQSC/USP, Lab. Eletroquímica, São Paulo, Brasil

Among the different fuel cell technologies, direct methanol fuel cells (DMFCs) working at low temperatures, are promising candidates to be used as power sources for portable equipment and in transportation applications [1]. In these systems, carbon supported platinum and platinum-ruthenium alloys (Pt/C, Pt-Ru/C) were considered the most active catalysts for the oxygen reduction (ORR) and methanol oxidation reactions, respectively. Additionally, alloy catalysts are being developed to improve the catalytic activity and reduce the cost. The advantage of bimetallic materials for the ORR in relation to Pt/C is attributed to several factors, such as, more favourable Pt-Pt distance, electronic effects, changes in the crystallographic structure or preferential crystalline orientation [1]. In this work, Pt3Co/C and Pt3Ni/C commercial materials were characterized by using X-ray diffraction and X-ray absorption spectroscopy. The performance in single DMFC fed with metanol/O2 of Pt3Ni/C and Pt3Co/C in the cathode was more satisfactory than that of Pt3Ni/C and Pt3Co/C as anode materials. The enhanced performance of Pt3Ni/C and Pt3Co/C as cathode materials was ascribed both to the improved activity for oxygen reduction (electronic effect) and to the higher methanol-tolerance (ensemble effect) of the alloy.

<u>C-P107</u> HIPERFINE INTERACTIONS IN INTERMETALIC SISTEMS RX (R = RARE EARTH, X = AG)

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In the present work, the Time Differential Perturbed Angular Correlation (PAC) was used to measure the magnetic hyperfine field (mhf) at the rare earth sites in intermetallic compounds RAg in order to study the behavior of the mhf with the variation 4f electrons density. 140Ce was used as probe nuclei in the PAC measurements carried out in the temperature range of 10 K to 300 K. X-Ray Diffaction (XRD) was used to compound caracterization. The results of the temperature dependence of the mhf show a standard antiferromagnetic behavior below the magnetic order temperature. However, for lower temperatures, it was observed a sharp deviation from the expected Brillouin-like behavior with an increase of the mhf values. This behavior was observed for all the compounds studied in this work The explanation for the additional magnetic interaction is believed to result from the polarization of 140Ce spin moments induced by the magnetic field from rare earth moments. A comparative analysis of the mhf and the magnetic moment at rare earth sites as a function of the rare earth J spin projection shows that both have the same behavior.

C-P108 SAXS AND XRD CHARACTERIZATION OF CHEMICALLY CROSSLINKED PVA HYDROGELS

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Poly (vinyl alcohol/PVA chemically crosslinked with glutaraldehyde has been characterized by Small Angle X-ray Scattering (SAXS) and X-ray Diffraction (XRD) techniques. The results obtained through synchrotron radiation curves and X-ray diffraction patterns have indicated the formation of nanostructured hydrogels, with crystal domains immersed in an amorphous polymer matrix. Also, swollen experiments have confirmed the crosslinking of PVA hydrogel by glutaraldehyde. We have successfully developed and characterized PVA hydrogels with nano-scale structure.

<u>C-P109</u> SYNTHESIS AND CHARACTERIZATION OF COPOLYMERS WITH DIFFERENT RATIOS OF PPV AND DCNPPV UNITS

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The use of PPVs type polymers (poly-p-phenylenevinylene) as active layer in organic light emitting diodes (OLEDs), has received much of attention in the last two decades, resulting in commercial projects developed by great companies like DuPont, Kodak and Philips. However some intrinsic problems related to the poor efficiency and short display life impossibility the utilization of this kind of technology. For this mentioned reasons, the search for PPV like polymers with CN connected to the backbone is justified by the diminishment of the electron injection barrier and by the improvement in the electron mobility in the polymer matrix. Nevertheless the synthesis of this kind of materials has been to much complicate and the obtained polymer showed a sequence of problems. Facing theses problems, this work describe the preparation of a series of copolymers prepared with different ratio of PPV and DCVPPV units using the Wessling methodology. These copolymers, after purification and thermal treatment were characterized by FTIR, UV-vis, GPC and cyclic voltammetry. The obtained results showed that the copolymers films presented a low conjugation defects degree, a high molecular mass and a ratio of PPV and DCNPPV unit correspondent to the monomeric proportion using to the polymers preparation.

#### <u>C-P110</u> SnO<sub>2</sub> - 3-AMINOPROPYLSILOXANE HYBRIDS H.W. Silva, R.R. Gonçalves, S.J. Ribeiro, Y. Messaddeq, UNESP-IQAr, Laboratory of Photonic Materials, PoBox 355, Araraquara-SP, 14801-970, Brazil

The possibility of combining the properties of organic and inorganic compounds in unique material is an old challenge that started with the beginning of the industrial era 1. Therefore the Sol-Gel processes together with the organic-inorganic hybrids appear as a creative alternative for obtaining new materials with unusual features. Organic-inorganic materials ally the favourable optical properties of inorganic compounds with the functionality and processing of polymeric materials. In particular, tin oxide has been used for many applications, including gas sensors, special conducting coatings, resistors and electro-optical devices 2-3. With the objective of prepare new organic-inorganic material for wave guide application, Eu3+ doped tin oxide nanoparticles was incorporated in a modified siloxane (3-aminopropyltriethoxysilane) matrix. The sol obtained was deposited by spin coating technique under the glass substrates. The structural characterization of the materials using MET, X-ray, PCS and NMR techniques as such as optical characterization using fluorescence spectroscopy for Eu3+ and m-lime apparatus (Metricon Model 2010) based on the prism coupling are reporting in this work.

#### <u>C-P111</u> PRODUCTION OF SELECTIVE MEMBRANES USING NANOCHANNELED PLASMA DEPOSITED THIN FILMS

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Tetraethoxysilane plasma polymerization films allow the formation of a nanochanneled silicone like structure when hydrolyzed. These nanochannels can be useful for the production of selective membranes. Therefore, the aim of this work is to test the use of these membranes for separation of organic compounds and/or water in gaseous phase and for salt permeation in liquid phase. The efficiency of separation or permeation was tested using quartz crystal microbalance (QCM) technique in gas phase and conductimetric analysis (CA) in liquid phase. The substrates used were: silicon for characterization of the deposited films, piezoelectric quartz crystal for tests of selective membranes, cellophane paper for tests of permeation and acrylic for test of adhesion on polymeric substrate. QCM analysis showed that the nanochannels allow the adsorption of organic compounds and water. The use of dodecane, hexane, acetone and 2-propanol as reactants showed that the adsorption efficiency is greater for more polar and/or smaller molecules. For water occurs not only adsorption but also permeation. CA showed that the film allows salt permeation. However, a time delay occurs in this permeation due to the necessary hydrolysis of the organic radicals within the film. The film also showed good adhesion in acrylic substrate. Due to the high amount of water used for hydrolysis, the films can be used for grains protection against microorganism proliferation during storage without preventing germination.

#### <u>C-P112</u> PHOTOLUMINESCENCE AND DIELECTRIC RELAXATION IN POLYANILINE/SURFACTANT NANOPARTICLES J.D. Ribeiro-Filho, H.P. de Oliveira, C.A.S. Andrade, C.P. de Melo, UFPE, Departamento de Física, Universidade Federal de Pernambuco, Rua Prof. Luiz Freire, S/N, Recife, Pernambuco, Brasil, CEP 50670-901

The possibility of controlling the intrinsic properties of polyaniline (PAN) either by changes in the oxidation state of the polymeric backbone or by varying the pH of the medium has made this material one of the most investigated conducting polymers. We report an investigation of the influence of protonation upon the photoluminescence and dielectric relaxation properties of PAN/surfactant nanoparticles. We have used surfactants to provide a convenient ambient for the emulsion polymerization of aniline, using ammonium peroxysulfate as the oxidizing agent. Polyaniline was obtained in the form of emeraldine hydrochloride salt (ES). ES was converted in the emeraline base (EB) by treatment with concentrated ammonium hydroxide.. After filtration, the resulting solutions were progressively diluted and had their fluorescence monitored for different excitation frequencies. Analyzing the corresponding excitationemission matrices, we could observe a progressive hypsochromic shift in the emission spectra and could identify the presence of two maxima (330 to 326 nm and 404 to 400 nm) for the ES/surfactant and only one (359 to 343 nm) for the EB/surfactant system. A dielectric spectroscopy analysis of these solutions shows that the real part of the impedance at 1MHz increases exponentially with dilution, a fact that can be explained by assuming that the micelles are preserved and are present in smaller concentration as the dilution process continues.

## <u>C-P113</u> PREPARATION AND CHARACTERIZATION OF NANOPARTICLES OF IRON AND POLYPYRROLE

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We report impedance spectroscopy (IS) results of aqueous solutions of surfactant micelles that envelope nanoparticles of iron and polypyrrole (PPy). A solution of lutrol (a surfactant), FeCl3 and pyrrole (Py) was stirred until micelles are formed. When iron nanoparticles are added to this solution under agitation, the FeCl3-induced polymerization takes place and the metallic particles are enclosed by the micelles together with some PPY chains. Separating the largest aggregates by filtration, micelles are present in the remaining dark color solution. We prepared different solutions in which the relative amounts in mass of Fe and Py are varied in a reciprocal manner. Scanning electronic microscopy established that the micelles have a spherical form only if PPY is present, while cubic ones were found in the sample prepared without Py. This is taken as evidence that the PPY chains are present in the interior of the micelles. IS was then used to examine the dielectric response of the different solutions, when we were able to identify the existence of two regimes of conduction accordingly to the relative amounts of PPY and Fe (one of metallic nature for the samples with larger amount of Fe and the other with the charge transport determined by the PPy chains), with a maximum in the real part of the impedance associated to the transition between the two. These systems can find application as anti-corrosive paints, magnetic memories or contrasting agents in medical diagnosis.

#### <u>C-P114</u> PREPARATION AND CHARACTERIZATION OF POLYANILINE NANOPARTICLES FOR USE IN ALL-POLYMER ELECTRONICS C.A.S. Andrade, H.P. de Oliveira, UFPb, Recife, Pernambuco, Brasil,

We report the preparation of conducting microwires using polyaniline (PAN) nanoparticles. Aniline was introduced in an aqueous solution of a surfactant (at a concentration in which micelles are present), containing ammonium peroxysulphate. The oxidant-induced polymerization takes place in the solution and some of the PAN chains become enclosed into the micelles. As the conductivity of PAN is affected by the pH of the medium, we have prepared the polymer both in the emeraldine salt (ES) and emeraldine base (EB) forms. Scanning electronic microscopy analysis has revealed that the micelles are spherical and homogeneous in size. The characteristic polaron band (800nm), present in the ultravioletvisible absorption spectra, had a discrete shift as the pH varies, in an indication of the conducting character of the PAN. An impedance spectroscopy investigation of the different solutions has confirmed that in fact the ES form is more conducting than EB. We have used solutions 0.25M of the ES to fill patterns drilled into a polystyrene dielectric matrix accordingly to a typical resistive-capacitive (RC) circuit. The characteristics of the resistive microchannels and capacitive microwells components so constructed could be controlled both by the preparation conditions of the PAN nanoparticles and by the physical parameters (length and depth) of the patterned circuit, so that an all-polymer operational device could be appropriately constructed.

<u>C-P115</u> EFFECT OF ANNEALING IN Ni BASED AMORPHOUS RIBBONS AND MICROWIRES A.E.P. de Araújo, M. Provêncio, K.R. Pirota, F. Batallan, M. Vazquez, M. Knobel, UNICAMP Campinas Sao Paulo, Brazil

In recent years many works has been studied the magnetic properties of amorphous microwires. In this work we compare the thermal treatment in amorphous microwires and ribbons with the same composition. Crystallisation behaviour and magnetic properties of melt-spun and annealed Ni73.5Cu1Nb3Si13.5B9 ribbons and microwires produced by Taylor-Ulstinov technique have been studied. The microwires has a metallic nucleus of 5 mm of radii and a glass cover of 3 mm thickness. The annealing was make in temperatures from 600 to 1000 oC in nitrogen atmosphere. The effect of the temperature and time of the thermal treatment was studied. XRD studies shows the formation of Nanocystalline composite diameter dispersed in an amorphous matrix. The as-cast samples do not present ferromagnetism at temperature ambient. After the annealed treatment the samples magnetization curve presents a ferromagnetic behaviour with a very small coercive field (10e). At the annealed temperature of 800 K for 1h we estimate the saturation magnetization of 410 emu/g for the microwire and 1.33 emu/g for the ribbon. In the work we discuss this difference how the effect of the glass cover in the microwire. It was also made measurements in microwires with composition Ni82B12Si6 with different diameters and glass cover thickness.

## <u>C-P116</u> CALCULATION OF THE MODULE OF BULK USING METHODS OF STRUCTURE OF BANDS

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With the evolution of the science of the material ones it also came the technological evolution, new leagues and its use, in the most diverse areas of the knowledge. Thus, in this work, we study the structures of bands of nitreto of Boron, in this case the structure of 3FeBN. To decide the structure of bands of the composition, we use the Linear Orbitals Method Muffin-Tin (LMTO) with the method of approach of the spheres (WING). Through this method we got as resulted of the energy of formation in function of the net parameter, a parameter of net of balance of 6,9569 u.a.. In elapsing of the work we will also argue I modulate it of Bulk, as well as the properties of the basic state.

<u>C-P117</u> XANES AND EXAFS INVESTIGATIONS OF THE PLATINUM-SILVER ALLOYS F.H.B. de Lima, E.A. Ticianelli, IQSC, Laboratório de Eletroquímica, Av. Trabalhador Sancarlense 400, São Carlos, Brazil, Caixa Postal, 780

Pt-Ag alloys with different compositions and dispersed on a high surface area carbon powder were prepared and investigated as electrocatalysts for the oxygen reduction reaction (ORR) for alkaline fuel cell application. The carbon-dispersed catalysts (20 wt.% metal/C) were prepared by chemical reduction of the precursors (H2PtCl6, Aldrich and Ag(NO3)2 Merck) with sodium borohydride (NaBH4) in the presence of the carbon powder, to form particles of Pt, Ag, and of Pt-Ag with 1:1, 1:2, 1:3, and 1:10 atomic proportions. The physical features of the materials were determined by XRD (X-ray diffraction) and in situ XAS (X-ray absorption spectroscopy), in the XANES (X-ray absorption near edge structure) and EXAFS (extended X-ray absorption fine structure) regions. Results showed formation of real alloys of Pt and Ag, resulting in an increase of the unit cell lattice parameter, a rise in the Pt 5d electronic band occupation, and an increase in the Pt-Ag coordination numbers with the increase of the insertion of Ag atoms. The electrochemical measurements indicated lower activity of the Pt-Ag/C alloys for the ORR compared to that of Pt/C, but higher activity compared to that of Ag/C. These electrochemical characteristics were correlated to the physical and electronics characteristics of the Pt-Ag catalyst particles.

<u>C-P118</u> PROTONATION AND OPTICAL PROPERTIES OF THE MACROMOLECULAR COMPLEX SULFONATED POLY(STYRENE):POLYANILINE A.A.A. de Queiroz, C.P.L. Rubinger, R.M. Rubinger, D.A.W. Soares, C.M.A. Freire, F.F. Brito, UNIFEI, Departamento de Física e Química/Instituto de Ciências Exatas, Av. BPS, 1303, CEP: 37.500-903, Itajubá-MG, Brasil

The synthesis and characterization of membranes with high protonic conductivities based on macromolecular complexes of sulfonated poly(styrene) and conducting polymers has received considerable attention in recent years due to their interesting electronic conduction and nonlinearity properties. In this work, the electrical and optical properties of the macromolecular complex sulfonated polystyrene:polyaniline (PSt/PANI) was investigated. The PSt/PANI were synthesized by the in situ redox polymerization of aniline in the sulfonated polystyrene matrix. The UV/VIS spectra of the PSt:PANI complex showed absorption bands at 730 nm and 817 nm characteristics of the polaron transition and protonation of the imine nitrogen of PANI by the sulfonic acid groups of PSt, respectively. The electrical conductivity at room temperature (298 K) was strongly dependent on the weight fraction of PANI in the PSt matrix, similarly to percolation systems with a low critical weight fraction of polyaniline in the stronglex. At low temperatures, the conductivity temperature dependence follows the s(T)=soexp[-(To/T)m] law, witch has been explained within the framework of Mott's variable range hopping model (m = 0.3).

<u>C-P119</u> ORGANIC-INORGANIC HYBRID FILMS INCORPORATING CHITOSAN AND IRON TETRASULFONATED PHTHALOCYANINE

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Chitosan [β-(1-4)-2-amino-2-deoxy-D-glucose] is the partially N-deacetylated derivative of chitin presenting both amino and hydroxyl groups. Chitosan has excellent properties as film forming material, including nanostructured layered films, as shown in this work, where chitosan was assembled in a layer by layer fashion with iron tetrasulfonated phthalocyanine (FeTsPc). Thin films containing up to 30 Chitosan/FeTsPc bilayers were deposited on glass slides and silicon wafers substrates. The growth of the multilayers was carried out via the immersion of the substrate in the chitosan and FeTsPc aqueous solutions, alternately for 5 min. After each immersion, the substrate was immersed for 1 min in water. The deposition process was monitored after each deposition step using UV-VIS spectroscopy. A linear increase in absorbance at 676 nm (assigned to the Q-band of the FeTsPc) indicated that the same amount of material was adsorbed at each deposition step. The presence of protonated amine groups from chitosan and sulfonated groups from FeTsPc allowed the formation of NH3+-SO3- salt bridges, which acted as binding sites in the chitosan/FeTsPc bilayers. The latter was revealed by Fourier transform infrared spectroscopy (FTIR) experiments, where the band at 1040 cm-1 (SO3 stretch from neat FeTsPc) was shifted to 1030 cm-1 in the PAH/FeTsPc films. The films were tested as sensors for neurotransmitter species (dopamine) using cyclic voltammetry and FTIR spectroscopy as detection techniques.