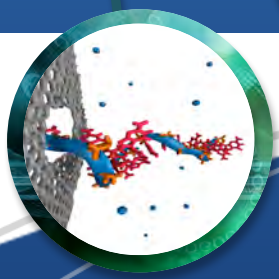
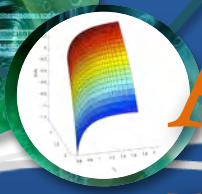
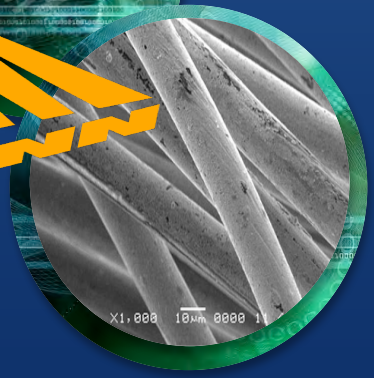




8th PREM Annual Meeting



November 18, 2011
University of Puerto Rico at Humacao

AGENDA

Friday November 18, 2011

9:00 AM Advisory Board meets in Palmas del Mar, Humacao, PR.

10:00 AM Group Meetings, PREM and UPR Faculty and Students: PREM Laboratories at UPRH

12:00 M Lunch: Faculty, Students and Advisory Board: Hall Physics Laboratories, Natural Sciences Building, UPRH

1:30 PM **Mathematical Modeling and Simulation of Materials** Group Meeting with members of Advisory Board: CNL 102

Moderator: Preston Moore

Brief Research Presentations (Progress Reports):

1. *A Nonlinear Model of an Actuator*, Pablo Negrón, UPRH (O1)
2. *Modeling and Simulations of Polymers and CNT Composites*, José Sotero, UPRH (O2)
3. *Layer Charge and Potential Distributions in Multilayer Graphene Films*, Natalya Zimbovskaya, UPRH (O3)

Discussion and Plans for the Future

3:00 PM **Materials for Nano-electronic Devices and Sensors Group** with members fo Advisory Board, CNL 112

Moderator: Jorge J. Santiago-Avilés

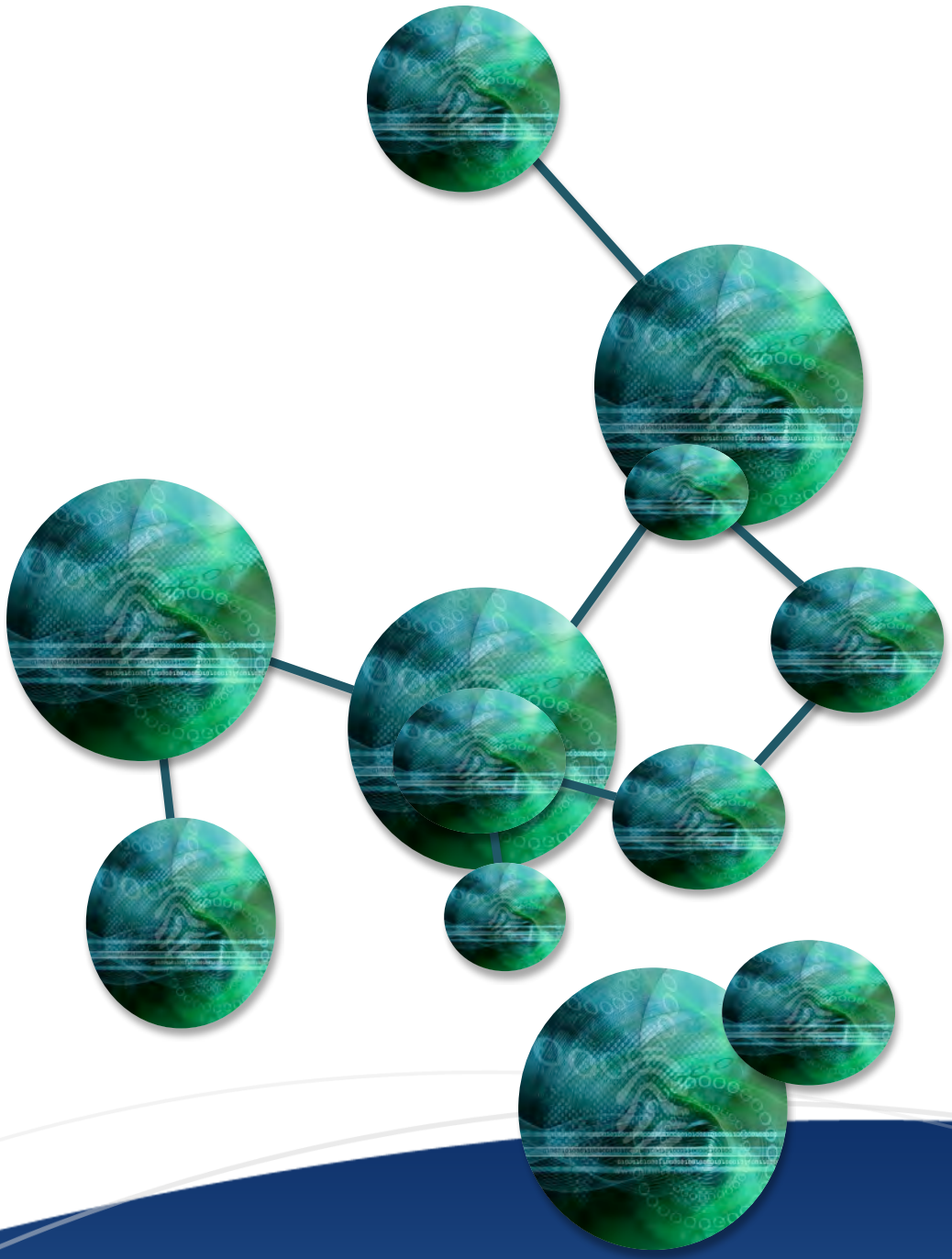
Brief Research Presentations (Progress Reports):

1. *Biochemical Pathways and Signals as Constructs for Electrochemical Sensors*, Ana Guadalupe, UPR-RP
2. *Fabrication of Palladium Nanoscale Structures for Hydrogen Sensing Applications, Wilfredo Otaño and Víctor Pantojas, UPRC (O4)*
3. *PEDOT-PSSA Nano-ribbon based Devices and UV doping of CVD Graphene, Nicholas Pinto, UPRH (O5)*
4. *Characterization of Electrospun Nitride Nanofibers,* Idalia Ramos, UPRH (O6)

Discussion and Plans for the Future

4:30 PM Student Poster Session with Refreshments at Natural Sciences Building Lobby

5:30 PM Advisory Board Meets to Write Report



Oral Presentations

O1 **A nonlinear model of an actuator**

Pablo V. Negrón[1] and Eva Campo[2]
[1]Department of Mathematics, University of Puerto Rico at Humacao
[2]Laboratory for Research on the Structure of Matter, University of Pennsylvania

We present two models based on the theory of nonlinear elasticity of a photoactuator consisting of a mixture of a polymer matrix with carbon nanotubes. Both models are generalizations of the one proposed by Ahir and Terentjev (2015) in which the actuation mechanism is modeled as a contraction of a given carbon nanotube in response to an external stimuli. In the first model, a slight variation is introduced in the projection onto the axis of the the pre-strain. This new computation improves the result reported in Ahir and Terenjev for carbon nanotube photo-contraction when a 10% pre-strain is applied. In our second model we use a nonlinear constitutive equation to describe the mechanical response of the composite. We show that by a suitable selection of the parameters in the model, consistent with the average constitutive parameters (Young modules) reported in the literature, we can further improve on the average carbon nanotube contraction for a 10% pre-strain threshold.

O2 ***Modeling and Simulations of Polymers and CNT Composites***

José Sotero and Pablo Negrón
Department of Mathematics, University of Puerto Rico at Humacao

The UPR-PENN-PREM's computational mathematics group is addressing the study of properties of composites of carbon nanotubes (CNT) and polymers being done by experimentalists working under the same project using continuous as well as discrete models. We study photo actuation effects on composites of CNT's with a polymer via macroscopic models from nonlinear elasticity. First, we improved on the results of Ahir and Terentjev regarding the predicted average compression ratio for CNT's, that induce a change in mechanical behavior due to actuation at a certain pre-strain. On another project, we study photo actuation properties of composite fibers that have been produced in the laboratory by the electro-spinning technique. Using an "inverse method" that employs the deformation of the fiber obtained from digitized pictures of the bended fiber, the corresponding internal forces and torques in the fiber are computed. We are also using the study of the structure of the CNT-polymer composites as the first test case for a Graphical User Interface (GUI) for molecular dynamics simulations called *NanoDevCAD*. This new application will serve as a front end to commonly used molecular dynamics simulation software such as GROMACS and NAMD running both locally or remotely on high performance servers. *NanoDevCAD*'s design is based on the experience gathered while collaborating with our partners at UPENN and USP as well as GUI plugins that our group has develop for the VMD molecular graphics software. The first prototype of the application is able to configure a MD simulation of a swCNT-PMMA-solvent mixture.

O3

Charge screening in few-layer graphene films

Natalya A. Zimbovskaya[1] and Eugene Mele[2]
[1]Department of Physics and Electronics, University of Puerto Rico at Humacao
[2]Department of Physics and Astronony, University of Pennsylvania

We present a non-linear Thomas-Fermi theoretical model, which describes the charge screening in the system including two charged substrate layers separated by a few-layered graphene film. We show that by increasing the charge at the interfaces the system could be turned from the weak screening regime where whole film responds to the external charge to the strong screening regime where the external charge is screened by a surface charge distribution confined to the bounding graphene layers. The transition from weak to strong screening is shown to turn on relatively quickly, and it happens when the applied external charge/external field reaches a certain crossover magnitude. The possibilities for experimental observation of the predicted crossover are discussed.

O4 **Fabrication of Palladium Nanoscale Structures for Hydrogen Sensing Applications**

W. Otaño and V. Pantojas; University of Puerto Rico at Cayey

Abstract:

Palladium (Pd) metal is one of the most prominent materials studied for the detection of hydrogen gas. Hydrogen rapidly dissociates on its surface and diffuses into subsurface layers forming palladium hydride with consequent changes in optical, mechanical and electrical properties that are easily detected. Materials with nanoscale morphologies are promising to improve sensor performance as they provide large surface areas for adsorption, and smaller crystallite size reducing the time needed for "bulk" diffusion. The amount of sites available for hydrogen adsorption per Pd atom is also higher in the surface and subsurface layers resulting in higher sensitivity. In this project, Pd nanoribbons and nanoshells are prepared by magnetron sputtering deposition on top of the mat of polymer fibers, which act as a template that shapes the morphology of the palladium being deposited while providing support to the metallic scaffold that is created. Sputtering is a line-of-sight deposition process and the fibers become a variable angle-substrate for the incoming Pd flux. A larger amount of palladium is deposited on top of the fiber where the incoming flux is perpendicular to the surface compared to the sides where the flux is incident at a glancing angle. The top and sides of the fibers shadow their bottom parts closer to the substrate preventing any substantial deposition there. The end result of the deposition is the formation of Pd nanostructures, thicker in the middle region than at the edges, with a large void network. Process parameters such as deposition time, sputtering pressure, and power can be used to produce nanoshells with different thickness and crystallinity. The high sensitivity and response time shown to 1% or less of hydrogen in nitrogen is understood to result from the reduced dimensions combined with this unique nanostructure. A description will be given of the conductance changes with hydrogen concentration as result of the competing mechanisms of percolation and scattering. This work shows the use of nanotechnology combined with unique processing approaches to produce new sensor geometries with different behavior and morphology than simple thin film or wire approaches.

O5 ***PEDOT-PSSA Nano-ribbon based Devices and UV doping of CVD Graphene***

Nicholas Pinto
Department of Physics and Electronics, University of Puerto Rico at Humacao

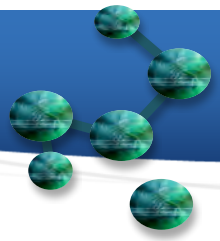
Our collaborative research this past year has included the study of two organic conductors, PEDOT-PSSA nano-ribbons and CVD graphene. The focus was to electrically characterize them primarily for use in various devices and sensors. The conducting polymer PEDOT-PSSA is commonly used as interconnects in devices mostly in the form of thin films. We have successfully used the electrospinning technique to fabricate PEDOT-PSSA nano-ribbons and used them for gas (alcohol, NH_3, HCl and NO_2) sensors and Schottky diodes. Due to the large surface to volume ratio and small quantity of active material used in their fabrication, these sensors have a similar or faster response time when compared to alcohol sensors based on PEDOT. Increasing the size of the alcohol molecule leads to longer response times, which is attributed to slower diffusion of the larger molecule into the polymer. The sensors were annealed in air at 70°C and used to sense NH_3, HCl and NO_2 gas. The response time for NH_3 was faster than HCl, and the sensors showed a large initial response to NO_2 at room temperature which is very desirable, as some NO_2 gas sensors only operate at elevated temperatures. Even though the sensors were exposed to such toxic and corrosive gases they did not get damaged, and after annealing they were reusable implying that the PEDOT-PSSA nano-ribbons are very robust. When used as a Schottky diode, we found that the diode parameters like the rectification ratio, the ideality parameter and the turn-on voltage could be tuned with a back gate bias making the device multifunctional. During the summer (2011) visit to PENN, we worked on CVD graphene with a post-doc at Johnson's lab. Upon return to UPR, CVD graphene was electrically characterized in a field effect transistor configuration in the presence of UV light. Our results indicate that UV light can dope graphene in a reversible fashion.

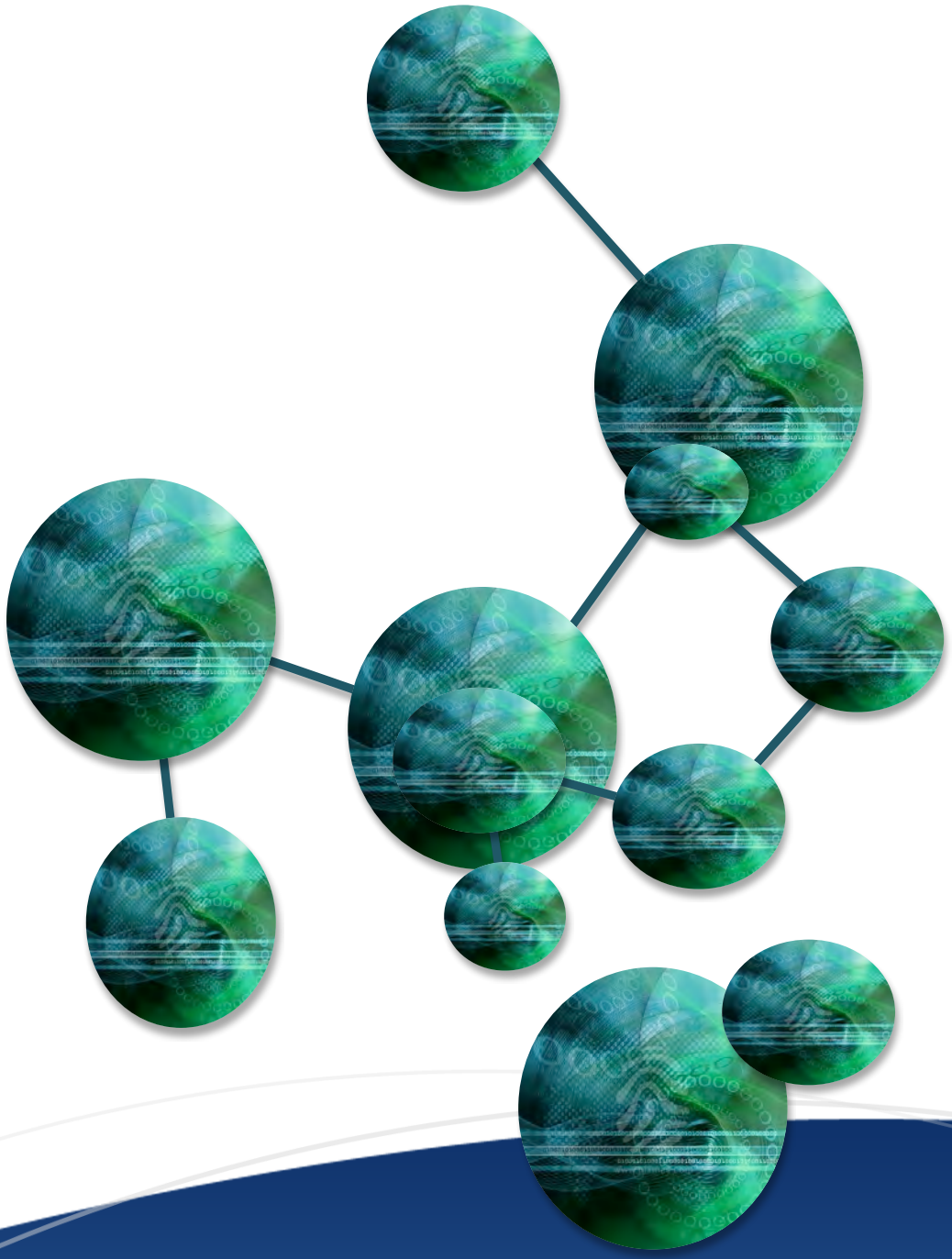
O6 ***Characterization of Electrospun Nitride Nanofibers***

Idalia Ramos
Department of Physics and Electronics, University of Puerto Rico at Humacao

Group III-nitrides are promising semiconductors with a wide direct band gap that covers a broad spectral range from infrared to deep UV (0.7 eV for InN to 6.2 eV for AlN). Binary, ternary and quaternary III-nitrides alloys of In, Al, Ga and N are important materials for optoelectronics, high temperature and high-power devices. We have fabricated GaN, AlN and In_xGa_{1-x} nanofibers using the electrospinning technique and nitridation under ammonia gas flow. The preparation, XRD, electrical and optical characterization of the fibers were done at UPRH. High resolution SEM and TEM were done at PENN during summer visits. GaN nanofibers are polycrystalline wurtzite-polymorph and photoconductive. X-Ray Diffraction analysis confirms dominant hexagonal 101-wurtzite preferential overall orientations. TEM analysis of GaN shows high orientational competition amongst grains. Current efforts focus on understanding nucleation and grain growth during the thermal treatment following electrospinning.

Our group has also produced AlN nanofibers with hexagonal wurtzite structure and a bandgap of approximately 6 eV. In a more recent effort we synthesized $In_xGa_{1-x}N$ nanofibers. Results confirm the formation of crystalline fibers.





Poster Session

P1 **Fabrication and characterization of poly (vinylidene fluoride-trifluoroethylene)/ poly (3-hexylthiophene) (PVDF-TrFE/P3HT) nanofibers via electrospinning**

William Serrano and Nicholas .J. Pinto.
Department of Physics and Electronics, University of Puerto Rico

The electrospinning technique has been used to fabricate nanofibers of PVDF-TrFE/P3HT blends in tetrahydrofuran (THF). Although many investigations of PVDF-TrFE and P3HT have been reported in the literature, mostly in the form of thin films, this work presents a new method of obtaining relatively long nanofibers of this material. Nanofibers have an inherently high surface to volume ratio compared to thin films and could serve as better sensors. Several concentrations of PVDF-TrFE in THF were prepared and electrospun either in the pure form or blended with P3HT. At very low concentrations it was difficult to obtain fibers in the pure material. Blending the solution with P3HT resulted in the fabrication of long fibers without the beading effect that is seen in the fibers formed from pure solution. The fiber diameters were found to increase for the higher concentration blends. UV-VIS spectra of the pure and the blended solutions show no significant differences, which imply a homogeneous blend of the two polymers in solution. A field effect transistor (FET) was fabricated and tested with the 1wt% blended solution. The device characteristics show *p*-type behavior with charge mobility of ~10^{-5} cm^2/V-S.

P2 **Aluminum Nitride Nanofibers fabricated using Electrospinning and Nitridation**

Idalia Ramos[1], Xenia E. Barbosa[1] and Jorge J. Santiago[2]

[1]Department of Physics Applied to Electronics, University of Puerto Rico at Humacao; [2] Department of Electrical Engineering, U-PENN

Aluminum Nitride (AlN) and other nitride semiconductors are important materials in the fields of optoelectronics and electronics. AlN nanofibere were synthesized using a precursor solution containing aluminium nitrate nano-hydrate $(Al(NO_3)_3 \cdot 9H_2O$ and cellulose acetate (CA). The electrospinning method and subsequent heating treatment were used to fabricate AlN nanofibers. The electrospun nanofibers were heated in nitrogen (N_2) to eliminate the polymer and produce Al_2O3. Then, they were nitridized in ammonia (NH_3) gas at a temperature of 1200°C. Scanning Electron Microscopy (SEM) observations demonstrate the production of fibers with diameters ranging from a few nanometers to several micrometers. X-Ray Diffraction (XRD) and UV-VIs analysis show the production of AlN nanofibers with hexagonal wurzite structure. Current-Voltage measurements on a single AlN fiber with gold contacts suggest the formation of Schottky barriers and high sensitivity to ultra-violet light. The fabrication method and results from the fibers characterization will be presented.

P3 **Electrical characterization of CVD graphene**

Yarely Davila[1], Nicholas J. Pinto[1], Zhengtang Luo[2] and A.T. Charlie Johnson Jr.[2]

[1]Department of Physics and Electronics, University of Puerto Rico at Humacao; [2]Department of Physics and Astronomy, University of Pennsylvania

Graphene is a one atom thick carbon sheet that can be obtained via exfoliation of graphite or via chemical vapor deposition (CVD). By using a very simple shadow masking technique, gold contact pads were evaporated over the graphene thereby eliminating chemical etching that is required when using photolithography and often leads to sample contamination. We electrically characterized CVD graphene in a FET configuration under different experimental conditions that include UV exposure, gas sensing and temperature. Our conductivity measurements yielded a carrier mobility of up to 3000 $cm^2/V\text{-}s$ for some devices. Exposure to UV leads to the doping of graphene in a very controlled manner. The doping level could be maintained indefinitely in vacuum or could be completely reversed by slight heating in air without loss of device performance. The FET's were also tested at different temperatures with little change in the characteristic curves. Exposure to ammonia gas *n*-doped graphene while exposure to NO_2 *p*-doped it. Results of these experiments will be discussed in this poster.

P4 **Electrical characterization of field effect transistors made from C-nanotubes covered with poly(3-hexylthiophene)**

Luis O. Pomales-Velázquez[1], Nicholas J. Pinto[1], Michael Lerner[2] and A.T. Johnson Jr.[2]
[1]Department of Physics Applied to Electronics, University of Puerto Rico at Humacao; [2] Department of Physics and Astronomy, U-PENN

Organic thin-film transistors (OTFT's) were fabricated using a thin film of regio-regular poly(3-hexylthiophene-2,5-diyl) cast from a 0.5 wt% solution in $CHCl_3$. By characterizing the material transport properties through IV curves, we compare the performance between devices with percolating networks of CVD grown single-wall carbon nanotubes (SWNT's) between the source and drain electrodes and ones without it. The SWNT's are used as a way to shorten the effective mean distance between source and drain terminals. We found that the devices made with SWNT's do not exhibit drain-source current saturation and have a carrier charge mobility of $1.2x10^{-2}$ $cm^2/V.s$ and an on/off ratio of 9; while the device without SWNT's it show clear saturation with a carrier charge mobility of $8.6x10^{-4}$ $cm^2/V.s$ and an on/off ratio of 870. The devices made with nanotubes appear to lose the saturation behavior due to the large off state current but they show a ~13X increase in the mobility.

P5 **Conducting threads for devices and sensors**

Manuel Bonilla[1], Anamaris Meléndez[1], Idalia Ramos[1,] Nicholas Pinto and Yajaira Sierra-Sastre[2]

[1]Department Physics & Electronics, University of Puerto Rico at Humacao ; [2]i Fyber, LLC, 950 Danby Road, Suite 300, Ithaca, NY 14850-1485

Conductive threads are attractive in smart textiles industry. It's most simple application is to conduct charge; another application of the conducting treads could be in the use of gas sensors. Nylon threads were made conductive by an aqueous solution of (Ag; Ag/ZnO NW_s Au NP`s) and with PEDOT-PSSA for cotton threads by a series of dip coatings. The threads were subsequently dried in air at 80°C. The silver coated threads were tested in the presence of methanol gas and had a response time of 113 seconds and a recovery time of 135 seconds for the control Ag sensor. The response time was 55 seconds and the recovery time was 52 seconds for the zinc oxide coated sensor. The conducting threads were electrically characterized and had a resistance of 1.2kΩ for the PEDOT-PSSA coated thread and a resistance of 2.3 Ω for the zinc oxide coated thread. The PEDOT-PSSA coated threads were tested as cables in a simple circuit and were found to work satisfactorily. The conductive threads combine strength, flexibility and ease of preparation making them good candidates for use in smart textiles.

P6 **Effect of Sb doping on Electrical Properties of SnO_2 Nanofibers**

Maritza Reyna[1], Idalia Ramos[1], Nicholas Pinto[1] and Jorge J. Santiago Avilés[2]
[1] Department of Physics and Electronics, University of Puerto Rico at Humacao
[2] Department of Electrical Engineering, University of Pennsylvania

Tin Oxide (SnO_2) is a semiconductor with important properties for electronic and optical applications. The addition of antimony (Sb) can enhance the conductivity of SnO_2. Electrospinning is an easy and fast method of producing nanofibers using a polymeric precursor solution and a high voltage source. This study started with the preparation of a precursor solution composed of Tin (IV) Chloride dissolved in Propanol and 2-Propanol, Cellulose acetate (CA) dissolved in a mixture of Acetone and Dimethyl Acetamide (DMA), and Antimonium (III) Chloride. After electrospinning the fibers were sintered in air for 2 hours at 700° C to decompose the polymer and produce Sb:SnO_2. Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Energy Dispersive Spectroscopy (EDS), and X-Ray Diffraction (XRD) tests were done to verify the size, composition and crystallinity of the nanofibers. The SEM and AFM analyses confirmed the production of continuous fibers with diameters ranging from 30 nanometers to several micrometers. EDS confirmed the presence of the Sn, Sb and O peaks. The XRD spectra showed the peaks characteristic of Sb:SnO_2 with rutile structure. Electrical measurements were done to a single Sb-SnO2 nanofiber with gold electrodes and as function of increasing and decreasing temperature to verify its conductivity. This analysis were done to these concentration of Sb 7.8% (original recipe), 10%, 13%, 15% showing that increasing Sb doping best enhance the conductivity of the nanofiber.

P7 **The study of Polydimethylsiloxane (PDMS) thin-film surface roughness properties and its resistance in high temperature and UV light resistant applications**

Gabriel A. Calderon Ortiz[1] and Josee Vedrine-Pauléus[2]
[1]Petra Mercado height school, Humacao; [2]Department of Physics Applied to Electronics, University of Puerto Rico at Humacao

Polydimethylsiloxane (PDMS) is an organic polymer with the basic physical properties of an elastic solid, and viscoelastic material, which means that it has a defined physical form, but can be molded to take the shape of any object. PDMS has many important and common applications such as contact lenses, and has also found wide use in nanofabrication and microcontact printing techniques. Our study investigates the surface roughness properties of this versatile polymer when fabricated as thin films, when cured at elevated temperatures, and when treated under ultraviolet light. We use an atomic force microscope (AFM) to analyze the nanoscale surface features-the surface roughness (R_a) to provide a quantifiable analysis under these experimental conditions, and show that UV exposure and high temperature drives degradation, but the overall degradation is substantially lower at thin films surfaces. Additionally, we found an interesting but inverted correlation in degradation for films heated at 200 ˚C and 250 ˚C, with respect to surface roughness and film thickness compared with other thin films.

P8 **Synthesis of ZnO fibers based on PVA for gas sensing applications**

Laura Amadeo, Nelson Granda, Victor Pantojas, Wilfredo Otaño
Math-Physics Department, University of Puerto Rica at Cayey

Zinc Oxide (ZnO) is an n-type semiconductor with the potential to be used as gas sensing element because of its favorable properties such as good transparency and high electron mobility. We produced ZnO fibers by electrospinning a mixture containing zinc acetate (ZnAc), and poly(vinyl alcohol)(PVA) in acidic and basic media. Zinc oxide forms after thermal treatment at 700°C in air. The fibers were characterized by Scanning Electron Microscopy (SEM), and X-rays diffraction (XRD). Our preliminary results show that fiber morphology was pH dependent. The average diameter size for fibers from acidic media was 0.126nm while for fibers from basic media was 0.146nm. XRD analysis confirmed the presence of a pure ZnO crystalline phase. The characterization of the fibers as hydrogen sensors elements in underway.

P9 **On the determination of photo-actuation effects for polymer/MWCNT composited fiber based cantilever**

Aixa de Jesus Espinosa and Pablo V. Negron
Department of Mathematics, University of Puerto Rico at Humacao

Composite fibers combining MWCNT and Sodyum dodecyl sulfate (SDS) have been produced in the laboratory by the electrospinning technique. These fibers exhibit photo-actuation properties (S. Rosa, J.P. Crespo 2011). In this project we use a model from nonlinear elasticity to determine the forces and internal torques that induce the photo-actuation effect. We use an inverse method in which starting from the the deformation of the fiber, obtained from digitized pictures of the bend fiber, the corresponding forces and torques are calculated.

P10 **Molecule classifier system**

Melissa López, Mirgery Medina, José O. Sotero Esteva
Department of Mathematics, University of Puerto Rico at Humacao

Graph theory has been used to model molecules for many years, making chemical graph theory a well established field of study. But, compared to the total volume of molecular dynamics software, those intended for the analysis of molecules and trajectories in molecular dynamics simulations based on graph theory results is scarce.We present a first prototype for an automated classifier of molecules represented in coordinate files for molecular dynamics simulations. The application uses a graphical interface based on the *QT GUI* tools. It represents chemical graphs using the *networkx* package. The application serves as a tool to read information from coordinate data that represent many molecules. It separates them into categories according to graph isomorphisms and similarities. The user may save some or all of them for later use. This software will be used as a basis for the analysis of trajectories produced by molecular dynamics simulations.

P11 **A nonlinear model of an actuator**

Pablo V. Negron[1] and Eva Campo[2]
[1]Department of Mathematics, University of Puerto Rico at Humacao; [2] LRSM, U-PENN

We present two models based on the theory of nonlinear elasticity of a photo-actuator consisting of a mixture of a polymer matrix with carbon nanotubes. Both models are generalizations of the one proposed by Ahir and Terentjev (2005) in which the actuation mechanism is modeled as a contraction of a given carbon nanotube in response to an external stimuli. In the first model, a slight variation is introduced in the projection onto the axis of the pre-strain. This new computation improves the result reported in Ahir and Terentjev for carbon nanotube photo-contraction when a 10% pre-strain is applied. In our second model we use a nonlinear constitutive equation to describe the mechanical response of the composite. We show that by a suitable selection of the parameters in the model, consistent with the average constitutive parameters (Young modulus) reported in the literature, we can further improve on the average carbon nanotube contraction for a 10% pre-strain threshold.

P12 **Prototype for CNT-polymer composites simulation.**

Mirgery Medina, Carlos Cortés, Melissa López, Frances Martínez, Giovanni Casanova, José O. Sotero Esteva
Department of Mathematics, University of Puerto Rico at Humacao

Molecular Dynamics is being used for simulating prototypes of nanodevice components that combine CNT, graphene and/or polymers. Students participating in the UPR-PENN-PREM program have worked on research with simulations carbon allotrope-biopolymer hybrids. For example, DNA translocation through graphene nanopores was studied last summer. There are plenty of difficulties with creating a system for simulations, especially if it has many different molecules or if you need to create the coordinate, topology and configuration files from scratch.
Based on those experiences, our group prepared plug-in for VMD a few years ago, called MoSDAS, which facilitated the process of building these systems or create coordinate files and topology files. The problem it had was that the TKinter library we used does not have a good variety of widgets to facilitate user-software interaction. In this occasion we will be presenting a prototype based on the QTGui library so that it can run independently from VMD. With this prototype we will demonstrate how to create a composition of CNT and PMMA and we will also demonstrate how to easily create different configuration files to be used with the NAMD simulator.

P13 **Electrochemical and Spectroscopical Studies on the Physicochemical Interactions of Bovine insulin and Meldola's Blue**

Maria del Mar Garcia, Liz Hernández Borrero and Ana R. Guadalupe
Department of Chemistry, University of Puerto Rico, Rio Piedras

Amyloid structures are related to severe health problems such as Alzheimer's disease and Creutzfeldt–Jakob disease. Bovine insulin, an inexpensive two chain peptide can form amyloid structures. To study the physicochemical interactions between bovine insulin and Meldola's Blue, the electrochemical and spectroscopy studies were carried out in Brinton Robinson buffer (pH 2.0) using $3x10^{-6}$ M Meldola's Blue in the presence of bovine insulin. Electrochemical characterization involved Cyclic voltammetry (CV), and Osteryoung's square wave voltammetry (OSWV), while spectroscopic characterization involved Circular dichroism (CD), UV-visible, and fluorescence spectroscopic studies. Bovine insulin fluorescence spectra showed an emission peak at 305 nm, when excited at 257 nm and 275 nm. We observed the energy transfer from phenylalanine to tyrosine, enhancing the emission intensity at 305 nm. The spectrum of bovine insulin in the presence of Meldola's Blue showed a decrease in the emission intensity at 305 nm, when Meldola's Blue concentration increases. CV of Meldola's Blue showed a diffusion and absorption controlled electrode reaction using glassy carbon working electrode. OSWV results confirmed that $3x10^{-6}$ M Meldola's Blue with bovine insulin was adsorbed to glassy carbon electrode surface. Experimental results showed changes in the electrochemical behavior of Meldola's Blue in the presence of different concentrations of bovine insulin. These results evidence the interaction between Meldola's Blue and bovine insulin.

P14 **Electrochemical characterization of ferrocene chalcones derivatives within nafion and b-cyclodextrin**

Rahul Singhal, Rocio del A. Cardona, Kenneth Hernandez and Ana R. Guadalupe
Department of Chemistry, University of Puerto Rico, Río Piedras

In the present work, we have studied the electrochemical behavior of various ferrocene chalcones (Fc's) [1-ferrocenyl-3-(G)-prop-2-en-1-one], immobilized in nafion and nafion/ b-cyclodextrin. 'G' represents 4-nitrophenyl, 3-nitrophenyl, 4-N,N-dimethylaminephenyl, 4-methoxyphenyl, 4-chlorophenyl, 2-fluorophenyl, 3-fluorophenyl, 2-pyridinyl, 3-pyridinyl, and 4-pyridinyl. In solution the formal potential for G = 4-methoxyphenyl was observed as 680 ± 2.0 mV, while the formal potential of 376.5 ± 5 mV and 389 ± 5.0 mV was observed in the presence of nafion and nafion/b-cyclodextrin, respectively. The apparent diffusion coefficients of the studied ferrocene chalcones were found to be the order of 10^{-9} – 10^{-10} cm^2/s, when immobilized within nafion. The detailed electrochemical results of Fc's in the presence of b-cyclodextrin will be presented during the meeting.

P15 **Development of an electrochemical biosensor for the detection of an ADP-Ribosylating Toxin, Exo A from *Pseudomonas aeruginosa***

Yanira Enríquez, Yashira Negrón and Ana R. Guadalupe.
Department of Chemistry, PO Box 23346, University of Puerto Rico, Río Piedras Campus, San Juan, PR 00931-3346

Pseudomonas aeruginosa (PA) is an opportunistic pathogen of clinical relevance. It secretes different virulence factors (such as enzymes and toxins) that are capable of causing infection. Exotoxin A (Exo A) is an extracellular toxin that PA produces and catalyzes the ADP-ribosylation of the eukaryotic elongation factor-2 (eEF2), inhibiting the RNA translational process and subsequently decreasing protein synthesis. We are interested in designing an electrochemical biosensor for the detection of Exo A. A free radical copolymerization of Styrene and NAS has been done in a range of 10:90 to 90:10 (Sty:Nas) molar ratios. These copolymers were characterized by FT-IR and HPLC-UV and will be used to generate a film on carbon surfaces to anchor a β-NAD^+ electroactive analog. Ferrocene-labeled NAD^+ (Fc-NAD^+) was prepared by attaching Ferrocene Succinimide (Fc-NHS) to the primary amine in the adenine moiety of the cofactor. This Fc-NAD^+ was characterized by H^1-NMR, CV and OSWV. The electrochemical analysis of Fc-NAD showed chemical reversibility and electrochemical quasi-reversibility. Presently we are working on anchoring the Fc-NAD^+ to the glassy carbon electrode surface using the 75:25, 50:50 and 25:75 (Sty:NAS) copolymer. Our OSWV results showed more current response when using copolymer 25:75 (Sty:NAS) when compared with 75:25 while a stronger attachment to the surface was observed for copolymer 75:25. The next step in our project is optimizing the attachment of Fc-NAD^+ to the electrode surface and separate, purify and characterize eEF-2 from *Saccharomyces cerevisiae* yeast. Our final goal is the electrochemical monitoring of the ADP-ribosylation process mediated by Exo A in vitro.

P16 **Microcontact Printing on Gold to Study the Interactions of Thiol Compounds**

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The interaction of thiol molecules when gold surface is modified using microcontact printing technique was studied by atomic force microscopy (AFM) and X-ray diffraction (XRD). The model was developed using polydimethylsiloxane (PDMS) as the stamp and the thiol as the ink. The results using alkanethiols or ferrocene thiols will be presented. We will continue to study other organic and organometallic compounds of interest.

P17 **A nonlinear model of an actuator**

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We present two models based on the theory of nonlinear elasticity of a photoactuator consisting of a mixture of a polymer matrix with carbon nanotubes. Both models are generalizations of the one proposed by Ahir and Terentjev (2015) in which the actuation mechanism is modeled as a contraction of a given carbon nanotube in response to an external stimuli. In the first model, a slight variation is introduced in the projection onto the axis of the the pre-strain. This new computation improves the result reported in Ahir and Terenjev for carbon nanotube photo-contraction when a 10% pre-strain is applied. In our second model we use a nonlinear constitutive equation to describe the mechanical response of the composite. We show that by a suitable selection of the parameters in the model, consistent with the average constitutive parameters (Young modules) reported in the literature, we can further improve on the average carbon nanotube contraction for a 10% pre-strain threshold.

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