PREM

Partnership for Research and Education in Materials

9TH ANNUAL MEETING

9TH NOVEMBER 16, 2012

EMBASSY SUITES HOTEL – ISLA VERDE

9th PREM ANNUAL MEETING

November 16, 2012

Embassy Suites Hotel, Isla Verde, Carolina, P.R.

PROGRAM

9:15 - 10:00 AM **Registration & Breakfast**

10:00 - 10:05 AM *Welcome Messages*
Idalia Ramos, UPRH, PREM PI
Arjun Yodh, UPENN, PREM Co-PI and Director PENN MRSEC
Andrew McGhie, Associate Director PENN MRSEC

10:05 - 10:15 AM *PREM Update*
Idalia Ramos, **Andrew McGhie**, and **Arjun Yodh**

10:15 - 11:15 AM Basics of IP and University Tech Transfer
Pamela Beatrice,
Center for Technology Transfer, University of Pennsylvania

11:15 - 11:30 AM Coffee break

11:30 - 11:45 AM *Wolffia as a Tool for Education and Research using Molecular Dynamics*
José O. Sotero Esteva, UPR-Humacao

11:45 - 12:00 AM *Super-Capacitors Development: From Electrodes' Materials to Self-Packaged Devices*
Rocío del A. Cardona-Couvertier, UPENN

12:00 - 12:15 PM *Computer Simulations of Wavefronts in Drosophila Embryos and Ion Movement through Porous in EDLC's*
Pablo Negrón, UPR-Humacao

12:15 - 1:30 PM *Working Lunch*

1:30 - *2:00 PM* *Carbon Nanoelectronics: Mimicking Biology to Create Novel* Nanomaterials
Mitchell Lerner, UPENN

2:00 - 2:15 PM *Electrical Response of CVD Graphene to UV Light and Organic Solvents*
Nicholas Pinto, UPR-Humacao

2:15 - 2:30 PM *Electric Charge and Potential Distribution in Twisted Multilayer Graphene*
Natalya A. Zimbovskaya, UPR-Humacao

2:30 – 2:45 PM *Break*

2:45 - 3:00 PM *Fabrication and Characterization of Organic Solar Cell Devices*
Josee Vedrine-Pauléus, UPR-Humacao

3:00 - 3:15 PM *Synthesis of Silver Nanoparticles for SERS Applications*
Wilfredo Otaño, UPR-Cayey

3:15 - 3:30 PM *Characterization of Aluminum Doped Zinc Oxide Thin Films and Nanostructures for H_2 Gas Sensing Applications*
Víctor Pantojas, UPR-Cayey

3:00 - 4:00 PM *Break*

4:00 - 5:30 PM *Student Poster Presentations*

5:30 - 6:30 PM *Advisory Committee meets to write Report*

6:30 PM *Closing*

Oral Research Presentations

Wolffia as a Tool for Education and Research using Molecular Dynamics

José O. Sotero Esteva[1], Mirgery Medina Cuadrado[1], Frances Martínez[1], Carlos Cortés[1], Wensy Cuadrado[1], Melissa López Serrano[1], Robert Johnson[2], and Preston Moore[3]

[1]UPR-Humacao, [2]UPENN, and [3]USciences

Wolffia is a graphical user interface (GUI) front end to software for Classical Molecular Dynamics software: currently NAMD and LAMMPS. With Wolffia a scientist may build mixtures from molecule in its molecule catalog, load them from coordinate files and/or fetch them from coordinates banks such as the Protein Data Bank. CHARMM force field parameters can be easily edited. Periodic boundary conditions may also be set and solvated with several solvents. Minimization, equilibration and test runs can be performed while monitoring changes in the molecule as well as energy and kinetics measurements. All the necessary configuration files cant then be packed to be transferred to high performance servers for production runs.

Wolffia's development began on August 2011. A prototype was presented at our previous PREM meeting. Further development incorporated important suggestions given by our collaborators at USiP and Penn. At this meeting we present our first stable version of the software. We report experiences of it use as a learning tool in workshops for high school students (Experimenta con PREM) and with scientists (Ibersensor 2012). We also report on current work related to the experiments being done by other PREM groups on electrospun nanofibers that contain carbon nanotubes dispersed with sodium dodecyl sulfate (SDS).

Super-Capacitors Development: From Electrodes' Materials to Self Packaged devices

Hitesh K. Sahoo,Jaewan Park, Rocío del A. Cardona-Couvertier, and Jorge Santiago

UPENN

Super-capacitors (Electrical Double Layer Capacitor, EDLC) are energy storage devices that function similarly to conventional capacitors, but instead of accumulating charges on two conductors, it is stored at the interface of a conductor and an electrolyte solution. In general, super-capacitors are classified in two major groups according to the material in the electrode, these are: physical super-capacitors (carboneous materials) and pseudo capacitors, which store charge indirectly through Faradaic chemical processes, but their electrical behavior is like that of a capacitor. Super-capacitors possess the attribute of having large specific capacitance, combined with large power densities (high charge per unit volume and can be charged and discharged quickly). These attributes make small super-capacitors ideal charge storage devices for distributed and embedded applications such as those for coupling or powering small robotic systems, distributed sensors / actuators and bio-medical devices, including those designed to be implantable. One of the drawbacks of super-capacitors is their low energy density in comparison with batteries.

For the past years our research group has invested efforts in decreasing the energy density gap between supercapacitors and batteries. Our efforts include the use of different new carboneous materials as CDC, carbon nano onions, modified single wall carbon nanotubes, and others for the electrodes, as well as, conducting polymers (p-ProDOT and PEDOT) and hybrid devices which combines both, carboneous materials and polymers. We have also explored the effect of the separating membrane on the performance of the devices, and how it can be optimized and the use of LTCC as packaging material for embedding EDLC applications. We will present the results obtained and the remaining challenges in the optimization of super-capacitors.

Computer Simulations of Wavefronts in Drosophila Embryos and Ion Movement through Porous in EDLC's

Pablo Negrón[1] and Andrea Liu[2]

[1]UPR-Humacao, [2]UPENN

In this talk I will describe several collaborations with faculty from the UPENN-PREM program. These projects originated from my visit to UPENN last summer. On the first part of the talk I will describe a collaboration with Andrea Liu which involves the modeling of wavefronts that propagate in Drosophila embryos during mitosis. One of the proposed models by Dr. Liu's group to explain this phenomena is based on mechanical signaling. In this model the embryo membrane is modeled using the equations of elasticity for thin membranes, including the effects of external (dipole type) forces and a damping term. We will show some preliminary results (including a movie) of a computer simulation for the propagation of wavefronts in an ellipsoidal shell. On the second part of the talk I will describe a project in collaboration with Jorge Santiago dealing with various aspects relating to the performance of super capacitors (EDLC). In particular, I will describe briefly a molecular dynamics type model for the motion of an ion into a pore on one of the capacitor's plates. The model is a first step in the problem of studying the observed phenomena of capacitance increase in the EDLC after a certain threshold of applied voltage is reached. Details of the simulations in this case will be presented by the student Aixa De Jesús in the poster session.

Carbon Nanoelectronics: Mimicking Biology to Create Novel Nanomaterials

Mitchell Lerner

UPENN

With their unique electronic, mechanical, and thermal properties, carbon nanotubes and graphene may have a tremendous impact across many scientific disciplines, uniting physics, chemistry, biology and engineering. Both carbon nanotubes and graphene are highly sensitive to ambient conditions since their surfaces are entirely exposed to the environment. This fact can be utilized to tailor a sensor for a particular chemical or protein, such as glucose, or an array of sensors capable of being measured simultaneously that function together in an "electronic nose"-type configuration. Such sensors can be used for generic vapor detection for environmental monitoring applications, specific protein detection for biomedical applications, and even as a UV photodetector. These high sensitivity biosensors could be used in parallel to test a single small volume patient sample for any number of potentially ominous biomarker proteins, thus affording better patient prognoses. These advanced nanobio-hybrid sensor modalities leverage the unique properties of nanomaterials. It may be possible that one day, functionalized carbon-based sensors could produce cost-efficient, easy to implement point-of-care immunosensors

Electrical Response of CVD Graphene to UV Light and Organic Solvents

Nicholas Pinto

UPR-Humacao

In this work a facile shadow mask technique of defining electrodes on graphene grown by chemical vapor deposition (CVD) is presented. This eliminates the use of detrimental chemicals needed in the corresponding lithographic process commonly utilized. Upon exposure to UV light we record a controlled, effective and reversible doping of graphene with minimal impact on charge mobility. The change in charge concentration saturates at ~$2x10^{12}$ cm^{-2} and the quantum yield is ~10^{-5} e/photon upon initial UV irradiation. In a separate study, some of the CVD graphene samples were repeatedly washed with toluene resulting in increasing electron mobility. Current work is underway to fabricate a glucose sensor based on CVD graphene. Results of these and other experiments will be presented.

Electric Charge and Potential Distribution in Twisted Multilayer Graphene

Natalya A. Zimbovskaya[1] and Eugene J. Mele[2]

[1]UPR-Humacao and [2]UPENN

The specifics of charge screening and electrostatic potential spatial distribution in rotationally faulted multilayered graphene films with decoupled layers placed in between charged substrates are theoretically analyzed. The analysis is carried out using a nonlinear Thomas -Fermi approach. It is shown that by varying the areal charge densities on the substrates and/or the thickness of the graphene pack one may tune the screening length in the graphene pack. When the charge densities on the substrates are weak, the screening length is of the same order as the pack thickness, which agrees with semi metallic properties of graphene. When the amount of the donated charge is sufficiently large the screening length reduces indicating the transition to a metallic-like behavior of the graphene layers. The transition is shown to turn on rather quickly, and in occurs when the charge on the substrates/external electric field reaches a certain crossover magnitude.

Fabrication and Characterization of Organic Solar Cell Devices

Josee Vedrine-Pauléus

UPR-Humacao

The fabrication of organic bulk-heterostructure solar devices, and their characterization will be discussed. Organic polymeric blends of P3HT (poly-3-hexyl-thiophene) and PCBM (phenyl-C61-butyric acid methyl ester) are analyzed under basic annealing conditions; in addition we look at the morphologies of solar cell devices and their performance when monolayers of PVDF(TrFE), an organic ferroelectric, is added. We are using AFM and C-AFM techniques to study the nanomorphologies of these blends to better understand how to improve solar cell efficiency.

Synthesis of Silver Nanoparticles for SERS applications

Bryan Vélez, Melissa Morales, William Ortiz, and
Wilfredo Otaño

UPR-Cayey

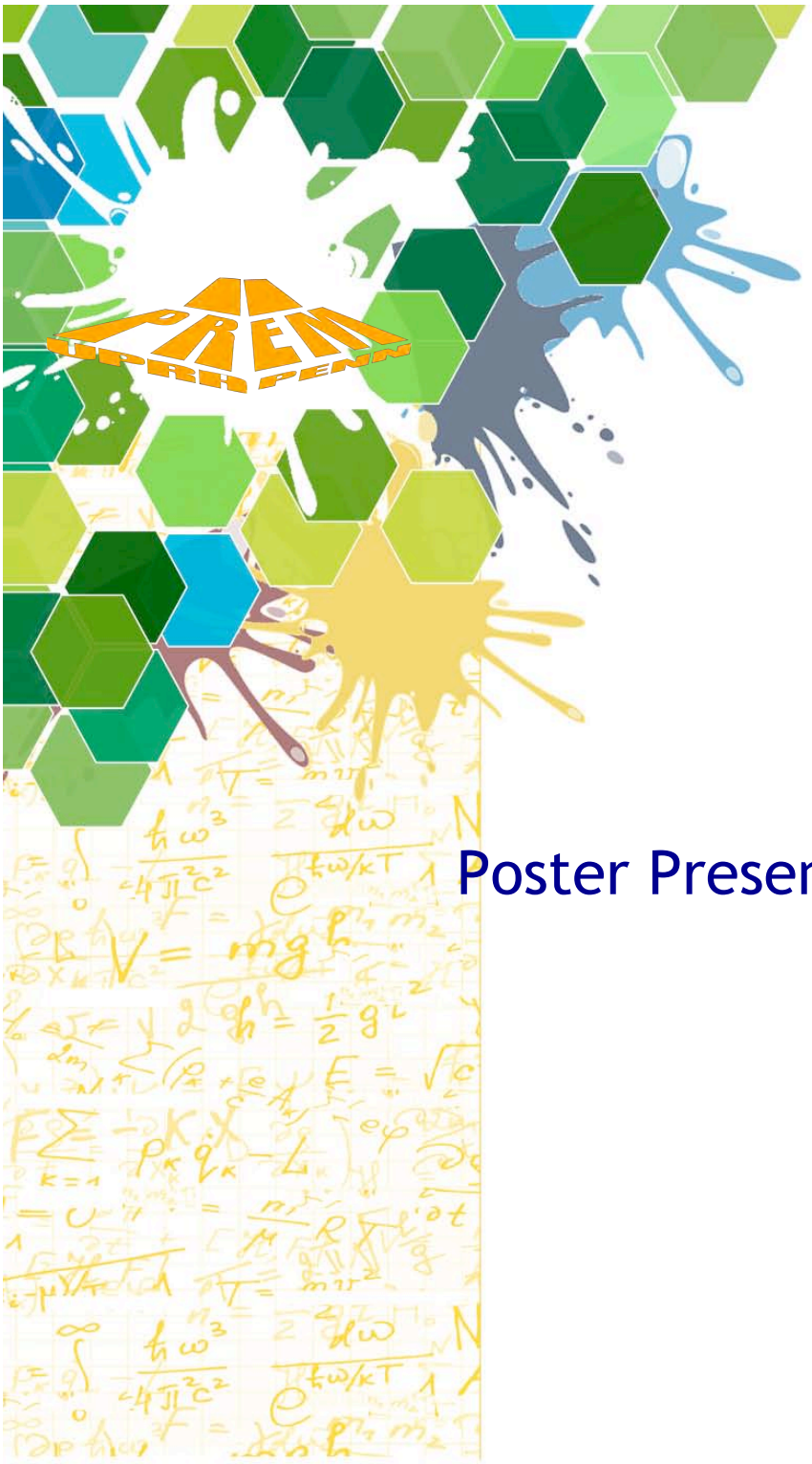
Silver nanostructures are actively studied for photonic applications while ultra-thin films are of interest for interconnections in ultra-large scale integration technology. In both applications, understanding of coalescence and film formation processes are of primary importance when the material is prepared by physical vapor deposition methods. Surface free energies, rate and angle of arrival of material, substrate temperature and energetic bombardment are process parameters that are used to change characteristics-properties of the material ranging from nanomorphology to epitaxy. Silver metallic nanospheres were prepared using the sputtering technique. In this method, several sputtering deposition process parameters were controlled to reduce coalescence of the silver being deposited resulting in the formation of nanostructures with different sphericity. Furthermore, the nanospheres form at random on the dewetted surface but it is possible to change their average separation. Therefore, the surface morphology can be selected to increase the surface enhance Raman signal (SERS). Initial results in the selection of the substrate surface and deposition process conditions required for the formation of the nanostructures will be presented and discussed.

Characterization of Aluminum Doped Zinc Oxide Thin films and Nanostructures for H_2 Gas Sensing Applications

Victor M. Pantojas, Laura Amadeo, Nelson Granda, Carlos Ortiz, and Wilfredo Otaño

UPR-Cayey

Metal oxides, such as ZnO, are especially attractive as sensing elements synthesized in the form of thin films and nanostructures. The influence of Al doping on the gas sensing performance of ZnO films and fibers are explored with the hope of improving the sensitivity or the selectivity of the sensor. The objective of this work is to obtain faster and more sensitive gas sensors by reducing the dimensions of the sensing elements and by doping. Zinc oxide fibers are formed by preparing a PVA solution containing zinc acetate which is deposited as a thin film by sol-gel or as fibers by electrospinning. A chamber was set up to test the sensitivity of the material to hydrogen gas.



Poster Presentations

Development of an electrochemical biosensor for the detection of an ADP-Ribosylating Toxin, Exo A from *Pseudomonas aeruginosa* P1

Yanira Enríquez, Yashira Negrón, Mónica Navarreto and Ana R. Guadalupe,
UPR-Río Piedras

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 used to generate a film on carbon surfaces to anchor a β -NAD+ electroactive analog. Ferrocene-labeled NAAD (Fc-NAAD) was prepared by attaching Ferrocene Succinimide (Fc-NHS) to the primary amine in the adenine moiety of the cofactor. The OSWV analysis of the new Fc-NAAD showed an anodic peak in 320 mV and the CV analysis showed chemical reversibility and electrochemical quasi-reversibility.

Simulation of Ion Movement in Activated Carbon Super-capacitor P2

Aixa de Jesús and Pablo Negrón
UPR-Humacao

It has been observed experimentally that as the voltage in a supercapacitor is increased, then for a certain threshold voltage, the capacitance increases abruptly. One possible explanation to this phenomenon is the liberation of charges around ions after their entrance through porous in the activated carbon. In this work we will describe a simple model of this process with some numerical simulations.

P3 Use of Ru-Fc Intercalation Complex as an Electrochemical Label for the Detection of *Salmonella* DNA

Madeline Díaz-Serrano[1], Arelys Rosado[1],
Dianicha Santana[2], Esther Z. Vega[2], and Ana R. Guadalupe[1]
[1]UPR-Río Piedras and [2]UPR-Humacao

Waterborne and foodborne diseases are one of the principal public health problems worldwide. Our particular interest is the development of nucleic acid biosensors (NAB) for the detection of pathogenic microorganisms in food and water samples. In this research, we report on the development of a NAB prototype using a polymer modified electrode surface together with sequences of different lengths for the OmpC gene from *Salmonella* as probes and Ruthenium-Ferrocene (Ru-Fc) bi-metallic complex as a label. We have optimized several PS films and anchored nucleic acid sequences with different lengths at gold and carbon surfaces. Non contact mode AFM and XPS were used to monitor each step of the NAB preparation, from polymer modification to oligos hybridization (conventional design). The hybridization event has been detected electrochemically by the conventional method, which is modifying the target with Fc-NHS.

This report describes the synthesis of $[Ru(Fe\text{-}Phen)_2dppz](PF_6)_2$ (Ru-Fe complex) for a label-free approach to detect DNA hybridization. The binding constant of Ru-Fe complex with CT-DNA obtained by UV-vis and OSWV were 8.0 x104 M-1 and 6.5 x 105 M-1 respectively. We used the Ru-Fe complex and the Ferrocene covalently attached to the target to monitor the hybridization event of a 70-mer oligo immobilized in 10.3KD NHS-PS-NHS. We also measured the hybridization event of a PCR amplified biotinylated OmpC gene of *Salmonella* using only the Ru-Fe complex. The lowest target detectable concentration for both DNA fragments was above 0.4 µM. Current work focuses on the sensor platform and its signal to noise ratio optimization by increasing the polymer hydrophilicity and thus the diffusion of molecules within film. Also, we plan to increase the intercalation capability of the complex by reducing the size and the number of biotins in the probe. This sensor could be used to study the hybridization of complementary oligo sequences of once optimized and their detection in real samples.

Synthesis of ZnO Fibers and Thin Films doped with Al for Gas Sensors

P4

Laura Amadeo[1], Nelson Granda[1], Victor Pantojas[1], Wilfredo Otaño[1], Jay Kikkawa[2], and Jorge Santiago[2]
[1]UPR-Cayey and [2]UPENN

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), poly(vinyl alcohol)(PVA), acetic acid (HOAC) and aluminum nitrate (AlNO3) and thin films with the spin coating technique of the same solution. Aluminum Nitrate was used to deliver the Al doping the fibers and films to improve their conductivity. The samples where characterized by Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and electrical characterization.

Electrochemical Characterization of Poly-(3,4 propylenedioxythiophene) Pseudo-Capacitor

P5

Hitesh K. Sahoo, Jaewan Park, Rocío del A. Cardona- Couvertier, and Jorge J. Santiago –Aviles
University of Pennsylvania

Pseudo-capacitors are a type of super-capacitors which are based on the principles of faradaic reactions. They also aid the formation of a double layer thus combining chemical and physical phenomenon as observed in a battery and capacitor respectively. The polymer based pseudo-capacitors being highly conductive are the preferred choice over the metal oxide based pseudo-capacitors. The polymers have an oxidized state and a reduced state and the charge storage mechanism involves the conversion of one state to the other. These forces an important dependence on the accessibility of the reaction sites on the polymer along with the number of reaction sites. We looked into the variation of the performance of the pseudo-capacitor having Poly-ProDOT as the polymer, with respect to the number of cycles of polymerization. The capacitance was measured over a range of scan rates and different voltage windows for various polymerization cycles which helped look into the competition between the chemical (redox reaction) and physical (Electrical double layer formation) mechanisms. A maximum capacitance of 109 F/g was obtained for the pseudo-capacitor corresponding to 20 cycles of polymerization.

P6 Poly-L- Lactic Acid Membranes Produced by Electrospinning for Applications in Electrical Double Layer Capacitors

Rocío del A. Cardona and Jorge J. Santiago-Avilés
University of Pennsylvania

Super-capacitors (Electrical Double Layer Capacitor, EDLC) are energy storage devices that function similarly to conventional capacitors, but instead of accumulating charges on two conductors, it is stored at the interface of a conductor and an electrolyte solution. In general, super-capacitors are classified in two major groups according to the material in the electrode, these are: physical super-capacitors (carboneous materials) and pseudo capacitors, which store charge indirectly through Faradaic chemical processes, but their electrical behavior is like that of a capacitor. Super-capacitors possess the attribute of having large specific capacitance, combined with large power densities (high charge per unit volume and can be charged and discharged quickly). These attributes make small super-capacitors ideal charge storage devices for distributed and embedded applications such as those for coupling or powering small robotic systems, distributed sensors / actuators and bio-medical devices, including those designed to be implantable. One of the drawbacks of super-capacitors is their low energy density in comparison with batteries.

For the past years our research group has invested efforts to decrease the energy density gap between EDLC and batteries. One key aspect in the construction and improvement of EDLC is the ion permeable separator that prevents electrical contact, but still allows ions from electrolytes to pass through. Most of the membranes currently used, are made from poly propylene, a thermoplastic polymer which, among other characteristics, can stand the chemical environment to which they are exposed. However, its use is limited due to UV-Vis degradation and low bio-compatibility. Therefore, we have prepared by electro spinning fibers' mats in the nano-micro size range of poly-L-lactic acid (PLLA), aliphatic polyester from renewable resources, in mixture with MWCNT of different sizes to use them as permeable separator in our devices. We will present the physical and chemical characterization of the mats as well as electrochemical performance of our devices using these materials in comparison to the benchmark poly-propylene

Wolffia: The Incorporation of LAMMPS and its use on Networks

P7

Carlos Cortés and José Sotero
UPR-Humacao

Wolffia is a program that is been developed for this past year that works as an assistant during Classical Molecular Dynamics Simulations (CMD). CMDs consist of simulating the movements of atoms based on their interactions in a system. The simulations help by giving an idea of how the atoms behave on that scale. *Wolffia* has been made so that it guides the user throughout the steps that you take during a successful simulation, e.g.: building the system, defining force parameters, defining boundary conditions, minimization and simulation. Since it is not a wizard-type application, it gives ample flexibility to an experienced CMD scientist. For a while now, the program has served as a graphical user interface to NAMD, a well-established MD package.

We report our results of the addition of support for LAMMPS (*Large-scale Atomic/Molecular Massively Parallel Simulator*), another CMD package. The reason for this is to allow the user to have more choices on which to use, depending on what he wishes to accomplish; for example, one could have certain parameters or is capable of doing things the other isn't. NAMD's development has been steered toward biomolecular simulations while LAMMPS is better suited for coarse-grained simulations. This new package is being coded into the program and will be available through the settings window by choosing either LAMMPS or NAMD via a radio button. Just like our implementation of NAMD into the program, *Wolffia* also shows the user how the simulation is progressing on LAMMPS by showing temperature and energy graphs as well as being able to preview the system.

Right now, *Wolffia* runs the simulations on the local computer it is being initiated in. We also report our progress towards getting the program to run simulations through a network. Being able to choose to use another computer to run the simulation has it's upsides as you don't need to be near it or it can be simulated on a computer that is better suited for the job. *Wolffia* will still keep track of the simulation and the program will keep you updated on how the simulation is going

P8 Dispersion of Carbon Nanotubes with SDS using Wolffia

Rósely I. Quiñones López, Wensy M. Cuadrado, Frances J. Martínez Miranda, and José O. Sotero Esteva
UPR-Humacao

Wolffia is a user friendly software that will guide the user through a simulation using NAMD or LAMPS (molecular dynamics simulators). We use a simulation of the dispersion of carbon nanotubes with Sodium dodecyl sulfate (SDS) in chloroform as a test-case to show Wolffia's capabilities. Nanotubes dispersed with SDS are being used as a component for electrospun nanofibers by other PREM experimental researchers. We use a configuration is similar to one obtained from specialized literature and compare results.

The procedure used to build and perform the simulation was as follows. A SDS molecule was downloaded from repositories (NCI-CADD Group) with Wolffia's molecule loader. AMBER force field parameters were found in references literature. Force field parameter values were changed from units used by AMBER to units used by CHARMMS. All the SDS molecules were placed together surrounding a carbon nanotube in a shape similar to a flower; a configuration similar to the one used by Duan et.al. Periodic boundary conditions were set and the box was solvated with chloroform using the Setup tab. Test simulations were performed within Wolffia to develop stable initial configuration and parameters for a production-grade simulation. Configuration files were packaged with the appropriate Wolffia's tool and transferred to a server. Simulation was performed for 20 ns of simulated time.

Radial distributions functions of the resulting trajectory were compared to the ones found by Duan et.al.. This software makes it easier because Wolffia have tools that help the user to: load molecules, changes force field parameter and delete, copy, paste, rotate or move the molecule in the mixture viewer, among others.

Fabrication and study of organic solar cells composed of P3HT/PCBM blend with monolayers of P(VDF-TrFE). P9

Héctor Carrasco and Josee Vedrine
UPR- Humacao

Organic polymeric materials that are conducting provide an added facility in device fabrication, particularly in solar cell applications. In this work, we study the electrical and morphological properties of bulk hetero-junction solar cells fabricated with poly (3-hexylthiophene-2,5-diyl) (P3HT) and phenyl-C61-butyric-acid-methyl ester (PCBM) blends, when a monolayer of the ferroelectric polymer poly[(vinylidenefluoride-co-trifluoroethylene] [P(VDF-TrFE)] is deposited between ITO conductor and blend. The bulk hetero-junction and ferroelectric film are annealed at 130 ºC under ambient atmosphere to increase their crystallinity, which may assist in enhanced charge transfer. We measure the solar cells photovoltaic properties with changing blend thickness, while keeping the ferroelectric layer constant. AFM and *C*-AFM are used to provide additional information on the film morphological properties. The *current-voltage* characteristics are measured and compared for the different film thicknesses. The study will help us better understand how to improve organic solar cell efficiency under these conditions.

The effect of thermal annealing on the efficiency of semi-transparent organic solar cells P10

Gabriel Calderón and Josee Vedrine
UPR- Humacao

Solar cells provide an alternative and environmentally friendly source of energy from the sun. In this project, we fabricated organic solar cells and characterized their conduction under a simulated solar light source. The organic cells have an active region composed of electron-donor poly(3-hexylthiophene) (P3HT) and electron acceptor penyl-C61-butyric acid methyl ester (PCBM) materials to form a *pn* heterojunction. In our study, we analyzed the effect of annealing P3HT:PCBM polymeric blends on cell efficiency while maintaining the substrates under ambient atmosphere. We investigated the effect of annealing on the solar cell efficiency by measuring their current-voltage characteristics given these conditions, and found an indirect correlation between efficiency and annealing temperature.

P11 Temperature-Dependent Electrical Properties of Antimony-doped Tin Oxide Nanofibers

Maritza Reyna[1], Anamaris Meléndez, Nicholas Pinto[1], Idalia Ramos[1], and Jorge Santiago Aviles[2]
[1]UPR-Humacao, [2]UPENN

Antimony-doped tin oxide ($Sb:SnO_2$) nanofibers with weight percentages of Sb from 0 to 18% were produced using electrospinning and thermal treating in air at 600ºC. FTIR analysis of the $Sb:SnO_2$ fiber show a broad band close to $625cm^{-1}$, which can be attributed to oxo-bridge functional groups. XRD spectra show all the characteristic peaks of SnO^2. No other phases are present indicating antimony ions susbstitute tin ions in the crystal lattice.

The resistivity of single fibers was measured for temperatures ranging from 300 to 20 K and from 20 to 300K. The data reveals a decrease in resistivity with increasing temperature indicating a semiconducting-like behavior, as expected. The resistivity decreases with Sb concentration up to 13%, a behavior that have been reported for thin films and other nanostructures with the percentage dependending on the growth process. The resistivity measurements for 7.8 and 18% show a large increment for temperatures below 70K.

Dual input logic AND device fabricated using an *n*-doped semiconductor: Effects of UV light on charge mobility

P12

Alexander Rosado and Nicholas J. Pinto
UPR-Humacao

An *n*-doped ActivInk™ N2200 [P(NDI2OD-T2)] thin-film transistor having a split gate architecture was fabricated on a doped Si/SiO_2 substrate. This device demonstrates AND logic functionality and was controlled by applying either 0 or 50V to each of the gate electrodes. When 50V was simultaneously applied to both gates, the device was conductive (ON state), while any other combination of gate voltage rendered it resistive (OFF state). We tested the device in the presence and absence of UV (λ=365nm) and measured a higher mobility in the presence of UV. The *n*-type carrier charge mobility in the device was *2.0* x 10−6 cm2V−1s−1 upon UV exposure, while without UV exposure the mobility drops to *3.3* x 10−7 cm2V−1s−1. The low mobility of these devices could be a result of the rough substrate surface. A possible explanation for enhanced mobility in the presence of UV is that electron trapping adsorbate groups on the ActivInk™ surface (possibly O2− or H2O−) inhibit charge transport and lowers mobility. Upon UV exposure, an electron-hole pair is generated that liberates the adsorbates via hole recombination (□.□. h++ O2− → O2(gas)) releasing electrons that contribute to charge transport and reducing the amount of charge traps, leading to enhanced mobility. One advantage of this architecture is the possibility of having multiple inputs and gate connections using a *single* ActivInk™ channel. The ability to affect the channel conductance via UV also makes this device more versatile and multifunctional

P13 Electrospun fibers of PLA/P3HT blends for device and sensor applications

William Serrano and Nicholas J. Pinto
UPR-Humacao

The thermoplastic aliphatic polyester, poly (lactic acid) (PLA) is a biodegradable polymer that is sometimes used in implant screws for bone repair. Our focus was to fabricate fibers of this polymer and its blends with *p*-doped poly (3-hexylthiophene)-(P3HT) in order to extend its use to devices and/or sensors. PLA/P3HT fibers were prepared in air at room temperature using the electrospinning technique that is cheap, fast and reliable. Scanning Electron Microscope images of the fibers reveal that the presence of P3HT does not affect the fabrication of PLA fibers at low or high polymer concentrations in chloroform, retaining the same morphological structure of pure PLA fibers. The fiber diameters were in the range 1-10μm. A slight increase in fiber formation results with the addition of P3HT, most likely due to a reduction of the solution surface tension. Results of the electrical characterization of this material will be presented.

P14 The Effect of Toluene on the Electronic Properties of CVD Graphene

M. Oquendo[1], N.J. Pinto[1], G. Hee[2] and A.T. Johnson Jr.[2]
[1]UPR-Humacao, [2]UPENN

Graphene was grown via chemical vapor deposition and transferred to a doped Si/SiO_2 wafer. Electrical contacts were placed over the graphene using a TEM grid as a shadow mask to define the source (S) and drain (D) electrodes. When characterized as a FET, the $I\text{-}V_g$ transfer characteristics showed poor electron mobility for the as received sample. Washing the sample with toluene, leads to improved device I-Vg curves that resemble high quality graphene. Our results show that repeated washing with toluene improves the electron mobility while the hole mobility remains unaffected. This leads us to conclude that toluene acts as a surface cleaner, removing microscopic debris and/or "ironing" out the graphene channel across the S and D electrodes, with concomitant decrease in defects.

Synthesis of silver nanospheres for SERS applications P15

Bryan Vélez, Melissa Morales, William Ortiz,
and Wilfredo Otaño
UPR-Cayey

Silver nanostructures are actively studied for photonic applications while ultra-thin films are of interest for interconnections in ultra-large scale integration technology. In both applications, understanding of coalescence and film formation processes are of primary importance when the material is prepared by physical vapor deposition methods. Surface free energies, rate and angle of arrival of material, substrate temperature and energetic bombardment are process parameters that are used to change characteristics-properties of the material ranging from nanomorphology to epitaxy. Silver metallic nanospheres were prepared using the sputtering technique. In this method, several sputtering deposition process parameters were controlled to reduce coalescence of the silver being deposited resulting in the formation of nanostructures with different sphericity. Furthermore, the nanospheres form at random on the dewetted surface but it is possible to change their average separation. Therefore, the surface morphology can be selected to increase the surface enhance Raman signal (SERS). Initial results in the selection of the substrate surface and deposition process conditions required for the formation of the nanostructures will be presented and discussed.

P16

Temperature Transformation of Electrospun $In(NO_3)_3$ Fibers into InN

Joshua L. Robles-García[1], Anamaris Meléndez[1], Andrew McGhie[2], and Idalia Ramos[1]

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The group III nitrides GaN, InN, AlN, $In_xGa_{x-1}N$ and $Al_xGa_{x-1}N$ are important materials for the development of optoelectronic devices. InN is especially interesting because a few years ago its bandgap was re-measured as 0.7 eV instead of its previously accepted 1.9 eV. The challenges of growing InN include the development of metallic indium when synthesizing at low temperatures (400-500°C) and the decomposition of InN above 600°C. In previous work we attempted to produce InN nanofibers using the electrospinning technique and a precursor solution composed of indium nitrate (III), and cellulose acetate dissolved in dimethylacetamide and acetone. After electrospinning, the fibers were sintered in nitrogen at 500°C to decompose the polymer and the nitrates and nitridized at 500°C-600°C under an ammonia gas flow to complete the production of InN. X-Ray Diffraction (XRD) analysis of the fibers showed the production of InN with In_2O_3 and metallic Indium peaks.

In this work, Themogravimetric/Diffferential Thermal Analysis (TG/DTG) was used to understand the chemical changes in the fibers during the heating process in nitrogen gas with the goal of improving the production of InN. The TG/DTG of the samples was done in a stream of nitrogen gas at a heating rate of 10°C/min from room temperature (RT) to 500°C. Then, the temperature was maintained constant for 30 min. TG/DTG was also done to separate Indium Nitrate and Cellulose Acetate samples. The results showed the incomplete decomposition of the polymer in nitrogen gas. The decomposition was completed by switching the gas to air and keeping at 500°C for another 30 min. Using this information the heating setup for the processing the electrospun fibers was modified by a adding a breathing air line. The XRD of the fibers with the new heating method shows the production of hexagonal and cubic InN with enhanced crystallinity.

Electrospun GaN Nanobridges for Self-Heated Gas Sensors P17

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Gallium Nitride (GaN) nanofibers were produced by electrospinning technique for the fabrication of nanobridges. In this work, GaN nanofibers synthesized by nitridation method (already produced and characterized in a previous work) were collected over designed high electrodes to create a bridge connection to be used as gas sensors. The main purpose of these structures is to enhance sensitivity by producing fibers with a larger area exposed to the sensed gas. The surface of the fiber expose to the gas is probably doubled in comparison with those fibers electrospun on solid substrates. The substrates used in the fabrication of these devices are favorable for well-controlled current settings and therefore, take advantage of self-heating effects to set appropriate temperatures for gas sensing. Small dimension structures are responsible for self-heating effects caused by dissipated power while operating in electrical devices. This leads to temperature gradients, which significantly reduce the lifetime of these components. However, effective temperatures for gas sensing applications could be settled by applying a well-controlled current value to the GaN nanobridge.

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