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POSTER PRESENTATION **ABSTRACTS**

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Por favor siga a numeração do resumo para
colocar seu poster.

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1. Theoretical NMR, IR/RAMAN calculations in sodium pravastatin: unraveling experimental results in drug carrier materials

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Layered double hydroxides (LDH) can be used as nanocontainers for immobilization of Pravastatin, in order to obtain suitable drug carriers. The material's structure and spectroscopic properties were analyzed by NMR, IR/RAMAN and supported by theoretical calculations. Density Functional Theory (DFT) calculations were performed using the Gaussian03 package [1]. The geometry optimizations were performed considering the single crystal X-ray diffraction data of *tert*-octylammonium salt of Pravastatin [2]. Tetramethylsilane (TMS), obtained with the same basis set, was used as reference for calculating the chemical shift of ^{13}C . A scaling factor was used to compare theoretical and experimental harmonic vibrational frequencies. Through the NMR and IR/RAMAN spectra, we were able to make precise assignments of the NMR and IR/RAMAN of Sodium Pravastatin.

We acknowledge support from CAPES, INEO and CNPQ.

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2. Optimally tuned hybrid DFT functionals for calculation of electronic properties of organic semiconductors
Funcionais DFT híbridos otimizados para cálculo de propriedades eletrônicas de semicondutores orgânicos

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The precise theoretical evaluation of band gaps and ionization potentials of organic semiconductors offers an useful guideline to design novel optoelectronic devices. In particular, the efficient performance of these devices crucially depends on the relative energy level positions between the metal and organic parts at hybrid interfaces. It is therefore desirable to find out a physical model that may describe the electronic structure of both metal and organic systems with the same level of accuracy. In this work, we perform first-principles calculations on the basis of Density Functional Theory (DFT) to investigate the electronic structure of a prototypical 1D conjugated polymer, trans-polyacetylene. We employ an internally consistent strategy to optimize the fraction of exact exchange (α -mixing) inserted in the Perdew-Burke-Ernzerhof hybrid functional (PBEh) such that the Kohn-Sham energy of the Highest Occupied Molecular Orbital (HOMO) reproduces the quasi-particle energy calculated with G_0W_0 approximation. Our findings show that the optimal fraction of exact exchange incorporated in PBEh decreases exponentially with chain length going from $\alpha=0.85$ for the ethylene molecule ($n=1$) up to $\alpha=0.75$ extrapolated for an infinite polymer chain. Furthermore, we observe that the HOMO-LUMO gap calculated with the optimally tuned PBEh reasonably fits also the electrical gap of G_0W_0 calculations. Finally we will discuss the adequacy of the PBEh optimized for organic systems to compute the electronic

properties of the stable geometries of gold clusters.

Acknowledgements

We acknowledge support from the Brazilian agencies CAPES, INCT-INEO and computational facilities of LCCA-USP and FHI-MPG.

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3. **Atomistic modeling of electronic transport in organic systems** **Modelagem atomística do transporte eletrônico em sistemas orgânicos**

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Organic conjugated polymers present several interesting properties and can be used as active layers in e.g. light emitting diodes (LEDs)[1] and field effect transistors (FETs) [2]. Even if the attainable efficiencies are lower compared to inorganic semiconductors, these organic counterparts have other advantages such as low weight and low cost, and in principle can be engineered for large area displays, and flexible devices. In this work we present an atomistic-based simulation of transport properties of poly- para-phenylene vinylene PPV. We employ Classical Molecular Dynamics (CMD) simulations of oligomeric films in order to generate atomistic models, using an in-home reparametrization to non-bonded energies of Universal Force Field (UFF) [3]. Transport was modeled via a non-linear Stochastic Master Equation SME [4,5] with parameters obtained from first-principles quantum calculations: conjugation length, site energies and transfer energies. For each film image generated by CMD, we built a topological connectivity network, from explicit calculations of inter-ring bond distances and bond angles. We calculated hole mobilities for different PV films (crystalline P5V4, amorphous P3V2, and P26V25) with several configurations (images) for the same film, representing a given temperature, and also with different carrier concentrations. We clearly see the dependence with morphology, and the need for averaging obtained values for all relevant quantities.

We acknowledge support from FAPESP, INEO, and CNPQ.

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4. **.Theoretical study of stretching of amorphous PPV films** **Estudo teórico do estiramento de filme amorfo de PPV**

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Poly (p-phenylene vinylene) (PPV) is a well-known organic semiconductor, usually deposited via spin-coating technique on a substrate and further treated to obtain the desired functionality;

generally, this system exhibits amorphous and crystalline regions. Changes in the molecular environment around the polymer chains can drastically affect the resulting properties and experimental results showed that mechanical stretching of PPV films can affect its electronic and optical properties such as the emission of polarized light, gap energies and the electronic conductivity [1, 2].

In order to simulate the evolution of the morphology during the mechanical stretching of PPV films, we carried out Molecular Dynamics simulations using an in-home reparametrized version of the Universal Force Field [4] concerning the non-bonded interactions, which improves the description of elastic properties of this system [5]. In this work we present analysis on the influence of stretching in the molecular conformations and induced variations in the intermolecular packing by means of statistical distributions obtained from the different images extracted from the dynamics realized over a set of different initial conformations. The work is still ongoing, so as to achieve larger statistical significance, however some initial findings and general trends can be discussed.

We acknowledge support from FAPESP, INEO, and CNPQ.

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5. Study of the electronic properties of the thienoacene derivatives

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Since the construction of the first organic transistor, based on thiophene, semiconductor polymers have been widely employed in the construction of organic devices such as: field effect transistors (OFET), organic light-emitting diodes (OLEDs) and organic photovoltaics (OPVs). A major advantage of using carbon-based materials is the flexibility with which they can be synthesized and functionalized, which combined with the low production cost and the possibility of obtaining ultra-thin and flexible devices, make these materials interesting technological point of view. The goal is to obtain materials with high stability and high charge mobility. Newly, were reported the synthesis of thienoacenes- based and derivatives with these characteristics. Single-crystal organic field transistors constructed with a derivative of the dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNNT) show saturation and the linear mobility of the order of 12.3 and 16 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, respectively.

Here, we use a the first principles methods, for investigation the three-dimensional band structure of DNNT and some of its derivatives (listed in reference [1]) and compared it with the electronic structure of acenes (crystalline pentacene, anthracene, naphthalene and phenanthrene) and thiophenes (crystalline polythiophene). We used LDA, GGA-PBE and GGA- PBE functional with the addition of van der Waals (VDW) correction. Based in on our results for each material, we try to gain insight about the possible reasons which lead to thienoacenes and its derivatives to exhibit mobility values higher than those obtained to acenes and thiophenes, from which they derive.

We acknowledge support from CENAPAD, CNPQ and INEO

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6. Theoretical study of electronic and optical properties of the trifluoromethylaniline oligomers

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In this work, the theoretical study of emeraldine and leucoemeraldine oligomers, where hydrogen atoms of the meta position of each ring were substituted with trifluoromethyl radicals, is reported [3,4]. We investigate oligomers containing from four up to eight rings, with two different configurations of the endings at each chain: H termination and NH₂ termination. All results are compared with pristine emeraldine and leucoemeraldine oligomers. We conducted convergence tests of the oligomers electronic properties as a function to the length of the chains. Differences of the HOMO-LUMO energy and the optical absorption spectrum were analyzed.

For this study we used the semi-empirical method AM1 [5], within the Hartree-Fock formalism. This method allows us to perform calculations related to stability as well as the structural, electronic and optical properties.

The optical absorption spectrum was obtained with the ZINDO-S method. We found that the inclusion of the trifluoromethyl radical in emeraldine and leucoemeraldine oligomers produces a decrease of up to 40% in the torsion angle. Also, we note that there is a reduction of the energy difference between the frontier orbitals, when comparing the substituted with the neutral systems. The reduction for the substituted systems reaches about 7% for leucoemeraldine and 5% for emeraldine. These variations of the structural properties are reflected in the optical absorption spectrum, the addition of trifluoromethyl radicals always lead to a red-shift in the absorption spectrum.

We acknowledge support from CNPQ and INEO

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7. **Analysis of structural and electronic properties of the poly(3-methylthiophene) oligomers**

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Thiophene derivatives are obtained when one hydrogen atom, which is bonded with a C \square , is replaced by an alkyl group. In this work, the structural and electronic properties of the poly(3-methyl-thiophene - P3MT) were investigated, using a Hartree-Fock (HF) and AM1 approximation. Three distinct conformations for the P3MT monomer were analyzed: Head-to-Tail (HT), Tail-to-Tail (TT) and Head-to-Head (HH). The results show that the HT and HH systems have total energies of 20 and 39 meV, higher than TT conformation respectively. The analysis of the potential torsion energy profile (\square) shows interesting effects of inclusion of alkyls at different positions on the backbone. For the bithiophene, one minimum of the energy structure corresponds to a torsion angle closed to 150 degrees. The second minimum is approximately 9 meV higher than the global one, in this case, the torsion angle was 40 degrees. The profile of the torsion energy barrier for the TT is similar to that obtained for the bithiophene and different from the results found for HH and HT. For these systems, the stabilization occurs for $\square = 180$ degrees. We also have investigated the effect of the conjugation length on the structural and electronic properties of the P3MT contained in 1 up to 8 thiophene rings. In all the cases, the Mulliken partition of the atomic charges shows that the electrons flow from the methyl radicals to the conjugated segment. The alkyl chains do not contribute to the frontier orbitals, consequently, the methyl groups are responsible for improving the solubilization of the polymeric chain.

We acknowledge support from CNPQ and INEO

8. **Statistical model of resistors network for studying the conduction processes in PANI /ITO nanocomposites**
Modelo estatístico de rede de resistores para o estudo dos processos de condução em nanocompósitos de PANI/ITO

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In this work, we study the conducting processes involved in electrical conductivity of polyaniline/indium tin oxide nanocomposites (PANI/ITO) from the application of a statistical model of network resistors and the analysis of the dc conductivity near the percolation threshold. The statistical model, developed in Fortran 90, generates the morphological structure of the nanocomposite and calculates the complex conductivity by applying a transfer matrix technique [1]. The impedance between two neighboring sites of the matrix was calculated by the modified Dyre's model [2,3], while the impedance between two neighboring sites of ITO was calculated by Drude's model [4]. From the analysis of experimental dc conductivity measurements determined percolation threshold of the nanocomposite, which represents 10,6% of ITO. The analysis of the theoretical and experimental settings showed that the conduction process between the two sites of the matrix obeys the modified Dyre's model (RFEB), while conduction process in the conductive areas is described by Drude's model. The analysis of the dc conductivity measurements carried out below the percolation threshold indicates that the conduction process occurs via hopping between sites of the polymer matrix. In the region of percolation, so hopping and tunneling can contribute to the conduction process. However, samples with concentrations of the conductive phase above the percolation threshold, percolation geometrical conduction mechanism is predominant.

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9. **Study of conductivity critical exponent in conducting polymers near the percolation threshold**
Estudo do expoente crítico da condutividade em polímeros condutores perto do limiar de percolação

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The ac conductivity of conducting polymers, as a function of doping concentration, obeys a power law of the form $\sigma \sim (p - p_c)^t$ near the transition, where σ is the bulk conductivity of the conducting polymer, p is the concentration of conductive component, p_c is the percolation threshold concentration, and t is the conductivity critical exponent. This exponent is associated with different conduction mechanisms involved in the electronic transport phenomena [1]. A statistical model of resistor networks is proposed to describe a conducting polymer structure and to

simulate the real and imaginary components of its ac conductivity. By the application of a transfer-matrix technique [2], it reproduces ac conductivity measurements carried out with polyaniline films in different doping degrees and at different temperatures. The structure was generated for a cell of 100 x 100 sites for the polyaniline with conduction chain formed by 60 segments. It was used a connections density of 0.5 that corresponds to bond percolation threshold for square lattice. The dc conductivity of polyaniline as a function of the pH of the HCl doping solution has been measured and fit to a power law, yielding a conductivity critical exponent ($t = 3.9 \pm 0.1$) above the percolation threshold is larger than the universal values described by the classical theory of percolation. This can be explained by non-homogeneous distribution of the conductive islands causing a distribution of the conductance in the bulk.

We acknowledge support from INEO, CNPQ and FAPESP.

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10. Study of organic MIS capacitors using equivalent circuit

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Organic electronics is very attractive for the manufacture of flexible circuits in large area. However, totally organic devices still need to be improved so that they become commercially viable. The MIS capacitor is a powerful tool to study the phenomena occurring in the semiconductor and its interfaces, and is the basis of the field effect transistor (OFET). One can characterize the MIS capacitor through measurements of capacitance and dielectric loss versus frequency and/or voltage. The major problems of the organic devices like MIS capacitor and OFETs are the low mobility of charge carriers, high degradation and doping with exposure to air. These characteristics may be related to the material properties as the energy bands distribution, charge transport mechanism and carriers response time, among others. Moreover, it is not appropriate to apply conventional equations of inorganic semiconductors to interpret the organic devices. In this work is shown that to study the MIS capacitor is necessary to make adaptations on equivalent circuit, considering the minority carriers mobility equal zero as well as one accumulation layer charge distribution of non negligible thickness. From these concepts, the curves of capacitance and dielectric loss are closer to the experimental results, and can be used as a good base, as a template, to add other phenomena like the interfacial states, degradation and the light effects.

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11. Photo-CELIV technique assembly and application for conduction parameters obtainment in electronic thin films polymers. **Montagem e aplicação da técnica Photo-CELIV para obtenção de parâmetros de condução em filmes finos de polímeros eletrônicos.**

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Organic Electronics is still an area that requires a lot of fundamental studies; the electrical properties of ultra-thin organic films is a branch that requires intense scientific research. For electronic and optoelectronic device applications it is necessary, for example, to know the value of the carrier mobility, which is not easy to obtain in ultra-thin films (from dozens to hundreds of nanometers). The technique Time-of-Flight [1-2] is extensively used to measure carrier mobility of

thin films, but its is limited to materials having conductivity relatively low, and thickness not smaller than 1 micrometer. The first direct measurements of carrier mobility in ultra-thin films appeared circa 10 years ago, by a new technique called CELIV [3]. The goal of this work was to build the Photo-Celiv technique in the Group of Polymer Bernhard Gross, and to apply it to study electrical properties of the polymer Poli[(9,9-dioctil-fluorenil-2,7-diil)-co-(1,4-benzo-{2,1'-3}-tiadiazol)], F8BT, which has been used with success as active material for organic photovoltaics and organic transistors.

We acknowledge support from CAPES, INEO, CNPQ, FAPESP

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12. Charge transfer in ordered/disordered conjugated polymer films on the TiO₂ nanoparticles

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In this work we investigated the effect of order/disorder in the charge transfer processes between thin (10 nm) conjugated polymer films and TiO₂ nanoparticles. Nanometer thick polymer films and TiO₂ nanoparticles [1] were dispersed on quartz substrates by spin-casting. Fluorescence confocal microscopy was used to characterize homogeneity and charge transfer. Absorption and luminescence data were compared with Monte Carlo simulations. The investigated polymers were blue emitter polyfluorene (PFO) containing the π phase chains, poly(p-phenylene vinylene) (PPV) and its precursor, the poly(xylyliden tetrahydrothiophenium chloride) (PTHT). We also used an inert spacer separating the active polymer layer and the TiO₂ nanoparticles. We observed the decrease of the polymer emission intensity deposited directly on the TiO₂ nanoparticles, consistent with exciton dissociation due charge transfer to the nanoparticles. The charge transfer process is very efficient in totally disordered polymer (PTHT and PPV). While exciton are efficiently transferred to ordered (lower energy) domains, reducing their migration path to the Polymer/TiO₂ interfaces and, consequently, affecting drastically the charge transfer. Ordered/disordered contribution for the charge transfer can be modified by thermal treatment around the melting temperature. Finally, optical confocal microscopy indicates that film morphology depends strongly on the solvent.

We acknowledge support from CAPES and INEO.

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13. Plasmonic nanostructures fabricated via nanosphere lithography

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When radiation of appropriate frequency focuses on metal nanoparticles, the conduction electrons spatially confined are subjected to a coherent oscillation known as Localized Surface Plasmon Resonance (LSPR) [1]. Plasmonic structures may also be generated by nanostructuring of a continuous metallic film, giving rise to localized as well as delocalized surface plasmons

[2,3]. It has been demonstrated that the use of plasmonic structures increases the performance of photovoltaic devices [4,5]. The evanescent electromagnetic field associated with the surface plasmon penetrates into dielectric materials for a certain distance. However, due to the recent use of the technique, little is known about the mechanisms that promote the increase in photocurrent in these devices, what makes plasmonics a promising field of study.

Here, we investigated the possibilities offered by nanosphere lithography, which allows the modulation of plasmonic properties of a metallic nanostructured film, by a convenient choice of the diameter of the nanospheres. Furthermore, the fabrication method used to fill the lithographic mold determines the type of structure generated. We focus here on two types of metallic nanostructures: a) a porous network of copper grown by electrodeposition and 2) a network of periodic triangular islands obtained by evaporation.

We acknowledge support from INEO, CNPQ, FAPESP.

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14. **Preparation and Characterization of Dyads with potential application on Photovoltaic Devices**
Preparação e aplicação de Díades com potencial aplicação em dispositivos fotovoltaicos

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Organic Photovoltaic devices (OPV) have been studied in order to prepare low cost, flexible and low environment impact materials. Devices based on inorganic materials are more efficient to convert solar energy into electric (around 25%), in comparison to organic devices that does not exceed 10%. With the objective to increase OPV efficiency, using materials that generates longer-lived charge-separated species by inhibiting energy wasting charge recombination process, organic compounds dual function as dyads, have been researched [1]. Dyads, compounds containing an electron donor (D) and an electron acceptor (A), separated by a bridge group (B), have found wide applications as the active layer of optoelectronic devices. Besides the advantages as the easily obtained, another important property to this end is the modulation of the HOMO and LUMO gap of conjugated molecules [2]. The presented work proposes two different dyads synthesis that contains the 1,8-naphthalimide as the donor electron group connected by aliphatic bridge to the different acceptor group fluorene and thiophene, doped with CN group in order to stabilize their energy levels [3].

We acknowledge support from CAPES, INEO and UEPG.

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15. **Photovoltaic investigation of new co-polymers based on fluorene-phenylene and fluorene-thiophene units**

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In this work a new series of electron donor copolymers was studied as active layer in organic thin-films solar cells. We have investigated five different polymers containing fluorene, thiophene and phenylene units that were synthesized through the Witting route [1] originating alternate copolymers with the combination of different rates of the following structures: poly(9,9-n-dihexyl-2,7-fluorenylenevinylene-alt-1,4-phenylenevinylene) and poly(9,9-n-dihexyl-2,7-fluorenylenevinylene-alt-2,5-thienylenevinylene). These co-polymers are composed of fluorene, phenylene and thiophene units, where the fluorene content is kept constant while the phenylene:thiophene ratio is varied in order to evaluate the effects on their photovoltaic properties. They are called as LaPPS 29 and LaPPS 30. For every copolymer ratio, we report results of photovoltaic devices in bi-layer structure using vapor-deposited C₆₀ as the electron acceptor. These bi-layer devices have shown higher efficiency when compared to previous PCBM bulk heterojunction devices [2]. Effects of annealing on the film morphology were also investigated. The best co-polymer showed a peak external quantum efficiency of 40% and AM 1.5 power conversion efficiency of 1.8 %.

We acknowledge support from CAPES, CNPQ and INEO.

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16. Hole mobility effect in the efficiency of bilayer heterojunction polymer/C₆₀ photovoltaic cells

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We have investigated the effect of temperature annealing on bilayer heterojunction solar cells based on poly[9,9'-hexyl-fluorene-alt-bithiophene] (LaPPS 43) as active layer. LaPPS 43 polymer was prepared by palladium catalyzed Suzuki coupling reaction between 9,9'-dihexylfluorene-2,7-diboronic acid and 5,5'-dibromo-2,2'-bithiophene monomers, according to the published procedure [1]. Film morphology for different temperature annealing was probed by atomic force microscopy (AFM) and the values of roughness range from 0.59 up to 2.15 nm. The best photovoltaic performance was found for devices with active layer annealed at 200 °C with power conversion efficiency (η) of 2.8% while devices without annealing presented only 0.4%. This performance enhancement is attributed to the reduction of traps and increased hole mobility after the thermal annealing [2].

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17. Composite films of TiO₂ and Poly-3-hexylthiopheno (P3HT) for application in organic photovoltaic devices

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Thin composite films of Poly-3-hexylthiophene (P3HT) and TiO₂ nanoparticles were prepared for application in organic polymeric photovoltaic devices. The film thicknesses were in the range of 100 to 300 nm and were characterized by voltage-current measurements. TiO₂ nanoparticles were produced by the sol-gel in aqueous suspension and showed dimensions in the range of 10 to 50 nm. Very homogeneous nanocomposite films were produced by an innovative process where TiO₂ nanoparticles were suspended in an organic solvent compatible with the solvent used for P3HT dissolution. The films were prepared by spin coating and were characterized by scanning and transmission electron microscopy. The composite processing conditions open a new way to produce fine and well homogeneous nanocomposites thin nanometric films. The authors acknowledge CAPES by the financial support.

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18. **Preparation and characterization of nanocomposites based on TiO₂/graphene and their application on inverted solar cells**
Preparação e caracterização de nanocompósitos TiO₂/grafeno e sua aplicação em células solares com configuração invertida

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The application of graphene in photovoltaic devices has received considerable attention due to their differential properties. The use of graphene incorporated into the oxide semiconductor film is an alternative to enhance the electron transport in the films, since this material has excellent conductive properties [1].

In this work, we characterized the graphene oxide samples obtained by the Hummers method [2]. Then, the reduced graphene oxide (rGO) was obtained by the method of ultraviolet irradiation-assisted photocatalytic reduction [3]. The TiO₂-rGO nanocomposites were characterized by X-ray diffraction and Raman spectroscopy. The FEG-SEM images showed that the rGO sheets were decorated with TiO₂ nanoparticles unevenly, but enough to prevent their agglomeration. In general, the inverted solar cells were assembled with the following configuration: Au / PEDOT-PSS / poly (3-hexylthiophene) (P3HT) / TiO₂-rGO / TiO₂ blocking layer / conductive glass (FTO). The solar cells were characterized by current-potential curves (I-V) under polychromatic light irradiation of 40 mW cm⁻². The TiO₂ electrode containing 0.24 wt.% of nanocomposite provided the following electrical parameters: J_{sc} of 0,08 mA cm⁻², V_{oc} of 0.26 V, and a conversion efficiency of 0,13 %. Compared with solar cell based on the TiO₂ porous films, devices based on the composite photoanode exhibited an increase in J_{sc} value attributed to the improved interconnectivity between TiO₂ nanoparticles and graphene, which further improved the electron transport through the film. In this case, the carbonaceous material introduced an alternative electrical conduction pathway which facilitates rapid electron transport in the photoelectrode.

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19. **Enhanced Open-Circuit Voltage and Hole Conduction in Multilayered Photovoltaic Device by Insertion of functionalized layers.**
Melhoramento da Tensão de Circuito Aberto e da Condução de Buracos em Dispositivos Fotovoltaicos de Multicamadas através da Inserção de Camadas Funcionais.

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The performance of the organic photovoltaic devices is limited by poor exciton dissociation and charge transport due in part to high rates of exciton recombination, low charge carrier mobility and low open-circuit voltage which should be equal to a difference of the work function of electrodes used [1,2]. However, the open-circuit voltage and charge carrier mobility into an organic photovoltaic devices can be improved by using either conducting layers or self-assembled layers of functionalized molecules deposited on the electrode in order to improve hole transporting and to reduce the Schottky barrier between the conductive electrode and the organic semiconductor, respectively. Furthermore, the polarizability of the molecules involved can also be oriented in order to increase the open-circuit voltage. Here, tetrasulfonated nickel phthalocyanine (NiTsPc) films were deposited onto ITO electrode by Layer by Layer technique as functionalized molecules and the conducting electropolymerized-PANI as hole transporting layer. The active layer of Poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV) and PCBM was spin coated to obtain ITO/NiTsPc/MDMO-PPV_PCBM/Al and ITO/PANI/MDMO-PPV_PCBM/Al device structures. Firstly the NiTsPc/MDMO-PPV with different number of bilayers and PANI/MDMO-PPV films were optically characterized and then the performance of multilayered devices were evaluated by dc conductivity (I vs V curves) and photocurrent spectroscopy. The data obtained suggest that the using of electropolymerized-PANI layers decreases the electrical resistivity of the devices with the increasing of charge carrier mobility to the collector electrode, improving the devices performance. Moreover, the number of electric polarized NiTsPc layers changes the open-circuit voltage V_{OC} values. (Acknowledgments: FAPEMIG, CNPq, INEO/MCT, Grupo de Polímeros BG/IFSC)

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20. **Investigation on the performance of organic photovoltaic devices by interface modification**

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In this work, the influence of interface modifications on the performance of organic photovoltaic devices (OPVs) was investigated. The modifications were achieved by inserting intermediate layers between the anode and the successive organic layers to improve the device efficiency [1,2]. The thin films used for this purpose were aluminum doped titanium dioxide (Al:TiO₂), poly(aminopyridine) (PAPy) and 2,3,5,6-tetra(pyrazin-2-yl)pyrazine (TPzPz). The PAPy and TPzPz compounds were synthesized at UNICAMP in Brazil and the Al:TiO₂ was produced by sol-gel technique at Inmetro laboratories. The OPVs devices were fabricated on ITO and FTO substrates. Both oxide and polymer films were deposited by spin coating technique whereas the small molecules were deposited by thermal evaporation under high vacuum environment. The PAPy presents high transmittance in the visible range offering a promising opportunity to improve the positive carrier charge extraction as well the built-in potential in OPVs. The device characterization was carried out analyzing the characteristic current density-voltage (J/V) under dark conditions and under illumination (1000 W/m², AM 1.5 G) through the transparent electrodes. Through efficiency measurements it was possible to evaluate the influence of the interface modification which depends on J_{sc}, V_{oc} and Fill Factor (FF) values. Preliminary results show that TPzPz molecule used in the metal interface allows an improvement in the direct dark current of about 25%. On the other hand, PAPy compound produced a rectification improvement of about two order of magnitude with respect to the standard OPV device.

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21. **Formation and characterization of resistive switching memories from of poly(3-hexylthiophene) and anodized aluminum oxide films**

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Metal-insulator-semiconductor-metal, MISM, devices were fabricated and studied aiming to obtain resistive switching memories, RRAM [1]. The devices were produced from thin films of aluminum oxide, Al₂O₃, and poly(3-hexylthiophene)P3HT. The Al₂O₃ film was grown through the anodization technique in a solution of tartaric acid, water and ethylene glycol containing, respectively, 1g, 40ml and 30ml at room temperature [2]. The P3HT was deposited by the Langmuir-Schaefer technique using chloroform as solvent. We examined the electrical procedure for the transformation of the pristine device into a RRAM memory using a ramp voltage and measuring the electric current [3]. The RRAM memories were characterized by measuring the ratio of electric current between the on and off states being that we have obtained values in order of 10⁻³A and 10⁻⁹A, respectively.

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22. **Electric properties study of polymer light-emitting electrochemical cells based on polyfluorene derivatives**

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Polymer light emitting electrochemical cells, PLECs, are devices that operate at low voltage and exhibit high performance without the need of specific electrodes such as indium tin oxide (ITO), calcium and others. This feature provides low cost of fabrication and flexible devices. The charge injection in the PLECs is facilitated by the action of ionic species, which are inserted in the polymeric material by adding a salt. This study treats with a controversy related to the device's operation mechanisms [1,2]. Currently, there is two opposite models. One that considers that transport is driven by diffusion mechanism [3]; and the other takes into account the formation of a PIN junction (p-type semiconductor – insulating layer – n-type semiconductor) [4,5]. Here, we proposed the fabrication and characterization of PLECs having different compositions and thickness, and the results were faced up to the models. We showed the existence of critical concentration of salt, below of which the operation of the PLECs are mainly due to injection stimulated by the ionic double-layer. For higher applied voltages, the injection still exists but it is followed by a PIN junction formation. We also verified that for voltages above the turn-on the device electrical resistance is proportional to the sample thickness and is temperature-independent. For low voltages the transport is dominated by diffusion, but as the voltage increases, the semiconducting layer starts to be doped: p-type in one side, and n-type in the other. Therefore, the conductivity of the semiconducting layer increases, and it finalizes by the formation of the PIN junction.

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23. **Doping of Polyfluorene with Two Red Emitters - White Light Emission**

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The photo- and electroluminescent properties of a single-layer multi-component blend composed of three luminescent materials were studied. The blue emitter poly(9,9 dihexyl-2,7-fluorene) (LaPPS10) was used as the matrix, and the two red emitters, poly[2-methoxy-5-(2-ethylhexoxy)-1,4-phenylene vinylene] (MEH-PPV) and 4 (dicyanomethylene)-2-methyl-6-(dimethylaminostyryl)-4H-pyrene (DCM), as the dopants. A detailed study of this system was performed in solution and in the solid state, focusing the photophysics aspects of emission spectra of the blend and those of the matrix with each one of the components. A white OLED device exhibiting CIE chromaticity coordinates $x=0.30$ and $y=0.31$ of very simple structure was built, and the possible photophysical phenomena involved in its emission spectrum were discussed. It was shown that a film-composite made with the blue emitter [poly(9,9-dihexyl-2,7 fluorene)], as a matrix, and the red emitters, poly[2-methoxy-5-(2-ethylhexoxy)-1,4 phenylene vinylene] (MEH-PPV) and 4-

(dicyanomethylene)-2-methyl-6 (dimethylaminostyryl)-4H-pyrene (DCM) as dopants has a great potential to be used as white light-emitting diode. A detailed photoluminescence study involving mixtures of the matrix with each one of two components, and of the complete blend, either in solution or in films, provided information about the photophysical mechanisms operating in PL and EL emissions. Electroplex emission is one possible explanation for a broad band at 571.4 that was observed only in the electroluminescence spectrum.

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24. Application of Salicylidene Zinc(II) Coordination Compounds in Organic Based Electroluminescent Devices

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The Schiff condensation occurs by a classic reaction, where a primary amine performs a nucleophilic attack on carbonyl group of an aldehyde or ketone, resulting in imine group (**RC=NR'**) [1]. Recent researches using Zn(II) Salicylidenes in electronic devices have showed interesting results in luminescence, electroluminescence and semiconducting properties, so being used in the manufacture of Organic Light-Emitting Diodes (OLEDs). These devices are based on fluorescent materials, as electroluminescent layer, or electron injector layer [2-3]. The papers available in the literature showed that these properties are enhanced when these Zn(II) coordination compounds are added to luminescent semiconducting copolymers, resulting in a host-guest system [3-4]. The aim of this work was to synthesize new salicylidenes and their Zn(II) coordination compounds, that were characterize them by FT-IR, UV-Vis and NMR ¹H and ¹³C spectroscopies, as well as melting point, thermal analysis (TGA/DTA) and electroluminescent analyses in order to investigate the application of these materials in a manufacture of organic devices. These researches were made in partnership with the Grupo de Eletrônica Molecular da Escola Politécnica da USP. The Salicylidenes as well as their Zn(II) coordination compounds, were successfully synthesized, with high purity and good yields. We carried out the study of salicylidenes synthesis assisted by ultrasonic irradiation, checking this methodology is more effective than reaction classic methods. Preliminary studies of luminescence and electroluminescence properties of these compounds were very satisfactory, presenting good

results in luminous efficiency, luminance and electrical conductivity. Finally, were obtained best results from the Zn(II) coordination compounds with respect to the free ligands.

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25. **Field-effect transistors based on polymer/transparent metal oxides heterostructures**

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Metal-oxide semiconductors like zinc oxide (ZnO), indium zinc oxide (IZO) and indium gallium zinc oxide (IGZO) and mixed composites have been recently considered as functional constituents of (opto-)electronic devices. Due to their large electronic band-gap, these materials allow for the preparation of see-through devices like OLEDs lamps, displays and semitransparent organic solar cells. One of the purposes of the present work is to build and characterize transparent thin-film transistors (TFTs) based on metal oxides obtained from low-temperature processed organic precursor solutions as the channel material. Owing to their superior device characteristics compared to TFTs based on amorphous silicon, metal-oxides are considered as the next-generation platform for high-performance driver electronics for active-matrix OLED displays and high-density 3D LCD screens. Aside from a high field-effect mobility ($> 10 \text{ cm}^2/\text{Vs}$) which is readily achievable in many oxide based TFTs, stability under various operating conditions is of paramount interest. This work will also discuss about recent insights and approaches to improve device stability. Another topic that will be also addressed is the use of metallic oxides like ZnO, In_2O_3 , Ga_2O_3 in heterostructures comprising conjugated polymers, organic semiconducting molecules and inorganic metallic oxides as an alternative method to obtain air-stable electrodes in order to improve electron injection from the electrodes in electroluminescent organic field-effect transistors.

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26. **Light Emitting Electrochemical Cells (LEC) Fabrication By Continuous Process** **Fabricação De Células Eletroquímicas Emissoras De Luz (LEC) Por Processo Contínuo**

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Organic electronics is already present in displays of mobile phones and gadgets and has great chances to come soon in dispute for TV market with advantages in relation to energy consumption, contrast and viewing angle, as well as creating new markets with the fabrication of flexible displays, manufactured entirely with organic materials, which can be processed in solutions. Recent national advances in the fabrication of lab-scale functional devices have generated a new need for series production ensuring reproducibility and low manufacturing costs. The *roll-to-roll* production is a continuous process that involves a variety of techniques for polymeric deposition, for example, slot die, gravure, flexographic, screen printing (manual and rotary screen) and spray [1]. In this work we propose the fabrication of LECs (Light Emitting Electrochemical Cells) for these low operating voltages and low influence of the thickness and electrodes materials on their optoelectronic properties [2]. In addition has been developed a laboratorial prototype for *roll-to-roll* techniques and simulated automation for use in industrial scale.

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27. **Fabrication of a flexible antenna of a conducting polymer (PEDOT:PSS) using printing techniques applied to the roll-to-roll process.**
Fabricação de um antena flexível a base de um polímero condutor (PEDOT:PSS) através de técnicas de impressão aplicadas ao processo roll-to-roll.

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The organic electronic is a new branch of the electronic technology that exhibits several advantages such as low cost and easy processing additionally, the structural flexibility of the active layers provides the development of flexible electronics. With this technology it is possible to manufacture electronic devices such as solar cells, light-emitting diodes, thin film transistors and sensors. However, the use of conventional techniques to process the components of the devices, like casting or spin-coating¹, are not adequate to large scale production. The present work is aimed to built an antenna based on PEDOT:PSS (conductive polymer) solution to apply in RFID (Radio-Frequency Identification) tags² using printing techniques like screen printing and gravure¹ in the roll-to-roll process. A determinant factor to fabricate a polymeric antenna is the electric conductivity of the employed polymer. Adding 5% in volume of DMSO (dimethylsulfoxide) in the PEDOT:PSS solution, we obtained an increasing magnitude in the electrical conductivity of the PEDOT:PSS film³. With the techniques of printing and roll-to-roll process that is being developed in our laboratory, we expect to obtain higher reproducibility and decrease the fabrication cost of the devices, avoiding the waste of material and enhancing the speed of the whole process.

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28. **Printed conductive tracks by inkjet printing technique using conducting polymeric suspensions**

Trilhas condutivas impressas por técnica de impressão por jato de tinta usando suspensões poliméricas condutoras

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The using of conducting polymers to build electronic devices allowed to reduce the manufacturing cost and facilitated their building, such advantages have become this application of conducting polymers an interesting area. One example of this application is in organic field-effect transistors (OFETs) [1]. Among the techniques can be used to deposit polymers, a technique that has attracted much attention to deposit polymers is the inkjet printing [2]. Several advantages are presented for this technique, as for example: the ability to deposit well-defined patterns using picolitre volumes of solutions or suspensions in each drop volume, therefore it removes the need for masks, which leads to cost-savings and waste elimination. In this work we prepared and printed, using the inkjet printing technique, inks based on conducting polymers PANI/PSS and PEDOT/PSS. We intend to use these polymers in OFETs. Modifications of suspension properties were carried out to adjust the best printing conditions. A commercial desktop printer was used, the canon pixma ip4500. Two flexible substrates were used: commercial transparency and Kapton[®]. The PANI/PSS films were doped using HCl vapor to increase the conductivity. The electric conductivity of the printed films was obtained using four point probe method. Comparing the conductivity values of the printed films were determined the best substrate to be used and the ink that formed the film more conductive.

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29. Inkjet printing of polyaniline tracks for application in printed circuit on paper

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The use of inkjet printing to produce devices on paper substrates have received great attention recently due advantages like low cost, lightness and easy processing [1]. To print one material in a commercial thermal printer is need to prepare a water based ink with viscosity and tension surface suitable [2]. Several methods can be used print a conductive material such as printing metallic nanoparticles, organic metallic compounds and solution of polymers. The design of pattern tracks and the ink penetration in the paper can determine properties and qualities of printed devices, therefore is as important as the ink preparation [3]. This work presents results obtained with polyaniline (PANI) printed on paper using a HP commercial inkjet printer. Geometrical parameters, such as the length and the width tracks, the deep of PANI penetration on paper and the drop diffusion were evaluated through electrical characterization. PANI lines can be printed with width of 100 μ m spaced one from others also by 100 μ m shown resistance ranging from 10⁴ to 10⁵ Ω . The characterization developed in this work provides the basic parameters to design sensor applications using PANI printed on paper by a commercial thermal

printer.

We acknowledge support from INEO and FAPESP.

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30. **Vibrational spectra and DFT calculations of the vibrational modes of Schiff Base C18H17N3O2**

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The Schiff base 4-[[1E)-(2-Hydroxyphenyl)methylidene]amino}-1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one (C18H17N3O2) is a synthetic compound with a variety of scientific and technological applications. In this work FT-Raman spectrum and FT-infrared spectrum of C18H17N3O2 were investigated at 300 K. Vibrational wavenumber and wave vector have been predicted using density functional theory (B3LYP) calculations with the 6-31 G(d,p) basis set. The description of the normal modes was performed by means of the potential energy distribution. A comparison with experiment allowed us to assign most of the normal modes of the crystal.

We acknowledge support from INEO, CAPES and CNPQ.

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31. **Vibrational spectra of (4E)-4-((E)-3-phenyl-allylideneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpirazol-5-one**

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This work presents through the X-ray diffraction method the crystal structure of ((4E)-4-((E)-3-phenyl-allylideneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpirazol-5-one as well as its vibrational properties and DFT calculations. The crystal is monoclinic with $a = 13.487 \text{ \AA}$, $b = 9.788 \text{ \AA}$, $c = 13.836 \text{ \AA}$ and the space group P21/n (C22). The equilibrium geometries, harmonic frequencies, infrared intensities and Raman scattering activities were calculated by density functional B3LYP method with the 6-31 G(d,p) basis set. The comparison between the calculated and experimental results covering molecular structure and, assignments of fundamental vibrational modes were investigated. The optimized molecular geometries have been compared with the experimental data obtained from XRD data, which indicates that the theoretical results agree well with the corresponding experimental values. For the compound, comparisons and assignments of the vibrational frequencies indicate that the calculated frequencies are close to the experimental data.

We acknowledge support from INEO, CAPES and CNPQ.

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32. **Fundamental and applied investigation on Luminescent Polymers**

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Luminescent polymers are commonly employed in light-emitting displays because of their good processability, and higher luminance with low power consumption. However, even though they are good candidates for optoelectronic devices, they are highly susceptible to photooxidation processes which dramatically change their color with light exposure time [1]. On the other hand, the change of color induced by radiation has been recently explored in the fabrication of light dosimeters since a relationship between the light intensity that reaches the sample and the color change can be established [2]. In this work we present a general overview on branches of researches related to the fundamental (theoretical and experimental) and applied studies developed in our group (LAPPEM). In this sense, we investigated the changes on the optical behavior of luminescent polymers under the effect of radiation and their application as radiation sensors.

We acknowledge support from CAPES, INEO, CNPQ, FAPESP and FAPEMIG.

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33. **Femtosecond spectroscopy investigation of polyfluorene solutions and films.**

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Femtosecond spectroscopy is used to study excited-state dynamics and coupling to the environment in polyfluorene solutions and films. Time-resolved Optical Kerr Effect (OKE) measurements revealed an ultrafast birefringence that essentially relaxed back to equilibrium within 2.5 picoseconds. When compared with the pure solvents OKE response, solution measurements show a decrease in the long-time component. This amplitude decrease in turn suggests over-damping of low-frequency solvent nuclear modes upon addition of polyfluorene solutions to THF. Upon further solute addition, low-frequency nuclear motion is nearly suppressed.

Linear pulse propagation measurements of polyfluorene solution were characterized by cross-correlation frequency-resolved optical gating (X-FROG). The spectrograms revealed intensity modulation 800 nm. Accordingly, the interaction of 50 fs pulses centered at 800 nm with both film and solution revealed bright two-photon-excited fluorescence emission. Interestingly: no X-FROG spectrograms could be recorded from pulse propagation experiments through polyfluorene films even when using 5 microjoules of 50 fs pulses at 1 kHz. This result further indicates strong two-photon absorption by the polymer. Two-photon absorption pump-probe measurements of polyfluorene solutions were performed in transient-absorption and polarization anisotropy mode. Both measurements indicated sub-picosecond vibrational relaxation and anisotropy decay in the excited state energy surface. All of the measurements were characterized by a home-built second harmonic generation frequency-resolved optical gating (SHG-FROG) apparatus, which

indicated

50 fs transform limited pulses. Kinetic modeling and comparative confocal fluorescence scanning microscopy measurements of the films before and after the pulse propagation experiments are underway.

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34. **Electrical conductivity of platinum-implanted PMMA nanocomposite** **Condutividade elétrica de nanocompósito de platina implantada em PMMA**

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Pt/PMMA (platinum/polymethylmethacrylate) nanocomposite material was formed by low energy ion implantation of Pt into PMMA, and the transition from insulating to conducting phase explored. In situ resistivity measurements were performed as the implantation proceeded, and transmission electron microscopy was used for direct visualization of Pt nanoparticles. Numerical simulation was carried out using the TRIDYN [1,2] computer code to calculate the expected depth profiles of the implanted platinum. The maximum dose for which the Pt/PMMA system remains an insulator/conductor composite was found to be $\phi_0 = 1.6 \times 10^{16} \text{ cm}^{-2}$, the percolation dose was $0.5 \times 10^{16} \text{ cm}^{-2}$, and the critical exponent was $t = 1.46$, indicating that the conductivity is due only to percolation. The results are compared with previously reported [3-6] results for a Au/PMMA composite.

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35. **Fabrication and electrical characterization of polythiophene derivative LB films**

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Among the several types of conjugated polymers used in recent investigations, polythiophene and its derivatives have attracted considerable attention due to their high mobility and other remarkable solid-state properties [1]. Films from these polymers may be fabricated with various experimental methods. These include the Langmuir-Blodgett (LB) technique, which is particularly suitable if some degree of molecular control is required [2]. In LB films, the thickness may be controlled down to the molecular scale, and the degree of order may also play an important role. In this work, we have investigated electrical properties of polythiophene derivative LB films, poly(3-hexyloxythiophene) (PHexOxT). Langmuir-Blodgett thin films were fabricated using a Langmuir trough model KSV5000 and an evaluation about the deposition parameters was done.

Electrical measurements, current versus voltage (I vs. V) and impedance spectroscopy, were carried out using Keithley 238 voltage source and Solartron 1260A impedance analyzer, respectively. The electrical measurements were performed using the parallel contact that was obtained by depositing the PHexOxT film on interdigitated electrodes (IDE). The I vs. V curve shows an ohmic behavior, and the device resistance, R , and conductivity, σ_{dc} , calculated from this adjustment are about 9.01 G Ω and 5.66×10^{-10} S/m, respectively. This low-valued electrical conductivity reflects in the a.c. measurements, in which not is possible to obtain the low-frequency conductivity. However it is possible to estimate the device resistance magnitude, which match with the results obtained in the d.c. measurements. The impedance values does not change regardless the bias (constant voltage superimposed on the ac signal) applied.

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36. **Electrical characterization of poly(amide-imide) films**

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The electric capacitance of dielectric layers in organic thin film transistors (OTFTs) is very important to get desirable electric OTFTs characteristics, for example, low threshold voltage. Many polymeric materials have been tested and used to fabricate OTFTs and cross-linked polymers are preferable because they are non soluble in solvents used to deposit the organic semiconductor film. A candidate material for organic electronics is the co-polymer poly(amide-imide) (PAI), which is amorphous, cross-linkable, with good mechanical, thermal and chemical properties.

In this work, ITO/PAI/Au MIM structures were characterized through AC measurements using the frequency response analyzer Solartron and current-voltage measurements under DC voltages. PAI layers were deposited by spin-coating technique. The cross-linking was achieved heating the layer at 300°C for 1h. Films were fabricated depositing several layers (1-4) and repeating the thermal treatment for each layer.

Impedance measurements carried out from 1Hz to 1MHz showed that the capacitance of MIM devices is almost frequency independent; varying from 500 to 900pF using PAI films with 2 to 4 layers, and the loss tangent is of order of 10^{-3} . Also the resistivity calculated for a 4 PAI layers film (~260nm) was $1,8 \times 10^{16}$ Ω cm under electrical field of 10MV/m.

We concluded that the co-polymer PAI is a good candidate for application as dielectric layer in OTFTs and metal-insulator-metal (MIS) devices. Furthermore, PAI/P3HT MIS devices were already fabricated and they showed electrical characteristics comparable to devices made from other high insulating polymeric materials. The paper describing the MIS devices is under consideration for publication in Organic Electronics.

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37. Structural and Morphological Characterization of Doped Polyaniline

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Emeraldine-salt polyaniline form (ES-PANI) was chemically synthesized at time synthesis ranging from 0.5 to 72h. As it is known polyaniline presents a characteristic diffraction pattern due to a semicrystalline phase superimposed with a characteristic broad background due to an amorphous phase. The aim of this work is the structural characterization of doped polyaniline using XRD and SAXD for the determination of the cell dimensions and crystallite size of the crystalline phase; SAXS for the determination of the size of the particle radius of gyration, pair distribution function and maximum dimension and SEM for the determination of the shape and sizes of the particle aggregates. XRD analysis showed that the ES-PANI crystallinity did not vary with the time synthesis. LeBail fit revealed that the crystallites were very small lamellae. By SAXS the maximum particle size (D_{max}) of 650Å was obtained from the Pair-distance distribution Function ($p(r)$). SEM images showed a fiber morphology formed by interconnected nanospheres. The obtained results might be essential for the structure understanding and properties of semicrystalline materials.

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38. Regioregularity improvement of Poly(3-hexylthiophene) by polymerization with slow addition of oxidant.

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Polythiophene derivatives has been exploited in several applications such as PLEDs, photovoltaic devices and sensors. The side chain, molar mass and the way in which the repeating units are linked in the polymer chain (head-to-head (HH), tail-to-tail (TT) and head-to-tail (HT)) influence the properties of these polymers and are resulting from the synthesis process [1,2]. In this work, the influence of oxidant slow addition of oxidant in the molar mass and regioregularity degree, (defined as the percentage of HT units) of poly(3-hexylthiophene), P3HT, is explored. Data from size-exclusion chromatography showed that the slower addition of oxidant has favored the growth of polymeric chain and, from ^1H RMN data, yielded a slightly higher regioregularity degree.

We acknowledge the support from FAPESP, CNPQ, CAPES and INEO.

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39. Synthesis and characterization of heteroaromatic derivatives 1, 2, 5-thiadiazole with electroluminescent potential.

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The heteroaromatic nucleus 1,2,5-thiadiazol is a strong electron acceptor, being incorporated into molecules for better formation of conductive material. Derivatives with different substituents showed a good fluorescence [1]. These heteroaromatic ring presents electronic configuration similar to the ring ortho-quinoid, a structure cyclic with conjugated π -bonding, allow large displacement in wavelength absorbing dye present in a chromophores with intense color. This displacement capacity is responsible for luminescence on the presence of a electric current [2]. These compounds can be synthesized by a addition of thionil chloride on a vicinal diamine, using triethylamine or pyridine how a catalyst under constant agitation for 15 minutes [3]. So, they were made the synthesis of four heteroaromatic derivatives, which were characterized by ^1H NMR, ^{13}C NMR, FT-IR and UV-Vis spectroscopies.

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40. Methodology evaluation of hybrid polyfluoreno/organophilized montmorillonite (OMMT)

Avaliação de metodologia para preparo de híbridos polifluoreno/montmorilonita organofilizada (OMMT)

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Conducting polymers with optical properties are good candidates for application in luminescent devices. However its fragility in terms if oxidation an degradation hinders implementation [1-6]. Thus, in order to improve the emission properties and thermal stability, the present study aims to evaluate which method is most suitable for clay incorporation, and preparation of the hybrid proposed material. There were two different methodologies, non-wetting (physical mixture) and wet incorporation. The hybrid preparation was synthesized via Suzuki reaction, using poly(9,9-dioctilfluoreno)-co-phenylene (PP), sodium montmorillonites clay, and modified clays with quaternary ammonium salt hexadecyltrimethylammonium bromide(HDTMA -Br).

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41. **Influence of the amount of variation in the properties of the composite polyfluorene SBA-15**
Influência da variação da quantidade de polifluoreno nas propriedades de compósitos de SBA-15

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Conjugated polymers derived from fluorene group are considerable interest because their great versatility color emission, thermal, chemical and oxidative stability and high solubility when have substituents at 9 position of the monomer, these characteristics make them candidates of many applications such as in light-emitting diodes (LEDs).¹ One problem attributed to those groups is related to their chain organization, with results in low chemical stability or low conductivity. This problem can be solved with the incorporation of the polymer in inorganic matrices, in this case, ordered mesoporous silica, which results in better conjugation along the same.²⁻³ In this work, the goal was to study the incorporation (*via* wet impregnation) of different percentage (by weight) of poly(9,9-dioctylfluorene)-co-phenylene (PF) on mesoporous silica SBA-15 type and verify the possible variations on the composite. Structural analyses of the composite revealed a decrease in the surface area (S_{BET}), pore size (D_p) and pore volume (V_p), which indicates the presence of the copolymer in the pores of the silica. The CHN elemental analysis showed a similar incorporation, independent of the amount of copolymer. The thermogravimetric analysis (TG) showed an increase in thermal stability after incorporation. The emission spectra showed a slight shift to the blue region of the composites, which indicates a smaller agglomeration of their chains.

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42. **Magnetoelectrochemistry: Influence of Magnetic Field on the Electrochemical Response of Magnetite Particles Modified with Prussian Blue**

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Magnetoelectrochemistry is the branch of electrochemistry in which electrochemical reactions and bioelectrocatalytic processes can be controlled by using external magnetic field. Since it was reported for the first time the magnetic control of bioelectrocatalytic reactions [1], the magnetoelectrochemistry can be applied to the development of biosensors and biofuel cells. Thus, in this work iron oxide Fe_3O_4 particles were modified with Prussian blue (Fe_3O_4 -PB) and the electrochemical properties of a suspension of Fe_3O_4 -PB were investigated in the presence (“switch on”) and absence (“switch off”) of an external magnetic field (0.24T) perpendicularly to the plane of an ITO (indium tin oxide) electrode. When “switch on” mode was applied, it was observed an increase of 60% in the current density (PB redox processes) when compared to “switch off”. The

latter, was attributed to the increase amount of mass on surface electrode. Results from chronoamperometry showed that the magnetic control of the Fe₃O₄-PB redox processes is very reproducible and these results indicate that the Fe₃O₄-PB can be used in several applications in bioelectrochemistry, when a reversible redox probe conjugated with magnetic switchable materials is required.

We acknowledge support from CAPES, INEO, CNPQ and FAPESP.

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43. **Effect of pressure on the magnetic properties of poly(3-hexylthiophene)**
Efeito da pressão nas propriedades magnéticas do poli(3-hexiltiofeno)

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Heterocyclic conducting polymers such as poly(3-alkylthiophene) that exhibit collective magnetic behavior are interest due to the possibility of new form of magnetic ordering in which the magnetic moments are located in the p orbital [1-3]. These polymers have a nondegenerate ground state that can lead to the formation of polarons by electron-phonon interaction. Polarons have spin 1/2, electronic charge ±e and plays an important role in the formation of the magnetic moments and therefore in the magnetic behavior of the polymer. In this work we present the effect of pressure on the magnetization of the poly(3-hexylthiophene). The results show that the pressure used in the preparation of the samples changes considerably the magnetic behavior of the samples. The changes could be associated with the reduction of the interchain distance, which leads to increased of the exchange interaction between the magnetic moments.

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44. **Photoassisted Poling: electro-optic measurements using the Mach-Zehnder interferometer**

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The *trans-cis-trans* photoisomerization of azobenzene groups increase their mechanical mobility allowing orientation of such groups under an excitation light and a *dc* electric field, at room or even at low temperatures. The photoassisted poling technique (PAP) allows azobenzene groups in polymeric films to be oriented to generate NLO properties and the orientation can be probed measuring the electric-optic coefficient, r_{13} , by a Mach-Zehnder interferometer (MZI). We use a MZI setup to track the poling process and its decays after poling in the PAP technique. The electro-optic r_{13} measurement during the poling process is possible since the excitation light, the *dc* voltage, the modulation MZI voltage and the light beam from the interferometer light source

are simultaneously applied to the polymeric film mounted in one of the MZI arms. We will present r_{13} measurements obtained using films prepared by casting of poly(methyl methacrylate), PMMA, containing disperse red-1, DR1, as azobenzene group at a concentration of 5 wt% in the polymer. PMMA/DR1 guest-host films were casted onto ITO glass slides and a semitransparent layer of aluminum was evaporated to have the second electrode to apply the voltage. Using the excitation light with wavelength of 488 nm with intensity of 64 mW.cm^{-2} , poling *dc* voltage of 100 V, during 10 minutes, at room temperature, a PMMA/DR1 film with 12 μm thickness exhibited electro-optic coefficient $r_{13} \cong 0.37 \text{ pm/V}$. Measurements of r_{13} under experimental conditions will be presented and the piezoelectric in the films will be also discussed

We acknowledge support from FAPESP, CNPQ and INEO.

45. **Time Correlation Single Photon Counting Technique in the Physics Department of UFMG**

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The lifetime of the quantum states of conjugated polymer structures can be very helpful in order to characterize a series of intra- or inter-molecular exciton energy transfer. The own knowledge of the lifetime can also determine the way to use the polymer material in device applications. The technique used to determine the lifetime of materials is the Time Correlation Single Photon Counting (TCSPC).

We were able to mount this technique in our laboratory. We have used a fast detector with a response time of 350 ps associated to the Pico Quant controller equipment. Initially our system was accomplished only for polymeric solutions. The results obtained for a polyfluorene (PFO) solution has given us a lifetime of 391 ps, which is agreement with values obtained in the literature [1]. As a continuation of this work we will perform lifetime measurements in thin films under different temperatures.

We acknowledge support from CAPES, CNPQ, FAPEMIG, INEO and INCT-DISSE.

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46. **Polymer nanostructures and nanocomposites for application in 2D photonic devices** **Nanoestruturas e nanocompositos poliméricas para aplicação em dispositivo fotônico em 2D**

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Production of nanostructures by soft lithography are widely applied in micro and nano-electronics and highly attractive for future applications in photonic devices, whose scales involved in these applications are between 100 to $0.01 \mu\text{m}$ ¹. In this work, nanostructures were prepared by microcontact printing for using as waveguides and resonant cavity with periodic distributions of different refractive indices. Structures of polymer blends of 2 μm to 370 nm polystyrene, polymethylmethacrylate with conductive polymer or light emitting showed good reproducibility and fidelity to the molds used. The results obtained in this study possibilitated to improve the

microcontact printing technique for obtain structures of polymers soluble in aqueous medium, which allow to make the structure of blends of PEDOT / PSS and single-walled nanotubes (SWNT). The phase difference in the AFM measurements showed the possibility of nanotube orientation in towers of PEDOT/PSS produced by the new technique. Thus, preliminary results show the possibility of obtaining "band gap" when achieve photonic structures in 2D below 200 nm. The structures with a periodicity of 200 nm will allow the development of distributed feedback lasers.

We acknowledge support from CAPES, INEO, CNPQ and FAPESP.

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47. **Anisotropy Study of F8BT Thin Films** **Estudo anisotrópico de filmes finos de F8BT**

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Since the first report of electroluminescence (EL) of conjugated polymers by Burroughes et al [1] a wide range of optoelectronic devices including LEDs, FETs, and solar cells have been constructed from semiconducting polymers. Many of the most commonly used conjugated polymers such as substituted poly(p-phenylenevinylene) (PPV), poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT), and poly(9,9-dioctylfluorene-co-bithiophene) (F8T2) have been found to exhibit thermotropic liquid-crystalline (LC) phases as a result of the stiff, conjugated backbone and the long alkyl side chains that are introduced to increase solubility [2].

The understanding of material orientation of those LC materials in thin films is important due to its influences in the final properties of diodes.

In this work, using decay anisotropy measurements, that are based on the principle of photoselective excitation of fluorophores by polarized light, in which fluorophores preferentially absorb photons whose electric vectors are aligned parallel to the transition moment of the fluorophore, it was measured the fluorescence decay anisotropy of F8BT thin films in a thickness range of 50-500 nm, and it was used glass covered ITO as substrate. The results showed F8BT was better aligned when the film was thinner.

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48. **Energy transfer from poly(vinyl carbazole) to a fluorene-vinylene copolymer in solution and in the solid state**

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The energy transfer processes were studied for mixtures of PVK and PFO-MEHPV, which are two polymers that have a strong overlap between the donor emission spectrum and the acceptor absorption spectrum, in both solutions and films and with several relative proportions of the two

components. The emission decay of neat PVK is much slower than that of PFO-MEHPV, which may favor the non-radiative energy transfer process [1]. The steady-state PL spectra of PVK exhibited an intensity decrease in the presence of PFO-MEHPV, but the decrease in the PVK lifetime does not follow the same trend upon increasing the donor concentration. Thus, it has been assumed that the intensity decrease was more strongly correlated with the trivial energy transfer than with FRET process by the Förster mechanism. The low FRET efficiency may be attributed to the presence of several types of the others PVK photophysical processes that quench the excited state via FRET process. Nevertheless, the solid-state polymer blends undergo Förster-type energy transfer more efficiently in addition to the trivial process, as demonstrated by the relative increase in the emission intensity of the acceptor following the donor excitation and the decrease in the donor PL lifetime. Moreover, in films, there are two concentration ranges in which the donor lifetime exhibited an additional decrease, and these concentration ranges are coincident with those at which changes in the morphology were observed using SEM. Further studies are required to explain these changes in the quenching efficiencies.

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49. **Different characteristics of the emission intensity in blends and bilayers of conjugated polymers induced by distinct excitation geometries**

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The optical properties of polymeric sequential bilayers and blends, fabricated by spin-coating on top of glass substrates, have been investigated.

The *Poly(thienylene,2,5dialkoxyphenylene)* (PTDP) and the *poly[(2,5-thiophene);(1,4-dialcoxyphenylene)]* (TPT) possessing a yellow-orange emission, has been used as an acceptor in the blend and bilayer films.

As a donors it was used the *poly[(9,9;dihexylfluoren,2;7;diyl);co;(9;ethylcarbazol2;7 diyl)]* (PDHF-ECZ), a copolymer from Aldrich, and oligomer derivate from the TPT, both with blue emission. Photoluminescence (PL) at room and low temperatures, and steady-state PL spectra, has been performed to characterize the samples at different geometries of excitation. In the PL spectra of the bilayer and the blend a new emission band has appeared. This band has been interpreted as being from exciplex emission complex, which is formed by donor and acceptor interaction at excited states. The exciplex normally comes from short range donor-acceptor interactions, in the range of the exciton dissociation length. Measurements with excitation made at 90° and PL emission detected from the edge of the samples reveal new spectra with different characteristics for the blend and for the bilayer. At this new excitation geometry the waveguide formation induces different effects, which are compatible with the architecture and structural conformation of the films.

Keywords: Conjugated polymer, oligomer, blend, bilayer, waveguide emission

We acknowledge support from CAPES, INEO, CNPQ, FAPEMIG e Pós-Graduação Física.

50. **Surface and bulk defects in layered titanate nanostructures induced by**

chemical and thermal treatments

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Layered titanate nanostructures are interesting materials for applications in (photo)catalysis, hybrid solar cells and sensors. The important (photo)physical properties of these nanostructures are due to the high surface area, reactivity of surface states and semiconducting properties. The photo-physical properties of titanate nanotubes, -fibers and -foils are strongly controlled by the stoichiometry of the material, i.e. submitted to reducing or oxidizing conditions. Such treatments control basically intrinsic bulk [1] and surface-related defects [2]. Therefore, a deep knowledge of the surface and bulk defect states in the titanate nanostructures is fundamental for a better understanding of their properties and optimization of their applications. One batch of titanate nanostructures was submitted to different thermal treatments in controlled atmospheres, while the other was treated by hydrogen peroxide. Titanate nanostructures were analyzed by scanning electron microscopy (SEM) for their morphologies and by Raman scattering and X-ray diffraction for their crystalline structures. Reflectance, photoluminescence and photo-electron paramagnetic resonance (EPR) were applied to the study of bulk and surface defects induced by the different chemical and thermal treatments under controlled atmospheres. While reducing treatments induce high concentration of surface O⁻ radicals and Ti³⁺ interstitial defects, H₂O₂ treatments produce high concentration of superoxide radicals. The latter material shows interesting catalytic properties in oxidizing processes of pollutions [3].

We acknowledge support from FAPEMIG, CAPES, INEO and CNPq.

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51. **Photophysical Properties of Chlorophyll-a/MDMO-PPV in Solution.** **Propriedades fotofísicas de clorofila/MDMO-PPV em solução.**

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Chlorophyll is photosynthetic pigment presents in chloroplasts of plants, algae and cyanobacteria. In organic solution the optical absorption shown the Soret band at 410nm (blue portion) and Q band at 668nm (red portion) and the luminescence spectrum of solution band at 673nm, when excited with 410 nm. The MDMO-PPV is a conjugated polymer which absorbs a broad band at 430 nm assigned to $\pi \rightarrow \pi^*$ transitions and shows luminescence band at 553nm. At this work we propose to study the photophysical properties of chlorophyll-a/MDMO-PPV system by increasing the polymer concentration. When excited at 410nm, the luminescence spectra has shown a quenching of chlorophyll-a luminescence intensity and an increase of MDMO-PPV PL intensity with the increasing MDMO-PPV concentration. For excitation at 600nm only chlorophyll absorbs, however the luminescence of each material has showed. The understanding of the photophysical properties in this system can be applied to harvesting solar energy..

We acknowledge support from CAPES, INEO, CNPQ, FAPEMIG.

52. **Different characteristics of the emission intensity in blends**

and bilayers of conjugated polymers induced by distinct excitation geometries

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The optical properties of polymeric sequential bilayers and blends, fabricated by spin-coating on top of glass substrates, have been investigated.

The *Poly(thienylene;2,5dialkoxyphenylene)* (PTDP) and the *poly[(2,5-thiophene);(1,4-dialcoxi-phenylene)]* (TPT) possessing a yellow-orange emission, has been used as an acceptor in the blend and bilayer films.

As a donors it was used the *poly[(9,9;dihexylfluoren;2;7;diy);co;(9;ethylcarbazol2;7diy)]* (PDHF-ECZ), a copolymer from Aldrich, and oligomer derivate from the TPT, both with blue emission. Photoluminescence (PL) at room and low temperatures, and steady-state PL spectra, has been performed to characterize the samples at different geometries of excitation. In the PL spectra of the bilayer and the blend a new emission band has appeared. This band has been interpreted as being from exciplex emission complex, which is formed by donor and acceptor interaction at excited states. The exciplex normally comes from short range donor-acceptor interactions, in the range of the exciton dissociation length. Measurements with excitation made at 90° and PL emission detected from the edge of the samples reveal new spectra with different characteristics for the blend and for the bilayer. At this new excitation geometry the waveguide formation induces different effects, which are compatible with the architecture and structural conformation of the films.

Keywords: Conjugated polymer, oligomer, blend, bilayer, waveguide emission

We acknowledge support from CAPES, INEO, CNPQ, FAPEMIG e Pós-Graduação Física.

53. Optical and Electrochemical Properties of Dendritic Gold Nanoparticles on ITO Electrodes

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Recently, the utilization of multilayer organic films has opened new paths for fabrication of supramolecular systems by modified surfaces with high control of thickness at nanoscale range and orientation level. Decher and co-workers [1] developed an interesting method based on layer-by-layer (LBL) to fabricate high oriented polyelectrolyte multilayer films. The LBL technique also enables to develop platforms with interesting optical [2] and charge transfer properties [3] using materials at nanoscale level. As an example, hybrids formed by polyelectrolytes and metal nanoparticles have been incorporated using LBL method due to the possibility to obtain modified surfaces with interesting properties [4]. This study reports the utilization of LBL method to modify ITO electrodes and also the obtention of gold nanoparticles (AuNPs) by a simple experimental method of immersion in a H₂AuCl₄ precursor solution in different times. The organic matrices consisting of polyamidoamine dendrimer (PAMAM) and poly (sodium styrene sulfonate) (PSS) self-assembled onto ITO (indium tin oxide) were utilized as platforms for chloraurate ions (AuCl₄⁻) adsorption and AuNPs were obtained by chronoamperometry. This experimental approach

shows the possibility to obtain ITO modified electrodes with enhanced electrochemical and conducting properties. Also, cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and optical measurements were used with the aim objective to investigate charge transfer and optical properties of the modified ITO electrodes.

We acknowledge support from CAPES, INEO, Rede NanoBioMed, CNPQ and FAPESP.

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54. **Spray layer-by-layer film of phospholipids applied in the detection of xanthene derivatives employing impedance spectroscopy and information visualization techniques**

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The layer-by-layer (LbL) technique via spraying (spray-LbL) has been applied as new and alternative methodology to fabricate ultrathin films due to its versatility in relation to the conventional dipping-LbL method, mainly in terms of faster layer deposition and larger coated area. In this work, the possibility of immobilizing phospholipid vesicles of DPPG onto alternating layers of the polyelectrolyte PAH using the spray-LbL method was investigated, being the results compared to the conventional dipping-LbL method. In addition, the Langmuir-Blodgett (LB), dipping- and spray-LbL films composed an array of sensing units successfully applied in the detection of diluted solutions of xanthene derivatives employing impedance spectroscopy measurements. To handle the large amount of generated data, it was used information visualization techniques, more specifically, multidimensional projection techniques, which also served to optimize the sensing performance.

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55. **Functionalization of chitosan-PEG blends with Layer-by-layer films of Concanavalin A and Frutalin.**
Funcionalização de blendas de quitosana-PEG com filmes automontados de Concanavalina A e Frutalina.

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Novel materials are now extensively studied for tissue engineering, as is the case of modified polyetheretherketone (PEEK-WC) membranes with potential for use in hepatocytes cell cultures [1] owing to their stability, permeability and biocompatibility [2]. Synthetic membranes for regeneration have been studied with regard to the interaction with biomembranes [3]. In our study, chitosan membranes were produced via solvent casting with purified chitosan and 20%

poly (ethylene glycol), and modified with layer-by-layer (LbL) films of frutalin and concanavalin A. The purification did not affect the chitosan properties such as the degree of acetylation (27% to 21%) and crystallinity, according to titration, $^1\text{H-NMR}$ and X-ray measurements. The fluorescence spectra indicated that a high intensity signal at 440 nm, with excitation at 370 nm, could be obtained if the membranes were not stored properly. This was probably due to adsorption of organic molecules from microorganisms. Membranes modified with frutalin displayed a fluorescence spectrum with peaks at 425nm, 440nm and 475nm, while those that contained ConA exhibited a spectrum with only one peak at 440nm. These results point to an efficient adsorption of biomolecules on the chitosan membranes.

We acknowledge support from CAPES, INEO, CNPQ, FAPESP, nBionet and ITM-CNR.

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56. **LbL films of lipid/phthalocyanine for sensing applications**

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The Layer-by-Layer (LbL) technique reported by Decher [1] has considerable advantages related to operating costs, time and efficiency. Dioctadecyldimethylammonium bromide (DODAB) is a cationic lipid that forms vesicles when dispersed in water under certain conditions and can be used as mimetic model of biomembranes [2]. Nickel tetrasulfonated phthalocyanine (NiTsPc) is an anionic organic semiconductor that is soluble in water and widely used in sensing applications [3]. Thereby, LbL films were fabricated by alternating layers of DODAB/NiTsPc. We compared LbL films grown using two concentrations of NiTsPc (0.05 and 0.5 mmol/L). The growth was monitored by UV-Vis absorption spectroscopy, the morphology was study by micro-Raman and AFM and the interaction between DODAB and NiTsPc was investigated by FTIR. UV-Vis absorption showed a linear growth of the film. Micro-Raman technique revealed that the LbL films are pretty homogeneous morphologically at micrometer scale. AFM results revealed the presence of DODAB vesicles for NiTsPc solutions at 0.05 mmol/L, being destroyed for 0.5 mmol/L. FTIR absorption spectroscopy showed that the electrostatic interactions between cationic $[\text{N}^+(\text{CH}_3)_2]$ and anionic $[\text{SO}_3^-]$ groups are weak, which was unexpected result. An electronic tongue [4] consisting of five sensing units was applied to detect dopamine as a proof-of-principle. These sensing units were composed by a bare Pt interdigitated electrode and Pt interdigitated electrode coated with LbL films of DODAB/NiTsPc (0.05 and 0.5 mmol/L) PAH/NiTsPc, and DODAB/CuTsPc.

We acknowledge support from CAPES, INEO, CNPq and FAPESP.

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57. **Analysis of the LbL deposition inside microchannels**

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The aim here is to check the influence of the time of deposition of self-assembled films (LbL, layer-by-layer) inside a microchannel. The establishment of the best conditions for the deposition of LbL films of different materials inside microchannels will contribute positively in the integration process to transform an “*electronic tongue*” system into “*lab-on-a-chip*” devices. Since part of this work involves photolithography, the fabrication of the microchannels and interdigitated microelectrodes are developed in cooperation with researchers at the Laboratory of Microfabrication, at the National Research Center for Energy and Materials (CNPEN), localized in Campinas. The microchannels were fabricated on poly(dimethylsiloxane) (PDMS) due to its good optical transparency, inertness, biocompatibility, good reproducibility and low cost [1]. The self-assembly growth of the LbL films inside the microchannels was monitored using Impedance Spectroscopy, more specifically through capacitance *versus* frequency plots.

We acknowledge support from CAPES, INEO and FAPESP.

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58. **Layer-by-Layer deposition of polymer-nanoparticle films and their application in hybrid solar cells**
Filmes crescidos por *layer-by-layer* de filmes de polímero-nanopartícula e sua aplicação em células solares híbridas

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Semiconductor inorganic nanoparticles such as CdSe with their tunable band gaps offer new opportunities to harvest light energy in the entire visible region of the solar spectrum [1]. One interesting approach is the construction of we call a “rainbow solar cell” [2], which employs an ordered assembly of nanoparticles of different diameters. By optimizing the solar cell configuration it should be possible to further improve the performance of these devices. In this work, CdSe nanoparticles of different sizes were synthesized in aqueous medium and characterized by HR-TEM, UV-vis absorption spectroscopy and X-Ray diffraction. Using the layer-by-layer technique, films of these nanoparticles with an inert polyelectrolyte and TiO₂ nanoparticles will be assembled to produce a solar cell configuration with enhanced solar light harvesting.

We acknowledge support from CAPES, INEO, CNPQ, FAPESP

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59. **Preparation and Characterization of Phthalocyanines and Polymers Thin Films Growth by Layer-by-Layer (LbL)**

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LbL technique is a powerful technique to deposit thin layers of molecules/polymers over a

solid surface or even a device, providing the growth of films of multiple layers. The surface is dipped in a polycation solution, washed, dried, dipped in a polyanion solution, washed and dried again. This sequence represents the simplest cycle of a film formation [1,2].

In this work, we carried out the growth of thin films of polymers and phthalocyanines to apply as active layers in organic solar cells. We chose for this experiment two types of film architecture. In the first architecture, n layers of phthalocyanine are grown over n layers of polymer, named "block architecture", and in the second architecture, layers of each material are intercalated, giving rise to an "intercalated architecture". These films were characterized by UV-Vis, AFM microscopy and photoelectrochemistry measurements. The UV-Vis spectra showed that the block architecture absorbs more light in the visible region of the solar spectrum. The AFM images showed that the block architecture has polymers that more agglomerated than the intercalated architecture.

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60. **Molecular architecture comparison in PVD films of perylene derivatives**
Comparação da arquitetura molecular de filmes PVD de derivados de perileno

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Nanostructured thin films of two perylene derivatives, *n*-butylimidoethylenamine perylene (PTCD-NH₂) and bis(2-carboxyethylimido perylene) (PTCD-COOH), were fabricated using physical vapor deposition (PVD) technique. The growth of the PVD films was monitored through ultraviolet-visible (UV-Vis) absorption spectroscopy and a linear behavior was observed (absorbance vs thickness). The molecular integrity of both perylenes in PVD films was confirmed by the similarity between powder and film spectra in Raman scattering measurements. The surface morphology was investigated in micrometric scale by optical microscopy coupled to Raman mapping and in nanometric scale by atomic force microscopy (AFM) and scanning electron microscopy (SEM). The results in micrometric scale show a smooth and homogeneous surface, however some aggregates were found in nanometric scale by AFM and SEM. The molecular organizations in PVD films for both perylene derivatives were determined using the selection rules of infrared absorption spectroscopy (transmission and reflection absorption modes). The results show that both perylenes have distinct molecular organization. Metallic nanostructures were used to promote localized surface plasmons (LSP) in order to achieve surface-enhanced Raman scattering (SERS).

We acknowledge support from FAPESP, INEO, CNPq and CAPES.

61. **Organic Semiconducting Materials with Discotic Structure**

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Columnar liquid crystals are formed of an aromatic rigid core, composed of disc-shaped molecules, surrounded by flexible peripheral chains. These materials combine the good charge-transport properties of single crystals with the good film-forming properties of viscous liquids. In these systems the disc-shaped molecules are stacked on top of one another resulting in columns [1]. Such semiconducting materials are well known to exhibit high charge mobilities and large exciton diffusion lengths along the column direction providing promising applications in organic electronics. An important issue to achieve high mobilities in the columnar mesophase is to control the structure and the organization of the discotic semiconducting material in oriented thin films. For solar cells, the face-on orientation (columns perpendicular to the electrodes) is required [2-4]. The synthesis of two discotic molecules, which exhibit antagonist solubility, allowing the formation of an oriented bilayer heterojunction, has been recently reported [5].

In this work we investigated the morphology, the optical and conductive properties of two discotic liquid crystals, a columnar donor and a columnar acceptor. The morphology of the films produced by spin-coating was monitored with atomic force microscopy before and after annealing. For the optical properties were performed absorbance and photoluminescence measurements. The conductive properties of the devices were investigated with current versus voltage and the HOMO and the LUMO of the materials were determined by cyclic voltammetry.

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62. **Progress of the sealing in a microfluidic device**

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Some effort was employed here to improve the sealing of a microfluidic device, aiming a reduction in some of the steps involved in the miniaturization process. The idea is the development of a new technology with strong commercial appeal due to a considerable reduction in the time of analysis, amount of sample(s)/reagent(s) used and waste. We have employed photolithography to build up gold interdigitated electrodes (IDEs) onto BK7 glass and replicated single microchannels in polydimethylsiloxane (PDMS), which are irreversibly sealed by oxygen plasma treatment. As the sealing is a critical and important step in the device fabrication, we present here recent results to improve the deposition of a thin SiO₂ layer onto the IDEs, the cleaning of the PDMS/microchannel previously to the plasma exposure and, the alignment between IDEs/microchannel.

We acknowledge support from CNPq, FAPESP and INEO.

63. **Use of self-assembled films in microfuel cells**

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This work envisages the use of self-assembled (LbL, layer-by-layer) films in the fabrication of a Direct Methanol Fuel Cell (DMFC), checking how these nanostructured thin films might help in the reduction of methanol permeation (in the cathode direction). Up to date LbL films were poorly explored in this sort of application, and our interest in micro fuel cells relies on their reduced size, integration using microfluidics and high commercial prospective for portable devices. Moreover, the LbL films might improve the efficiency as recent results in the literature point out that the deposition of nanostructured films in Nafion® membranes results in higher proton conduction and lower methanol permeation [1]. Here, a first step was taken choosing a DMFC structure, made at Microfabrication Laboratory (CNPEM-LNNano), allowing the incorporation of distinct supramolecular architectures and rapid prototyping alterations in the device, if some modifications are needed during the developments proposed.

We acknowledge support from CAPES, INEO, FAPESP and CNPq.

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64. **CdWO₄-on-MEH-PPV:PS as a candidate for real-time dosimeters**

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We report on the investigations about the modification of optical properties induced by X-rays onto film detectors based on cadmium tungstate (CdWO₄), poly[2-methoxy-5-(2'-ethylhexyloxy)-p-phenylenevinylene] (MEH-PPV) and polystyrene (PS). This device takes advantage of reduction of spectral overlap between the radioluminescence of CdWO₄ and the absorption of MEH-PPV as it is exposed to radiation, forming the basis of a new radiation detector that is capable of converting the orange-red radioluminescence of PS:MEH-PPV:CdWO₄ into green. We also propose an explanation of the optical processes occurring in MEH-PPV:CdWO₄ under X-rays exposure in terms of the radiation hardness of CdWO₄ combined to the radioluminescence-induced photodegradation of MEH-PPV.

We acknowledge support from CAPES, INEO, CNPQ, NANOBIOMED, FAPESP and FAPEMIG.

65. **Microdevice from natural rubber for fluids applied as biological sensor (Lab-on-a-Ship)**

Micro-dispositivo de borracha natural para fluídos aplicado como sensor biológico (Lab-on-a-Ship)

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This work presents a research proposal involving the construction of micro-devices (lab-on-a-ship) of natural rubber prepared from latex of *Hevea brasiliensis* (clone RRIM 600), carried out by casting technique to investigate fluids. Studies published in the literature show the development of hard technology, in some cases using synthetic polymeric supports, for the sensor build [1,2,3]. The fluid under analysis will be injected in the channels generated in the polymeric matrix by means of a peristaltic pump with both flow control and pressure, through the use of catheters in order to be measured internally in the optical window. Sensors based on the use of carbon micro-electrodes (fibers extracted from carbon's tissue) with immobilization of enzymes such as glucose oxidase to evaluating glucose in liquids as well as the deposition of platinum on surface of the electrodes to evaluating the oxygen present will be addressed the main routes, studied by electrochemical techniques. This sensor will be a way to create new clinical diagnostics technology after tests in vivo (implanted in animals) for biochemical analysis and monitoring of blood plasma, for example. The choice of materials is based on the mechanical properties, high flexibility, which makes the device's sustainability as well as both the biocompatible, mechanical and electrical properties from natural rubber and carbon fibers used to build the sensor.

We acknowledge support from CAPES, INEO, CNPQ, FAPESP, NanoBioTec and NanoBioMed groups.

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66. **The Influence of gold nanoparticles on the horseradish peroxidase and cytochrome C bioelectrochemical properties**

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In this study we report the immobilization of horseradish peroxidase (HRP) and cytochrome C (CytC) with gold nanoparticles (AuNPs) on gold electrode surface. The electrode was firstly modified with poly(sodium 4-styrenesulfonate) (PSS) *via* layer-by-layer (LBL) self-assembly technique. After, AuNPs and HRP or CytC were utilized on the films formation, leading a two configurations, Au/(PSS/AuNP/PSS/CytC)_n and Au/PSS/(AuNP/HRP)_n, where *n* is the number of layers. From quartz crystal microbalance with dissipation (QCM-D) data, it was observed a steady growth for both films with mass of 26 $\mu\text{g cm}^{-2}$ of 7 $\mu\text{g cm}^{-2}$ for Au/(PSS/AuNP/PSS/CytC)₃ and Au/PSS/(AuNP/HRP)₅, respectively. Finally, the electrocatalytic activity was studied by cyclic voltammetry measurements, where was observed a catalytic current in the presence of 0.5 mmol L⁻¹ of H₂O₂, for onset potential at -0.10 V for Au/(PSS/AuNP/PSS/CytC)₃ and -0.15 V for Au/PSS/(AuNP/HRP)₅. When compared with films without AuNPs, was verified an increase in these catalytic current from -1.29 to -3.39 $\mu\text{A cm}^{-2}$ for Au/(PSS/AuNP/PSS/CytC)₃, and -1.87 for -3.28 $\mu\text{A cm}^{-2}$ for Au/PSS/(AuNP/HRP)₅. The currents were obtained at onset reduction potential. The abovementioned results suggests that the HRP and CytC when immobilized with AuNPs enhanced charge transfer from bioelectrocatalytic processes.

We acknowledge support from CAPES, INEO, CNPQ and FAPESP.

67. **Nanostructural Modifications in Stretch-Induced Crystallization in PVDF Films as Measured by Small-Angle X-Ray Scattering**
Modificações Nanoestruturais Induzida pela Cristalização por Estiramento de Filmes de PVDF Medida por Espalhamento de Raios-X a Baixo Ângulo.

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Previous works demonstrated that stretching α -PVDF films reduces the intensity of the dielectric relaxation α_c [1,2]. With base in those results, it was suggested that the metastable polarization, as well as, the dielectric relaxation α_c should be caused by dipolar orientation in the interfacial amorphous-crystalline region of the PVDF [3]. In this work the nanostructure of stretched and non-stretched PVDF samples was studied by small-angle X-ray scattering (SAXS). The crystallinity of the samples were determined by wide-angle X-ray diffraction (WAXD) and differential scanning calorimetry (DSC), and crystalline phases by Fourier Transform Infrared Spectroscopy (FTIR). The nanostructure can be described by a lamellar stacking of crystalline and amorphous layers, with a fairly well defined long period D and a diffuse-boundary in the interface between the crystalline and amorphous phases. The crystallinity of the stretched sample was found to be greater than that of the non-stretched sample. The long period D and the thicknesses of the crystalline lamellae T_c were found to be greater in the stretched sample than those in the non-stretched sample. The thickness of the diffuse-boundary was evaluated as being approximately 1.4 nm in the non-stretched sample and 1.1 nm in the stretched sample. It was concluded that the growth of the thickness of the crystalline layer induced by the stretching process (stretch-induced crystallization) occurs partially at expense of the diffuse boundary and also by the coarsening of the structure with the stretching process, because of the diminution in the surface area to volume ratio observed.

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68. **Development of novel genosensors for HPV detection and diagnosis**

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Genosensors refer to a class of analytical devices capable of recognizing specific DNA sequences upon transducing a biochemical event into a measurable signal, e. g., optical, electronic or electric. Genosensors have a diagnostic potential, since they can be used to detect genetic disorders, viruses, bacteria and parasites upon recognition of their DNA. Recently, efforts have been made to achieve a device that can be used routinely at clinical analysis with good sensibility and low-cost. However, these devices still exhibit drawbacks regarding lack of sensibility and high cost. The aim of this study is develop a fast-response and low-cost genosensor for *Human Papilloma Virus* (HPV) detection. The devices comprised specific, small DNA sequences (primers), or capture probes, immobilized on a solid platform, which is capable of hybridize with a target sequence (a specific sequence from HPV virus). Silicon and quartz

surfaces were functionalized via silanization and muconic acid was used as a crosslinker between the modified surface and the capture probes. The detection is performed via Impedance Spectroscopy.

We acknowledge support from CAPES, INEO, CNPQ and FAPESP.

69. **Use of conceptual maps for management of projects and scientific dissemination**
Uso de mapas conceituais para a gestão de projetos e difusão científica

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The main goal of this work is to present a methodology for knowledge management by using conceptual maps. The research is focused on the activities carried out by the INEO network which involves research groups from different universities in nine Brazilian states. Due to the complexity of subjects it becomes necessary to figure out an appropriated tool capable of giving a whole sight of the project in order to permit its management with a clear recognition of the goals to be met. The use of conceptual maps makes easier the collection as well as the disclosure and dissemination of scientific results achieved [1]. The scientific dissemination in this project is intended to be used as a motivational tool for science and math teaching in elemental and high school levels. Presentation of fundamental science and math concepts and relate them to advances in scientific research and technology developments is a strategy for encouraging students to become interested in Engineering and Exact Sciences careers. This is a secondary goal of the project since Brazil is nowadays demanding a number of human resources above its universities' capacity of training.

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70. **PEDOT:PSS Films treated by UV-Ozone: Electrical Behavior Analysis**

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The electroluminescent devices called P-OLEDs and organic photovoltaic are currently mounted using the base of organic electronic. They use a polymeric film known as PEDOT:PSS generally deposited by wet process. This layer has been deposited on another film called by TCO (transparent conductive oxide) deposited on glass substrate. Both layers have important electrical and optical properties as transparency and low sheet resistance, together they actuate as anode electrode during the polarization. The active polymeric material is deposited on the PEDOT:PSS and then, it is deposited a metallic film (aluminium or silver). In this work is presented a study of samples that it has the objective of optimization on the electrical

performance of complete electrode anode (TCO - PEDOT:PSS). The processes parameters unchanged for the formation of PEDOT:PSS films were: time/rotation of spinner (for the formation of films), type/supplier of PEDOT:PSS, temperature and evaporation time of solvent (water) used inside the oven. Then the PEDOT:PSS films were placed inside the UV-Ozone reactor and were irradiated during a period of time and at this same period of time the electrical resistance of films were sampled [1,2]. The electrical resistance of PEDOT:PSS film deposited on the ITO (indium tin oxide used as TCO) presented a parabolic behavior of variation, it was produced during the elapsed time of exposition inside the UV-Ozone reactor. It was obtained different values of electrical resistance for different samples at different temperatures of annealing (range from 80 °C to 160 °C). Under the UV-Ozone reactor condition a decrease of the electrical resistance was observed (it was reduced by the half way, at the middle, compared it initial value) and then an increase of the electrical resistance was obtained during the last part of the elapsed time.

The experimental methodology and all particular result will be presented with details.

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71. **Luminance Reference for the Measurement of OLEDs / PLEDs** **Referência de Luminância para a Medição de OLEDs / PLEDs**

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Electroluminescent devices can be characterized in terms of light output and the reading register performed based on the concept of luminance, the light intensity per unit area (usually sampled in the direction of normal to the surface) is to be used in the calculation of efficiency and a figure of merit. The photometer may have offset that needs to be documented. To seek knowledge about possible drift in relation to the instrument class of accuracy set by the manufacturer an experiment was designed and conducted in Nov./01/2011, at Tucumán, Argentina. The experiment was called by the partners from Argentina: an operation of verification since it does not involve absolute method or luminance standard [1]. The performance check was conducted between two luminance meter, Argentina: LMT brand, model L1009; and Minolta brand, model LS110 (Brazil), luminance produced from an incandescent light bulb radiating a reference white were sampled. The range of luminance considered in terms of reading in the LMT, whose field of view was set according to the LS 110 (one third of degree) during the sampling process was (3.05 to 417) cd/m². The relative difference found indicates the need to multiply the reading of the instrument LS 110 (Brazil) by the base factor "1.067" for it reading to be equivalent to the reading obtained at the LMT (Argentina). Survey was conducted over a distributed part of the reference white sample (by the LS 110 instrument) to assess the uniformity of luminance. In the central region of the white reference plate the uniformity of luminance calculated indicate a dispersion factor that is not greater than 0.7%.

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