Monday 14.04

08:00 Registration

08:15 Opening session (Marília J. Caldas & Roberto M. Faria)

08:30-10:30 Focus Session 1: INEO: Balance of Activities 2009-2013
Chair: Marília J. Caldas

08:30-10:05 Statement of the Teams (2 minutes each)
10:05-10:30 Overview of results obtained by INEO
Roberto M. Faria - IFSC/USP

10:30-10:50 Coffee Break

10:50-12:30 Focus Session 2: INEO - Advances in Theoretical Research
Chair: Marília J. Caldas

José A. Freire
Departamento de Física – Universidade Federal do Paraná.

11:20-11:40 “Correlations between anisotropy and optical behavior in amorphous stretched PPV films”
R. Ramos (1), M. F. Siqueira (2)
(1) Instituto de Física, Universidade de São Paulo. (2) Departamento de Física, Universidade de Ouro Preto.

11:40-12:00 “Recent Advances in Research at LABMADE Laboratory”
Liliana Yolanda Ancalla Dávila, R. Lelis-Sousa
Curso de Licenciatura em Física; Campus Universitário de Araguaína - Universidade Federal do Tocantins.

12:00-12:30 “Perspectives and Challenges in Modeling Nanostructures”
Douglas S. Galvão
Instituto de Física Gleb Wataghin – Universidade Estadual de Campinas.

12:30 -14:00 Lunch

14:00-17:00 Free discussion of projects and collaborations

17:00-19:00 Posters
19:00-20:00 Invited Talk
“Modifying graphene”
Helio Chacham
Universidade Federal de Minas Gerais

20:00 Dinner

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Tuesday 15.04

08:30 Focus Session 3: Organic Devices and Related Phenomena
Chair: Paulo B. Miranda
08:30-09:00 “Experimental design in searching smart organic dosimeters”
R.F. Bianchi,
Laboratory of Polymers and Electronic Properties of Materials, Department of Physics – Federal University of Ouro Preto
09:00-09:30 “Electroluminescence and electric current response applied to the characterization of polymer light-emitting electrochemical cells”
L.F. Santos
Departamento de Física, Instituto de Biociências, Letras e Ciências Exatas, Universidade Estadual Paulista - UNESP, São José do Rio Preto, SP.
09:30-10:00 “Advances in Organic Devices: Photovoltaics and Field-Effect Transistors”
Roberto M. Faria
IFSC/USP

10:00-10:30 Coffee Break

10:30-11:10 Invited Talk
“OLEDs, PLEDs and QLEDs for displays and lighting”
Peter Kember
Kember Associates, UK

11:10-12:30 Focus Session 4: Projects with Enterprises (Round Table)
Chair: Rodrigo F. Bianchi
A. Lucrécio (Instituto de Tecnologia Flextronics, BR ), P. Kember (Kember Associates, UK), V. Cegal (Fast Company Brazil, BR) and R.M. Faria (INEO)

12:30-14:00 Lunch

14:00-17:00 Free discussion of projects and collaborations
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<th>Time</th>
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<tr>
<td>17:00-19:00</td>
<td><strong>Posters</strong>&lt;br&gt;Scientific contributions; experimental and computational facilities</td>
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<td>19:00-20:00</td>
<td><strong>Team Leaders Meeting: Future and Perspectives</strong></td>
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<td>20:00</td>
<td><strong>Dinner</strong></td>
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**Wednesday 16.04**

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<th>Time</th>
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<tr>
<td>08:30-10:30</td>
<td><strong>Focus Session 5: BioMaterials and Biosensors</strong>&lt;br&gt;Chair: Osvaldo Novais de Oliveira Jr</td>
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<td>08:30-08:50</td>
<td>“Processing of nanomaterials and biomolecules in nanostructured films for sensing applications”&lt;br&gt;Jose Roberto Siqueira Junior&lt;br&gt;Institute of Natural Sciences and Education, Federal University of Triângulo Mineiro, Uberaba, MG</td>
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<td>08:50-09:10</td>
<td>“Printed Biosensors and Biomedical Devices”&lt;br&gt;F. J. Pavinatto&lt;br&gt;Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos -SP.</td>
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<td>09:10-09:30</td>
<td>“Sensors and Biosensors development at Grupo de Pesquisa de Nanociência e Nanotecnologia Aplicada ao Sensoriamento”&lt;br&gt;Marystela Ferreira&lt;br&gt;Universidade Federal de São Carlos, CCTS, DFQM</td>
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<td>09:30-09:50</td>
<td>“Atomic Force Microscopy used in Developing Nanobiosensors “&lt;br&gt;Fábio L. Leite&lt;br&gt;Grupo de Pesquisa em Nanoneurobiofísica, Universidade Federal de São Carlos, Sorocaba</td>
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<td>09:50-10:10</td>
<td>“Recent progress on molecular modeling of bio-molecular systems”&lt;br&gt;H. M. Petrilli&lt;br&gt;Ínstituto de Física, Departamento de Física de Materiais e Mecânica – Universidade de São Paulo.</td>
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<td>10:10-10:30</td>
<td>Brief Discussion on plans for the future</td>
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<td>10:30-11:00</td>
<td><strong>Coffee Break</strong></td>
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<td>11:00-12:30</td>
<td><strong>Focus Session 6: Synthesis, Characterization and Other Studies Related to Molecules and Thin Films</strong>&lt;br&gt;Chair: Roberto Mendonça Faria</td>
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<td>11:00-11:20</td>
<td>“Polypyrrole nanostructured fibers for solid phase microextraction”&lt;br&gt;E. F. Jasinski (1, 2)&lt;br&gt;(1) LabSiN - Departamento de Física – Universidade Federal de Santa Catarina.&lt;br&gt;(2) Campus Araranguá – Universidade Federal de Santa Catarina.</td>
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| 11:20-11:40  | “Control of the Energy Levels in Donor-Acceptor Copolymers”  
P.C. Rodrigues  
Departamento Acadêmico de Química e Biologia – UTFPR |
| 11:40-12:30  | **Invited Talk**  
“White emission in polymeric light-emitting diodes”  
Teresa D. Z. Atvars  
Grupo de Fotofísica e Fotoquímica - Universidade Estadual de Campinas |
| 12:30-14:00  | Lunch                                           |
| 14:00-17:00  | Free discussion of projects and collaborations   |
| 18:00-19:00  | **Closing session**                            |
| 20:00        | Dinner                                          |
Abstracts / Resumos

Focus Session 2: INEO - Advances in Theoretical Researches
Chair: Marília J. Caldas

1. Localization in the Gaussian Disorder Model and Extended Hückel Method for Computing Polarization Energies of Random Molecular Ensembles

José A. Freire (1), Rodrigo P. Rocha (2) and Raphael M. Tromer
(1) Departamento de Física – Universidade Federal do Paraná.
(2) Departamento de Física – Universidade Federal de Santa Catarina.
e-mail: jfreire@fisica.ufpr.br

We obtained the density of eigenvalues of the rate matrix that describes the electron hopping motion in the Gaussian Disorder Model (GDM) [1], the simplest model for disordered organic materials. The spatial localization of the eigenvectors is also obtained by means of the Inverse Participation Ratio. We discuss how the diffusion and the speed of thermalization in the GDM are directly related to these two quantities.

We present an adaptation of Hoffmann’s extended Hückel method [2] to study the polarization of a molecule and apply it to obtain the polarization energy of a charged benzene dimer [3]. The ultimate goal of the method is to compute the polarization energy of a large disordered molecular ensemble and we discuss how to obtain this quantity.

We acknowledge support from CAPES, INEO and CNPQ.


2. Correlations between anisotropy and optical behavior in amorphous stretched PPV films

R. Ramos (1), M. F. Siqueira (2), M. J. Caldas (1), T. Cazati (2) and R. M. Faria (3)
(1) Instituto de Física, Universidade de São Paulo, C. P. 66318, São Paulo, SP, Brazil.
(2) Departamento de Física, Universidade de Ouro Preto, C. P. 35400-000, Ouro Preto, MG, Brazil.
(3) Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 13560-970 São Carlos, SP, Brazil.
e-mail: melissa@iceb.ufop.br;

Poly (p-phenylene vinylene) (PPV) is a well-known organic semiconductor, usually deposited via spin-coating technique on a chosen substrate, and exhibits amorphous and crystalline regions.
Modifications in the molecular arrangement and the induced variations in the chain packing are expected to affect drastically the resulting optoelectronic properties, but such local structural fluctuations are not easily probed by experimental measurements only [1,2]. In this work we present classical molecular dynamics simulations, building an atomistic scale picture of local morphological changes due to an applied external uniaxial strain, as well as experimental results on polarized UV emission and absorption spectra of stretched PPV films [2]. In the simulations we employ statistical correlation functions to evaluate the anisotropic behavior during the stretching procedure. In addition, we characterize the molecular arrangement distortions, the relative orientation and the packing evolution of the chains. Comparisons between ab initio calculations for crystalline models [3] and our simulations indicate that the detected optical behavior of polarized emission spectra can be attributed to the increase of local π-stacking in the amorphous regions.

This work was supported by INEO, CAPES, CNPq, and FAPESP.


3. Recent Advances in Research at LABMADE Laboratory

Liliana Yolanda Ancalla Dávila, Alexsandro Silvestre da Rocha, Nilo Maurício Sotomayor Choque and R. Lelis-Sousa
Curso de Licenciatura em Física; Campus Universitário de Araguaína - Universidade Federal do Tocantins.

E-mail: lydavila@mail.uft.edu.br; rlsousa@uft.edu.br

The LABMADE is dedicated to characterization and computational study of materials used to conversion from solar light to electrical energy. We have work with support from INEO in: nanostructuring of materials, electroanalytical methods for detection of herbicide in water, manufacturing colloidal crystals, synthesis of colloids, modeling of electron transport in semiconductor systems and computer simulation of materials with applications on organic electronics. In this presentation, we briefly discuss some results that have been obtained through computational simulations using semi-empirical and first principles methodologies. The focus is the study of structural and electronic properties of materials which can be interesting as active layer in photovoltaic devices, solar cells, light emitting diodes and transistors.

We present results obtained by semi-empirical methodology of structural, electronic and optical properties of copolymers composed by fluorene in association with benzotiodiazole or benzoselenodiazole molecules. This work is been development in collaboration with other INEO members. We also investigate the effect of insertion of substituent groups into the polymeric structure. In general, these side chains are used to get a better solubility of organic semiconductor. In the last year, we have studied the effects of addition of methyl and methoxy groups on polypryrrole (PPY) conjugated backbone. More recently, we improved our methodology employing first principles methods to investigate electronic structure of thienoacenes, graphite, graphene, fullerenes, CdSe and CdTe with Density Functional Theory with and without empirical corrections also dispersion forces. Our preliminary results indicate that the organic semiconductor investigated here can be interesting alternatives to those traditionally employed in the construction of devices. This conclusions are supported by experimental findings [1].
entre outros. Discutiremos brevemente alguns resultados que têm sido obtidos em simulações computacionais empregando métodos semi-empíricos e métodos de primeiros princípios. O foco é o estudo das propriedades estruturais e eletrônicas de materiais que possam ser interessantes como camada ativa em dispositivos fotovoltaicos, células solares, diodos emissores de luz e transistores.

Apresentaremos resultados obtidos por meio de métodos semi-empíricos de propriedades estruturais, eletrônicas e ópticas de copolímeros produzidos por diferentes concentrações de fluoreno com moléculas de benzotiodiazole e benzoselenodiazole em colaboração com outros membros do INEO. Ainda com metologia semi-empírica, foram realizados estudos para equacionar o efeito da adição de grupos substituintes à cadeia dos polímeros com o intuito de torná-los mais solúveis. No último ano, dedicamos à adição de grupos metil e metóxi no polipirrol (PPY). Quanto às simulações empregando métodos de primeiros princípios, destacamos a obtenção da estrutura eletrônica de tienoacenos, grafite, grafeno, fulerenos, estaneno, CdSe e CdTe empregando Teoria do Funcional da Densidade e também correções empíricas de forças de dispersão. Muito interessantemente, nossos resultados indicam que dentre os materiais investigados, alguns [1] podem ser alternativas interessantes àqueles tradicionalmente utilizados na construção de dispositivos. Estas conclusões corroboram recentes dados experimentais [1].

We acknowledge support from INEO, CNPq, UFT and FAPT. Computer resources were provided by CENAPAD-SP and INEO.


4. Perspectives and Challenges in Modeling Nanostructures

Douglas S. Galvao
Instituto de Física Gleb Wataghin – Universidade Estadual de Campinas. Campinas/SP
e-mail: galvao@ifi.unicamp.br

With the technological advances and crescent demand for smaller and more complex electronic devices, we are approaching the physical limits of our present day silicon technology. This has motivated, in part, the creation of a new scientific area, generically called nanoscience. This is a particularly appealing scientific area because of the existence of new and unique nanoscale phenomena, which promise to revolutionize basic science and technology.

In this presentation we will discuss the challenges and perspectives to develop new computational tools to be applied to nanomaterials. In particular we will discuss new results from our group for modeling structural and mechanical properties of graphene, graphene oxide and carbon nanotubes.

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

5. Modifying graphene

Helio Chacham (1)
(1) Departamento de Fisica - UFMG
e-mail: chacham@fisica.ufmg.br

Graphene is a 2D material with high optical transparency, conductivity, and mechanical resistance. Many of possible applications of graphene depend on the modification of its properties relative to the pristine material. Here we will present experimental and theoretical results on the modification of graphene properties through doping, functionalization, compression, and deposition either at
surfaces or at other 2D materials. In particular, we will report the effect of oxygen doping [1],
alloying with nitrogen and boron [2], compression [3], deposition of organic molecules [4], and
deposition of graphene atop boron nitride [5], iron/nickel [6], and graphene itself at an angle [7].

We acknowledge support from CAPES, CNPQ, FAPEMIG, and INCT de Nanomateriais de Carbone.


Focus Session 3: Organic Devices and related phenomena
Chair: Paulo B. Miranda

6. Experimental design in searching smart organic dosimeters

R.F. Bianchi,
Laboratory of Polymers and Electronic Properties of Materials, Department of Physics –
Federal University of Ouro Preto
e-mail: bianchi@iceb.ufop.br

This work describes a variety of experiments that reveal the potential application of semiconducting
dosimeters to improve the performance of dosimeters for therapeutic radiation dosimetry. We report our
experimental design in searching a smart dosimeter used to detect x-rays, gamma rays and blue-
light for improving patient safety in radiation oncology and neonatal phototherapy. The dosimeters
are based on radiation-induced color change of a blue-light sensitive polymer-based film, gel or
nanofiber consisting of a light stable green emitter cooper phthalocyanine (C_{32}Cl_{16}CuN_{8}) and a
blue-light sensitive red emitter polymer (OC_{10}OC_{6}-PPV). The optical properties of the dosimeter
have been examined as function of radiation dose, and the effect of radiation is observed to be
strongly correlated with the efficient spectral overlap between C_{32}Cl_{16}CuN_{8} emission and the
absorption of degraded OC_{10}OC_{6}-PPV, which alters the color and photoemission of OC_{10}OC_{6}-PPV/
C_{32}Cl_{16}CuN_{8} from red to yellow, and then to green. The rate of this change is more sensitive when
the dosimeter is irradiated in the presence of benzoyl peroxide than when in the presence of
hindered phenolic stabilizers, respectively, an accelerator and an inhibitor to activate or inhibit free
radical formation. This gives rise to optimize the response curve of the dosimeters. It is clear from
the experimental results that organic emissive semiconductors have potential to be used as
dedicated and low-cost dosimeters to provide an independent check of radiation/light beam output
and therefore to give patients the opportunity to have information on the dose prescription or
equipment-related problems a few minutes before being exposed to radiation.

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


7. Electroluminescence and electric current response applied to the
characterization of polymer light-emitting electrochemical cells
Light-emitting electrochemical cells (LECs) are optoelectronic devices which had been proposed as an alternative to organic/polymeric light-emitting diodes (OLEDs/PLEDs) due to advantageous characteristics like low operation voltage, simple device structure and bipolar electroluminescence behaviour almost irrespective to the work-function of the metals used as electrodes. In the present work, frequency-dependent electroluminescence and electric current response spectroscopy were applied to polymeric light-emitting electrochemical cells (LECs) in order to obtain information about the operation mechanism regimes of such devices. Three clearly distinct frequency regimes could be identified: a dielectric regime at high frequencies; an ionic transport regime, characterized by ionic drift and electronic diffusion; and a electrolytic regime, characterized by electronic injection from the electrodes and electrochemical doping of the conjugated polymer. From the analysis of the results, it was possible to evaluate parameters like the diffusion speed of electronic charge carriers in the active layer and the voltage drop necessary for operation.

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


8. Advances in Organic Devices: Photovoltaics and Field-Effect Transistors

Roberto M. Faria
IFSC/USP
e-mail: faria@ifsc.usp.br

The field of organic semiconductor devices is still in its infancy. This area consists of either polymers or large molecules technologies, and has been expanding fast, driven by an increasing number of groups worldwide. Displays of OLEDs have already made their way into commercial products such as mobile phones and TV sets, as well as in lighting panels. Organic solar cells (OSCs) and field effect transistors (OFETs) are treading similar development, and their technology is being rapidly improved. In this presentation, we intend to describe results related to organic devices that have been obtained in the Group of Polymers Bernhard Gross. In OSCs, we present recent results achieved by Douglas J. Coutinho, in his doctoral thesis. He worked with ITO/PEDOT:PSS/rr-P3HT:PCBM/Al-Ca structures, and after numerous series of measurements he devised an analytical model for the electric transport, in the specific case where charge carrier mobility and lifetime were equal for electrons and holes. This model provided excellent fits of the experimental J-V curves. In OFETs, devices using P3HT as the semiconducting channel and PMMA as the dielectric material showed to be promising technology for plastic electronics. Four different structures were used in this investigation and a semi analytical model was proposed to explain the electrical operation of the device. These results are part of the PhD thesis of Alexandre C. Maciel, and now Lilian S. Cardoso is making her research in the same subject. Finally, we present some recent progress in the area of printed electronics, carried out by Josiani C. Stefanelo. She is finishing her doctoral research in printable inverter devices, and she has obtained promising results in p-OFETs and n-OFETs, and also for inverter circuits.
9. Processing of nanomaterials and biomolecules in nanostructured films for sensing applications

José Roberto Siqueira Junior
Institute of Natural Sciences and Education, Federal University of Triângulo Mineiro, Uberaba, MG

The integration of nanomaterials and biomolecules have been investigated in nanobiotechnology applications, especially for sensing and biosensing. The processing of these materials can be obtained in the form of nanostructured films by the layer-by-layer and Langmuir-Blodgett techniques, in which materials are disposed in a controlled nanoarchitecture. The interaction between the materials by these techniques is attractive for the development of new sensing units with improved properties, leading to creation of sensors and biosensors with optimized characteristics and performance. In this talk, it will be presented the research that has being developed at the Federal University of Triângulo Mineiro regarding the manipulation of carbon nanotubes, metallic nanoparticles, quantum dots, and biomolecules in the form of nanostructured films. Some hybrid systems and their properties will be presented, as well as their applications in sensors and biosensors.

10. Printed Biosensors and Biomedical Devices

F. J. Pavinatto
Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos -SP.

*e-mail: pavinatto@ifsc.usp.br*

Printing techniques have been extensively used for the fabrication of organic electronic devices, as transistors and light-emitting diodes. Furthermore, these techniques (remarkably inkjet printing) are being employed for the localized dispensing of solutions containing biological molecules and cells, aiming at the fabrication of bio-functional microarrays and biosensors. Here, the potential applications of printing for the fabrication of biosensors and biomedical devices will be discussed. Firstly, printing techniques will be introduced, with special attention devoted to inkjet and rotogravure printing and to advantages of these techniques over traditional processes as lithography. The fabrication of an all-printed and flexible impedance-based biosensor for antioxidants will be presented as an example. Such biosensor is constituted by sub-100 µm inkjet-printed gold (Au) interdigitated electrodes (IDEs) and a rotogravure-printed active layer, which was deposited from a tailor-made bioactive enzyme (Tyrosinase) containing ink on a plastic substrate. The final all-printed device is flexible, light-weight and disposable, and illustrates how inkjet and rotogravure can be used, respectively, when high resolution or large-area printing are desired. Finally, applications of printing in the fabrication of biomedical devices will be speculated, and a few examples in which the author is currently working will be cited. The main goal of this talk is to illustrate how printed electronics can be used in biosensors and biomedical devices research, opening doors for the deployment of technological products using roll-to-roll processes.

We acknowledge support from INEO, FAPESP project # 2011/05742-0.

11. Sensors and Biosensors development at “Grupo de Pesquisa de Nanociência e Nanotecnologia Aplicada ao Sensoriamento”

Marystela Ferreira
Universidade Federal de São Carlos, CCTS, DFQM
In our research group we have developed and characterized nanomaterials using Layer-by-Layer (LbL) and Langmuir-Blodgett (LB) techniques and aiming the synergy between materials or better conformation of the enzyme. These sensors after spectroscopic characterization (UV, Raman, FTIR, SPR) and morphological characterization (AFM, SEM) and electrochemical characterization are applied in food samples or samples of environmental contaminants. Beyond this line, we are developing materials for applications in drug delivery.

We acknowledge support from CAPES, INEO, CNPq, FAPESP, Rede nBioNet and all our students and collaborators.

12. Atomic Force Microscopy used in Developing Nanobiosensors

(1) Grupo de Pesquisa em Nanoneurobiofísica, Universidade Federal de São Carlos (UFSCar), Sorocaba-SP.
(2) Departamento de Engenharia de Alimentos, Universidade Regional Integrada do Alto Uruguai e das Missões, Erechim-RS.
(3) Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos-SP.
(4) Instituto Federal de São Paulo, Itapetininga-SP.
(5) Instituto de Química, Universidade Federal de Uberlândia, Uberlândia-MG.
(6) Departamento de Química, Universidade Federal de São Carlos, São Carlos-SP.
(7) Laboratório Nacional de Nanotecnologia para o Agronegócio (LNNA), Embrapa Instrumentação, São Carlos-SP.
(8) Instituto de Química, Universidade de São Paulo, São Paulo.

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The development of sensitive methodologies for detecting agrochemicals has become important in recent years due to the increasingly indiscriminate use of these substances. In this context, nanobiosensors based on atomic force microscopy (AFM) tips are useful because they provide higher sensitivity with operation at the nanometer scale. In this work, we exploit specific interactions between AFM tips functionalized with enzymes, antibodies and microparticles for development of nanobiosensors used in the detection of environmental contaminants and autoimmune diseases. The nanobiosensors are studied using theoretical models (molecular docking and molecular dynamics simulations), force measurements between AFM tips and target-molecules and variations in the deflection of the microcantilevers when exposed to a diversity of compounds and humidity. We show that the specific, biorecognition force plays a crucial role in the higher sensitivity of the nanobiosensor, thus opening the way for the design of similarly engineered tips for detecting herbicides, volatile organic compounds and other analytes [1-7]. Computational methods were used to determine the binding energies associated with the enzyme-herbicide interactions which were compared with experimental results for adhesion forces [8, 9].

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

13. Recent progress on molecular modeling of bio-molecular systems

H. M. Petrilli
Instituto de Física, Departamento de Física de Materiais e Mecânica – Universidade de São Paulo.

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Here we review some recent achievements performed at our group in the Instituto de Física da Universidade de São Paulo on the theoretical modeling of bio-molecular systems with potential applications as biosensors. The work is performed in the framework of the INEO and also with experimental collaborators from the Instituto de Química da Universidade de São Paulo and Europe. An overview of the procedures used in the simulation of some examples will be made.

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


Focus Session 6: Synthesis, Characterization and other studies related to molecules and thin films
Chair: Roberto Mendonça Faria

14. Polypyrrole nanostructured fibers for solid phase microextraction

E. F. Jasinski (1, 2), I.M. Santos (1), B.L.D. Grilo (1), P.J. Manso (1) and M.L. Sartorelli (1)
(1) LabSiN - Departamento de Física – Universidade Federal de Santa Catarina.
(2) Campus Araranguá – Universidade Federal de Santa Catarina.
e-mail: everton.fabian@ufsc.br

This study aimed at the development of new fibers for use in solid phase microextraction technique (SPME) [1]. The fibers are formed by a pyrrole (PPy) polymer layer that coats nitinol wires (nickel-titanium alloy). This work consists in obtaining a nanostructured coating using the method of nanosphere lithography combined with electrodeposition technique. A methodology was developed based on a original vertical deposition process [2], which ensures the production of large thick and homogeneous colloidal masks over large cylindrical areas. We present the process of fabrication and characterization of nanostructured coatings obtained by nanosphere lithography and electropolymerization of PPy/ DBSA on NiTi wires. The extraction capacity of the fiber was tested for coffee and beer. The performance of the nanostructured fibers was shown to be up to 5 times higher than compact fibers of the same mass for n-hexadecanoic acid and 2.5 times for caffeine.

We acknowledge support from INEO and CNPq.
15. Control of the Energy Levels in Donor-Acceptor Copolymers
P. C. Rodrigues
Departamento Acadêmico de Química e Biologia – UTFPR

Invited Talk
Chair: Roberto Mendonça Faria

16. White emission in polymeric light-emitting diodes

Atvars, T. D. Z.
Grupo de Fotofísica e Fotoquímica - Universidade Estadual de Campinas
e-mail: tatvars@iqm.unicamp.br

This work describes a new approach for producing white-emitting electroluminescent diode using an electroluminescent polymer in a one layer, which was obtained with a single layer of an electro-active greenish component (poly[(9,9-dioctylfluorene-2,7-diyl)-alt-(9,9-di(pent-4-en-1-yl)fluorene-2,7-diyl)]) (PFP) and an external photoluminescent (PL) layer of a red-emitting material, poly[2-methoxy-5-(3′,7′-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV), in a diode configuration of MDMO-PPV/glass/ITO/PEDOT:PPS/PFP/Ca/Al. This was the first example that we showed of a quite general concept. To demonstrate this concept was quite general, several other examples were presented. White emission was produced by adjusting the absorbance of the layer thickness and the blue-greenish component until it reached the CIE white coordinates. The photophysical and morphological properties of the materials in this systems under the same conditions of the device were detailed.

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