



# PROGRAM

9:15 - 10:00 AM	Registration & Breakfast
10:00 - 10:10 AM	Welcome Messages Idalia Ramos, UPRH, PREM PI Arjun Yodh, UPENN, PREM Co-PI and Director PENN MRSEC Andrew McGhie, Associate Director PENN MRSEC
10:10 - 10:30 AM	PREM Update Idalia Ramos, Ramón Rivera, Andrew McGhie, and Arjun Yodh
10:30- 11:00 AM	Liquid-crystalline nanoparticles: Organizing nanometer-scale core- shell nanohybrids <b>Bertrand Donnio</b> , Université de Strasbourg (France) & UPENN
11:00 - 11:20 AM	Coffee break
11:20 - 11:40 AM	Wolffia: improvements and applications José O. Sotero Esteva, UPR-Humacao
11:40 - 12:00 AM	A theoretical model for the characterization of molecular cavitation in liquids <b>Pablo Negrón</b> , UPR-Humacao
12:00 - 1:30 PM	Working Lunch
1:30 - <i>1:50 PM</i>	High Power Electric Double-Layer Capacitors based on Room- Temperature Ionic Liquids and Nanostructured Carbons <b>Carlos R. Pérez</b> , UPENN



1:50 - 2:10 PM	Mobility enhancement in an electrospun poly(3-hexylthiophene) FET using crossed nanofiber architecture Nicholas Pinto, UPR-Humacao
2:10 - 2:30 PM	The effect of Coulomb interactions on thermoelectric properties of quantum dots Natalya A. Zimbovskaya, UPR-Humacao
2:30 - 2:50 PM	Coffee Break
2:50 - 3:10 PM	Fabrication and study of organic solar cells composed of P3HT/PCBM blend with monolayer of P(VDF-TrFE) Josee Vedrine-Pauléus, UPR-Humacao
3:10 - 3:30 PM	Resistivity of Al-doped ZnO thin films Víctor Pantojas, UPR-Cayey
3:30 - 3:40 PM	Colsing Message Dr. Carmen A. Miranda, Chancellos UPR-Humacao
3:40 - 5:00 PM	Student Poster Presentations
5:00 - 6:00 PM	Advisory Committee meets to write Report
6:00 PM	Closing





# **Oral Research Presentations**



# Liquid-crystalline nanoparticles: Organizing nanometer-scale core-shell nanohybrids

#### Jean-Louis Gallani, Bertrand Donnio\*

#### Université de Strasbourg (France) & UPENN

Nanostructured materials provide one of the greatest potential for improving performances and extended capabilities of products in a number of industrial sectors. Research in this area aims at promoting *functional molecular objects* able to self-organize into periodic arrays, whose functions can be ultimately addressed by external stimuli. Ordered assemblies of monodisperse, spherical nanoparticles (NPs) that provide 2D or 3D superlattices constitute an attractive class of nanostructured functional materials for a wide range of applications from high-density recording media, single-electron microelectronic devices to nanoscale metamaterials.

The controlled solvent evaporation technique of surface-passivated NPs mostly leads to bcc, hcp or fcc compact arrays of spheres, since primarily governed by close-packing and geometrical criteria. Long-range ordering, in the cm-scale, of simple and binary lattices can be achieved by this method. Alternatively, since selforganization takes also place in systems that have some fluidity during the process, liquid crystals appear as ideal candidates, and therefore self-assembling NPs using mobile liquid crystalline (LC) phases seems a promising approach. In addition, a higher modularity in the organization is anticipated due to the softening of interparticles boundaries. Our methodology towards nanostructured materials consists in the covalent functionalization of spherical metallic nanoparticles, endowed with electronic/magnetic/optical properties, by proto-mesomorphic structuring ligands to enforce LC mesophases formation.

The induction of such LC mesophases, whose supramolecular arrangements and physical properties are controlled by their surface derivatization, is reviewed. It will be shown that the nature of the proto-mesogenic capping agents gives rise to specific organizations of the hybrids into nematic,' smectic,' columnar,' cubic,' and more complex mesophases.' We thus can provide by self-organization, structures whose symmetry can be pre-determined. It will also be shown that the rational organization of functional nanoparticles can enhance existing properties or promote their collective behaviors and the emergence of new ones by synergistic effects upon ordering into such complex, low-dimensional lattices. This concept may be extended to other types of nanoparticles (e.g. oxides, semiconductors, alloys) and of different shapes (rods, discs, triangles, rings, cubes, etc..).



# Wolffia: improvements and applications

#### José O. Sotero Esteva, Melissa López, Frances Martínez-Miranda, Radamés Vega Alfaro, Wensy Cuadrado Dávila

#### **UPR-Humacao**

Improvements done to the computer application Wolffia during the last year include usability features that ease the manipulation of molecules in the mixture, add flexibility to the process of adding multiple copies of molecules (as when adding solvents) and to the force field parameters editor. Another notable improvement is the possibility of submitting and running simulations on a server and monitor from a laptop or desktop running Wolffia. A side product of this effort is the PyIMD Python language module that implements the Interactive Molecular **D**vnamics communication protocol (IMD) widely used molecular dynamics simulators. The module is written in a object oriented fashion, it is easily extensible, and provides additional tools not present in the original C language implementation. Ideas for these improvements came from suggestions made by our PREM collaborators Preston Moore and Robert Johnson, as well as from our own efforts to use the program to produce simulations relevant to experimental work being done by other PREM researchers.

Wolffia is still being used in outreach activities such as *Experimenta con PREM* as well. Results from standardized usability tests performed during this activity will also be reported.



# A theoretical model for the characterization of molecular cavitation in liquids

#### Pablo Negrón Marrero<sup>1</sup>, Melissa López<sup>2</sup> and José O. Sotero Esteva<sup>1</sup>

# <sup>1</sup>UPR-Humacao, <sup>2</sup>UPR-Río Piedras

The phenomenon of void formations in solids and liquids have been studied extensively in the literature mostly from the experimental and computational point of views. In solids, within the frame of the continuous theory of nonlinear elasticity, the concept of volume derivative has been recently used to give a mathematical characterization of the pressures or the pre-specified volumes of the deformed body that lead to the formation of voids. For the so called elastic fluids, this criteria provides an exact characterization of the pressures or prescribed volumes that lead to the formation of voids.

On the other hand, for molecular models of liquids, the formation of voids in liquids for pressures at certain ranges has only been observed via molecular dynamics simulations. In this talk we review the basic equations of molecular dynamics including the one for the pressure, as a first step to obtain a mathematical characterization of the pressures leading to the formations of voids. We discuss as well the concept of Voronoi polyhedron and graphs as a tool for defining a discrete density function such that regions of very low density would correspond to places where voids may or have formed.



# High Power Electric Double-Layer Capacitors based on Room-Temperature Ionic Liquids and Nanostructured

#### Carlos R. Pérez

#### UPENN

The efficient storage of electrical energy constitutes both a fundamental challenge for 21st century science and an urgent requirement for the sustainability of our technological civilization. The push for cleaner renewable forms of energy production, such as solar and wind power, strongly depends on a concomitant development of suitable storage methods to pair with these intermittent sources, as well as for mobile applications. In this regard, supercapacitors represent a vibrant area of research due to their environmental friendliness, long lifetimes, high power capability, and relative underdevelopment.

The objective is to better understand the interplay of electrode and electrolyte parameters in the ultimate performance of RTIL-based supercapacitors in terms of power, energy, and temperature of operation. For this purpose, carbon nanomaterials such as nanoporous CDC nanopowders, vertically aligned carbon nanotube arrays, and single wall carbon nanotube aerogels, were synthesized and used as electrodes, alongside RTIL electrolytes with systematically varying ion sizes and compositions. While electrode/electrolyte development can take place along parallel lines, both must be properly matched to the device's ultimate operating conditions. The devices exhibit good performance characteristics, and the best temperature range of any electrochemical storage device to date.



# Mobility enhancement in an electrospun poly(3hexylthiophene) FET using crossed nanofiber architecture

#### Nicholas Pinto

#### UPR-Humacao

Nanofibers of P3HT and PEDOT-PSSA were electrospun sequentially to form junctions over a doped Si/SiO<sub>2</sub> substrate with the PEDOT fiber lying over the P3HT. Near the intersection, the fibers were contacted with Au electrodes at either end and the resulting device had a crossed fiber architecture. When characterized in a FET configuration, the P3HT fiber exhibited *p*-type behavior with mobility ~ 8.0 x  $10^{-5}$  cm<sup>2</sup>/Vs. Applying a bias to the PEDOT fiber injected charge into the P3HT channel under it. Subsequently, by sweeping the back gate bias and subtracting out the non-field effect current due to the bias on the PEDOT fiber, an enhanced device transconductance and an order of magnitude increase in the mobility was observed. This result is proposed to be due to a reduction of the internal series resistance, reduction of the energy barrier for hole injection at the metal-semiconductor contact and a higher current density in the channel that fills charge traps. The effect was reversible and indicates a novel way of enhancing mobility in organic FET's.



# The effect of Coulomb interactions on thermoelectric properties of quantum dots

#### Natalya A. Zimbovskaya

**UPR-Humacao** 

Thermoelectric effects in a quantum dot coupled to the source and drain charge reservoirs are explored using nonequilibrium Green's functions formalism beyond the Hartree-Fock approximation. We concentrate on theoretical analysis of the influence of Coulomb interactions on thermopower and thermoelectric efficiency described by the dimensionless figure of merit ZT. Obtained results show that Coulomb interactions between charge carriers on the dot significantly contribute to its thermoelectric properties, as was repeatedly suggested in earlier works, both theoretical and experimental. In the present work, we trace the transition from the Coulomb blockade regime to Kondo regime in the thermoelectric properties of the quantum dot, which occurs when we gradually strengthen the coupling of the dot to the charge reservoirs. We show that within the Coulomb blockade regime (when the coupling of the dot to the leads is weak compared to the characteristic strength of the charge carriers interactions) thermoelectric characteristics of the dot display distinct features caused by Coulomb interactions. These features indicate possibilities of enhancement of thermoelectric efficiency of the considered systems. Within the Kondo regime, when the couplings of the dot to the leads became stronger, the influence of Coulomb interactions declines bringing a decrease in the thermoelectric efficiency.



# Fabrication and study of organic solar cells composed of P3HT/PCBM blend with monolayer of P(VDF-TrFE)

#### Josee Vedrine-Pauléus

#### UPR-Humacao

Probing the nanomorphology of the bulk heterojunction (BHJ) has implications on device performance; this can also provide insight on structural ordering of the polymer when induced with heat. We present results of the morphology of P3HT:PCBM BHJ using atomic force microscopy (AFM). The BHJ depicts a network of dispersed nanofibrils at room temperature, but these networks aggregate in clusters with increasing annealing temperature. Quantitative measurements such as surface roughness and electrical conductive properties show a distinct difference between films annealed from 100  $^{\circ}$ C to 140  $^{\circ}$ C.



# **Resistivity of Al-doped ZnO thin films**

#### Victor M. Pantojas

#### UPR-Cayey

Aluminum doped ZnO (AZO) is a transparent conducting oxide with applications in photovoltaics, gas sensing and spintronics. Doping with aluminum increases the number of charge carriers, which should lower the resistivity of the material. On the other hand, doping can be detrimental to charge transport due to impurity scattering, segregation and/or changes to microstructure of the film due to the incorporation of the dopant. AZO films were deposited by sol-gel spin coating with 1, 2, 3, 5, and 10 at.% Al. The resistivity ( $\rho(T)$ ) as a function of temperature was measured by the Van Der Pauw method. Indium and Gold/Aluminum contacts were tested for ohmic behavior. The resistivity was found to decrease with temperature, which is typical of semiconducting materials. Several conduction models for the temperature dependence of the resistivity were tested. A minimum resistivity  $\rho = 1.94 \ \Omega$ -cm was measured for 2 at.% Al at room temperature.





**Poster Presentations** 

# Dielectric properties of the n-doped polymer [P(NID2OD-T2)] P1

#### Pablo I. Sepúlveda and Nicholas J. Pinto UPR-Humacao

Poly[N,N'-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyll-alt $5,5'-(2,2'-bithiophene)]-[P(ND12OD-T2)]_n$  is a *n*-doped polymer that is stable in air. Since this polymer exhibits a high resistance, our goal was to characterize its dielectric properties using an impedance analyzer. Materials that have a high dielectric constant and low loss tangent are important for improving device parameters. To determine the dielectric properties we designed a capacitor using this polymer as the active layer between two parallel silver electrodes. An Agilent 4294A precision impedance analyzer was then used to measure the device capacitance (C) and conductance (G) as a function of frequency. Measurements were made on the device in air as a function of temperature and after exposure to UV irradiation. All of the measurements were done using a Visual Basics program that was written to control the frequency steps at which the measurement of the parameters (C, G) were made and were analyzed using SigmaPlot<sup>TM</sup> software. Knowing the geometrical capacitance of the sample, the polymer complex dielectric permittivity ( $\epsilon^* = \epsilon' - i\epsilon''$ ) was then calculated. At high frequencies,  $\epsilon'$  is seen to be relatively constant while at low frequencies  $\varepsilon'$  increases representing additional contributions to the dielectric response with an almost Debye like relaxation mechanism as seen from the nearly semi-circular Cole-Cole plots. As temperature was increased, the impedance increased and the relaxation times decreased. Increasing the exposure to UV light caused a decreased in impedance and an increase in its relaxation time. The charge relaxation mechanisms and potential use of this polymer in devices will be presented.

# Effect of ultraviolet irradiation on an *n*-doped semiconductor thin film transistor

#### Alexander Rosado and Nicholas J. Pinto UPR-Humacao

Spin coated thin film field effect transistors were fabricated from the *n*-doped semiconductor poly[N,N'-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarbo-ximide)-2,6-diyll-alt-5,5'-(2,2'-bithiophene)] [P(ND12OD-T2]<sub>n</sub> with charge mobility of  $3.0x10^{-3}$  cm<sup>2</sup>/V-s. UV irradiation however leads to an increase in the channel current with concomitant increase in the charge mobility and on/off ratio. There is also a shift of the threshold voltage in the negative direction with an induced change in charge concentration of  $3.0x10^{12}$  cm<sup>-2</sup>. The device was also tested as a UV light sensor and had a response time of ~20s making it multifunctional. Desorption of electron trapping species and photo-excitation are suggested as possible mechanisms. These results show that one can improve the device parameters via UV irradiation without cumbersome chemical purification techniques.



# Electrical Characterization of CVD grown MoS<sub>2</sub>

William Serrano<sup>1</sup>, Nicholas J. Pinto<sup>1</sup>, Anamaris Melendez<sup>1</sup> Idalia Ramos<sup>1</sup>, and Alan T Johnson Jr<sup>2</sup> <sup>1</sup>UPR-Humacao, <sup>2</sup>UPENN

Graphene and molybdenum sulfide ( $MoS_2$ ), 2-D materials, are proving useful in low dimensional electronics devices. Unlike graphene, which is a semimetal with zero bandgap,  $MoS_2$  on the other hand has a direct bandgap of 1.8eV. Our work has focused on the chemical vapor deposition (CVD) technique to fabricate thin flakes of  $MoS_2$  on doped Si/SiO<sub>2</sub> substrates. We have thus far tried two different starting precursor materials to grow  $MoS_2$ . In one method we placed a few mg of molybdenum trioxide on the substrate and heated it in an O<sub>2</sub> environment at 800C after which we lowered the temperature to OC and then had a gas of sulfur flow over it at 450C. In the other method, we used molybdenum chloride and heated it together with pieces of sulfur at 800C. We noticed a thin film deposit on the substrate in both methods and proceeded to electrically characterize them in a field effect transistor configuration. Some of the thin film deposits appeared to have a crystalline structure while the other just yielded uniform coverage of the substrate. The results of these experiments will be presented in this poster.

**P4** 

# Simulation of Ion Movement in Activated-Carbon Based Supercapacitor

#### Aixa De Jesús and Pablo Negrón UPR-Humacao

Electric Double Layer Capacitors (EDLC) or supercapacitors, are devices that store electric energy in the electric double layer that is formed at the interface between the electrode and the electrolyte. 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. We present some molecular dynamics simulation of ion transport in activated carbon supercapacitor using the Wolffia software. Using carbon atoms and single wall CNT, the model incorporates some of the geometry of carbon pores whose diameter tapers from 1.6 nm to 0.6 nm. We use sulphate and hydronium to simulate the ions of the electrolyte. The model predicts ion transport into the activated carbon pores.

# Fibers of MEHPPV prepared via electrospinning

Clarissa D. Vázquez<sup>1</sup>, Nicholas J. Pinto<sup>1</sup>, Alan T. Johnson Jr.<sup>2</sup> <sup>1</sup>UPR-Humacao, <sup>2</sup>UPENN

Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]-(MEHPPV) is a *p*-doped organic conducting polymer that is commonly used in light emitting diodes (LED) and field effect transistors (FET). Most devices use this polymer in the form of thin films during the manufacturing process. We have successfully fabricated fibers of this polymer in air and at room temperature using electrospinning. The fibers were several cm's long and had diameters in the range 0.5-5.0mm. The advantages that a fiber has over a thin film include: reduced dimensionality, smaller size and it consumes lesser material. A thin film FET was fabricated using this polymer and electrically characterized. The field effect mobility was calculated to be  $72.1x10^{-6} \frac{cm^2}{V \cdot s}$ . Individual fibers of MEHPPV were also captured on doped Si/SiO<sub>2</sub>

wafers and connected in a FET configuration. Our poster will summarize the FET performance parameters obtained using a thin film and a nanofiber of this polymer.

### A molecule editor for Chitosan Polymer

Wensy Cuadrado Dávila, and José O. Sotero Esteva UPR-Humacao

Chitosan is a polisaccharide obtained from crustacean shells. It has biomedical uses. For example, when used in bandages, it allows blood to clot rapidly, and serves as an antibacterial agent. It can also be electro-spun to form nanofibers which have the potential to be used as a bio-compatible nanomaterial. In this work, a *Chitosan Homopolymer Editor* has been built for *Wolffia*: a graphical user interface that integrates diverse Molecular Dynamics software to guide the user throughout the setup, execution, monitoring, and analysis of simulations. The new editor, gives the user the opportunity to select the length of the *Chitosan polymer* or the quantity of monomers.

To construct the editor, first, a Chitosan monomer was downloaded from the NCI/CADD database using Wolffia. After downloading the monomer to Wolffia, it was observed that it's Force Fields were not parametrized. In order to parametrize the Force Fields, the monomer was separated into its constitutive parts. A search was done using Wolffia's parameter finder, to find each of the monomer's Force Field parameters. A prototype of the Chitosan monomer was created using the monomer's components. Preliminary simulations show agreement to known behavior of the polymer.

**P6** 

**P5** 

# Flow Programming for Molecular Dynamics

#### Brian Matta Rosado and José O. Sotero Esteva UPR-Humacao

Flow-based programming (FBP) is a programming paradigm in which applications are built as networks of components that run as separate processes exchanging data across predefined connections. These components can be reproduced and reconnected to form different applications without having to be changed internally. FBP has been shown to increase productivity as well as software performance by exploiting process concurrency.

Wolffia is a user friendly molecular dynamics simulator software being developed by our group, which is based on input from scientists with experience in molecular dynamics. It guides the user throughout the simulation process, analyzing it's parameters and monitoring it's behavior. Our goal in this project is to integrate this type of programming to our research group's molecular dynamic simulator to analyze simulation trajectories while the simulation is running and to facilitate the development of new tests done in the program by bringing more parameters and make the processes more efficient and faster.

This presentation shows prototypes of different measures for molecular dynamics simulations made using FBP inside Wolffia. Once the feasibility of the method is proved, a plan for further development is presented.

# P8 Mining Force Field Parameters Using Graph Embeddings

### Radamés Vega Alfaro and José O. Sotero Esteva UPR-Humacao

Obtaining reliable Force Field parameters is somewhat cumbersome when working with Molecular Dynamics simulations, specially when these simulations have numerous types of molecules or large molecules with various types of bonds within it. Wolffia, a Graphical User Interface (GUI) designed to help its users set up and run Molecular Dynamics Simulations. It aims to facilitate the whole procedure from setting up a mixture to specifying the details for each configuration file needed to run the desired mixture and then pack up everything that's needed to execute the simulations in a dedicated environment. In this work, we will be describing Wolffia's current approach to acquiring Force Field parameters using types of bonds in already existing Force Field parameters files. The results will be compared to simulations reported in literature. This approach will be used as a base to build a more reliable technique to aid our probe for more consistent Force Field parameters.

# Bubble formation with water and chloroform in presence of nanotube

#### Frances Martínez Miranda and José O. Sotero Esteva UPR-Humacao

Sonication is the act of applying ultrasonic energy to a solution. The ultrasound high-low pressure oscillations in the solvent cause a cavitation process. This process consists in generating many microscopic bubbles that expand and then collapse. The shock waves produced cause the dispersion of molecules. Sonication is the most commonly used method for dispersing carbon nanotubes (CNT). Sonication protocols could be critical in experiments. Stronger and longer sonication disperses better the CNTs at the risk of fracturing them. Weaker and shorter sonications do not risk fracturing CNTs but could hurt dispersion efficiency. The process of formation of cavitation has been simulated before using classical molecular dynamics (CMD) using single-atom liquids. Works reported in literature show time-void volume plots that start with an initial period without voids, then a sudden appearance, grow and, eventual stabilization of the cavities.

Using Wolffia, a software that assembles CMD simulations to be run using NAMD, we performed molecular dynamics simulations of different systems consisting of two CNTs varying the solvent used, chloroform or water, and the solvent density. A new piece of software, called Nucleation, was programmed to see the bubbles and to know what is the volume of the biggest bubble and the sum of all bubbles in the simulation. This program was used to make time vs void volume plots as in the literature. Pressure-temperature plots were also produced using the energy data produced by NAMD. Significant differences were observed between systems solvated with water and chloroform. Water-solvated systems form bubbles protruding from the CNT walls while in the systems with chloroform the bubbles are strewn away from the CNT walls. This result is consistent with previous singleatom liquid simulations with walls in which the place of nucleation varied according to surface wettability. Density ranges where cavitation starts to occur were obtained from time vs void volume plots. Pressure-temperature plots show interesting patterns that deserve further study.



**P9** 



P10

# Void Detection Using Voronoi and Delaunay Triangulation

### Melissa López<sup>1</sup>, Pablo Negrón Marrero<sup>2</sup>, and José O. Sotero Esteva<sup>2</sup> <sup>1</sup>UPR-Río Piedras, <sup>2</sup>UPR-Humacao

The geometric characterization of molecules is a very useful technique for gathering information of the physical properties of molecules arrays. One can for example obtain information of the structure of the molecules, as the location of the atoms, determine the density or intensity of points, and detect the cavities between them. In this work we are interested in the use of Voronoi diagrams and its complementary Delaunay triangulation to determine the existence of voids or cavities in molecules arrays. The Delaunay triangulation can give us information about the local density of the points: in areas with low density, we will find big triangles and vice versa. Therefore, we could use the size of the triangles as a measure of the local density of the points. We used the Voronoi Diagram and Delaunay Triangulation method to study a system of liquid argon and analyzed the local densities, in order to characterize the voids in the system. For our simulations we used the software *Wolffia* that is an open-source graphical user interface to prepare and monitor classical molecular dynamics simulations.

# P11 Simulations of Carbon Nanotubes (CNTs) and surfactants in water and cloroform

#### Giovanni Casanova Sepúlveda and José O. Sotero Esteva UPR-Humacao

Carbon nanotubes (CNTs), with their exceptional mechanical and electronic properties can be integrated into a variety of devices such as chemical and biological sensors, and electromechanical actuators. To be used effectively as reinforcement of polymer nanocomposites, a proper dispersion of the CNTs and adhesion to the polymer matrix are necessary. In this work, we use computational techniques to study the influence of the CNTs-dispersion in the properties of the precursor solution and CNT/polymer nanofibers fabricated using electrospinning. The dispersion was done using the ionic surfactants Sodium Dodecyl Sulfate (SDS) Sodium dodecylbenzenesulfonate (SDBS) in Chloroform (CHCl<sub>3</sub>). and The interactions between CNTs, surfactants, and polymers were simulated using the Wolffia graphical user interface to NAMD. To understand the behavior of the surfactant about the CNTs in chloroform, two simulations were prepared: SDS and SDBS micelles and CNT dispersed in water to validate the method by comparing to results in literature and SDS and SDBS micelles and CNT dispersed in chloroform. Results of simulations using water as solvent were used to validate the method. The simulations were prepared setting a specific value for the periodic frontier conditions with the purpose of simulating a infinite CNT and verifying that the values of the force fields where the correct ones. Both SDS and SDBS aggregate around the nanotube as cylindrical and hemispherical micelles, respectively. Results are consistent with literature (Tummala, et al., ACS Nano, 2010). MD simulations suggest that the SDS or SDBS used in CNT dispersions when incorporated to the polymer leave the nanotubes free to occasionally interconnect forming conductive paths.

# Effect of CNTs Dispersion on the Properties of CNT/PMMA Nanofibers

Valeria Capel<sup>1</sup>, Sabrina Rosa<sup>1</sup>, Xenia Barbosa<sup>2</sup>, Idalia Ramos<sup>1</sup>, and José O. Sotero Esteva <sup>1</sup>UPR-Humacao, <sup>2</sup>Florida International University

Electrospinning was used to fabricate Carbon Nanotubes (CNT)/ Poly(methylmethacrylate) (PMMA) composite nanofibers. We studied the influence of the CNTs-dispersion method on the properties of the precursor solution and the CNT/PMMA nanofibers. The dispersion was done in the solvent chloroform  $(ChCl_3)$ with and without the addition of the ionic surfactants Sodium Dodecyl Sulfate (SDS) and Sodium dodecylbenzenesulfonate (SDBS). The solutions were stirred and sonicated before electrospinning. The properties of the solutions and fibers were analyzed using UV-visible Spectroscopy, Optical Microscopy, Scanning Electron Microscopy, and Electrical (I-V) measurements. In a complementary computational work presented in this conference, Sotero and his group simulated the interactions between CNTs, surfactants, and polymers using the software Wolffia.

## Simulation of Fullerene Electrodes for Capacitors

#### Jordan Caraballo<sup>1</sup>, Génesis Ayala<sup>1</sup>, and José Sotero Esteva<sup>2</sup> <sup>1</sup>Esc. Sup. Petra Mercado, <sup>2</sup>UPR-Humacao

A super capacitor is composed of two electrodes and a dielectric material that unites working like a battery and acquiring its energy fast. Fullerenes and carbon nanotubes may work as the electrodes based in their conductivity owed to their electrical properties. At the same time the sulfuric acid  $(H_3OSO_4)$  is one of the most common dielectric materials or electrolyte in the scientific field. The Wolffia program is a software that works making basic molecular dynamics simulations based in their initial and boundary conditions and is the one used to make the simulations. Added to this we used a program called "Nucleation" inside of Wolffia that computes us the volume of the biggest void cavities inside of the simulation. Procedures were divided in two phases. The initial phase was to view the interactions between the fullerenes of  $C_{100}$  making agglomerates with (H<sub>2</sub>O). The second one was based in mixing the sizes to view their interaction and then use them as electrodes. A way of adding solvent without filling the fullerenes was implemented and tested with the Nucleation program. Charges were alternated between positive and negative values to view their attraction/repulsion and it was found that the electrolyte flowed in and out of the cavities. Therefore, the effective surface area of the electrode is considerably larger than when using a plate.





P14

# Composite Activated Carbon/Carbon Nanotubes Electrode for Electrical Double Layer Capacitors

Génesis Ayala<sup>1</sup>, Idalia Ramos<sup>2</sup>, and Jorge Santiago<sup>3</sup> <sup>1</sup>Esc. Sup. Petra Mercado, <sup>2</sup>UPR-Humacao, <sup>3</sup>UPENN

Electrochemical double layer capacitors (EDLCs), are one of the most promising A simp compo energy storage devices due to their high power density, rapid charging/discharging ability, and long cycle life. Two simple EDLCs were fabricated using electrodes were p composed of Activated Carbon (AC) and Carbon Nanotubes (CNTs). The electrodes dissolv were prepared using a solution containing 90 wt% AC and 10 wt% polystyrene (PS), the siz in chloroform (ChCl<sub>3</sub>). The solution was stirred and sonicated to reduce the size of films. the AC particles and increase their surface area, before fabricating the films for solutio the electrodes. In a second capacitor, 0.15 wt% SWCNTs was added to the solution. filter | The capacitors were constructed by inserting two electrodes with a piece of filter aqueo paper between them (separator) inside a small seal bag with KOH as the aqueous proper electrolyte, and two pieces of nickel foam for the electrical contacts. The Electro properties of the electrodes were studied using Optical Microscopy, Scanning the de Electron Microscopy (SEM), and electrical (I-V) measurements. The capacitance of the device was measured using an impedance analyzer.

# P15 Effect of Urea addition on the Gallium Nitride Nanofibers Optical and Electrical Properties

Anamaris Meléndez<sup>1</sup>, Joshua Robles<sup>1</sup>, Carlos Camargo<sup>2</sup>, Jaume Esteve<sup>3</sup>, and Idalia Ramos<sup>1</sup> <sup>1</sup>UPR-Humacao, <sup>2</sup>CNM-Spain

Gallium Nitride technological importance is related to its wide bandgap (3.39 eV at Galliur 300K), large heat capacity, and thermal conductivity. GaN polycrystalline electro nanofibers have been produced using electrospinning and a precursor solution of dimeth gallium nitrate, cellulose acetate, dimethylformamide, and acetone, followed by a at 450° heat treatment in flowing nitrogen at  $450^{\circ}$ C, and then in ammonia (NH<sub>3</sub>) at 950of the 1000°C. The development of devices using the electrospun fibers have been limited proper by leakages on the substrates produced during the heat treatment in ammonia. In The ra this work, we study the effect of the addition of urea to the precursor solution in compa maintaining or enhancing the properties of the fibers, while lowering the hours temperature necessary to produce GaN and preventing reducing damage to the were a substrates. The ratios of urea to gallium nitrate in the precursor are 1.5 M and 1.7 and Cu M, and 0 M for comparison. The electrospun fibers were sintered under nitrogen gas flow for 3 hours at 450°C, and then under NH<sub>3</sub> flow for 5 hours at 900°C. The GaN were analysed using diffraction, UV-Vis fibers X-Ray Spectroscopy, Photoluminiscence, and Current-Voltage measurements.

### Nanomorphology study of P3HT:PCBM Bulk Heterojunction thermally annealed *pre*-encapsulation

#### Gabriel Calderón and Josee Vedrine UPR-Humacao

Thermal annealing of the bulk heterojunction has implications on device performance and probing the nanomorphology can provide useful insight on the mechanism of crystallization and ordering in the organic polymer mix. In this study we investigate the morphology of thermally annealed organic bulk heterojunction polymer thin films before deposition of the cathode layer using atomic force microscopy (AFM). The organic blend or active region is composed of electron-donor poly(3-hexylthiophene) (P3HT), and electron acceptor phenyl-C61butyric acid methyl ester (PCBM). Polymer photovoltaic cells were fabricated from the thermally annealed BHJ films and analyzed to measure their light-to-electricity conversion efficiency with increasing annealing temperatures before the aluminum layer is deposited. P3HT:PCBM thin films depict a morphological network of dispersed fibrils throughout the thin film at room temperature, while these networks tend to aggregate in clusters with increasing annealing temperature. The solar cells devices fabricated under these conditions showed increase in device efficiency for increasing thermal annealing temperature contributing to primarily to network aggregation and increase surface roughness at 140 C. Although the driving force that contributes to the aggregation of the P3HT fibril network is not well understood, their formation is related to increase roughness and improved charge transport properties of solar devices.

# Fabrication and study of organic solar cells composed of P3HT/PCBM blend with monolayer of P(VDF-TrFE)

#### 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 °C 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. 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.





# P18 Electrical characterization of Al doped ZnO sol-gel thin films

Carlos R. Pérez<sup>1</sup> and Víctor Pantojas<sup>2</sup> <sup>1</sup>UPR-Río Piedras, <sup>2</sup>UPR Cayey

As part of the master's thesis research, a sample holder was designed, built and tested for the electrical characterization of thin film samples. Multiple LabVIEW™ routines were developed for the automation of the characterization processes. In addition, the sample holder was used for resistivity measurements and Hall Effect calculations of Al doped ZnO sol-gel films on fused glass of various Al content. The resistivity measurements were performed using Indium contacts and repeated using sputtered Aluminum-Gold contacts. The resistivity results as a function of temperature were compared for both cases and Hall Effect measurements were conducted when possible.

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### Development of Electrochemical Biosensors for the Detection of Pathogens

#### Yanira Enríquez, Mónica Navarreto, Madeline Díaz, Andrea G. López, and Ana R.Guadalupe UPR-Río Piedras

Gram negative and gram positive bacteria outbreaks, in particular from antibioticresistant strains, are a serious worldwide problem. Not only because of the direct consequences for human beings in terms of morbidity and mortality, but also because it represents a significant burden to an already afflicted public health system. New tracking systems that aid in the successful monitoring and timely recognition of pathogens and their resistant variants are needed. These methods can help in the early identification of pathogens and resistant strains, the design of strategies for their effective control and outbreaks prevention, and the gathering of scientific information for new vaccines development.

Our research aims to develop unique fingerprinting signatures for pathogenic microorganisms based on the development of electrochemical biosensors. These signatures could be constructed from microorganism's complex cell machinery and can include detection signals for specific DNA sequences, proteins, metabolites and cell processes. Currently, we are exploring the detection of *Salmonella* and *Pseudomonas aeuroginosa*, in the first case by monitoring DNA hybridization and, for *Pseudomonas aeuroginosa* by measuring the ribosylation of eEF<sub>2</sub>. Both processes are monitored using ferrocene derivatives as redox labels and glassy carbon electrodes modified with polymeric films. These polymers are synthesized from monomers with reactive groups for anchoring the biosensor recognition elements onto the electrode surfaces. Our results point to the potential use of these organometallic compounds for detecting oligos hybridization and proteins modification, and for the construction of biosensors.

### Gas Sensors based on PEDOT - PSSA Thin Film and Electrospun Fibers

#### Shamir Maldonado Rivera<sup>1</sup> and Nicholas Pinto<sup>2</sup> <sup>1</sup>Specialized in Science and Math School Thomas Armstrong Toro, <sup>2</sup>UPR-Humacao

The conducting polymer poly(3,4-ethylenedioxythiophene) doped with (poly styrene sulfonic acid)-PEDOT-PSSA was used in the form of a thin film and in the form of a fiber to make a gas sensors. These sensors were tested in the presence of methanol which is a very toxic gas. Since the fiber has a higher surface to volume ratio than the thin film, the sensors made from fibers have a faster response time and higher sensitivity. Annealing the sample at 80C removes the effect of the alcohol and the sensors can be reused without loss of sensitivity. The advantages of these sensors are that they are robust, cheap to fabricate and are reusable.

# Charge transport in CVD graphene

Marishka Oquendo Mustafá<sup>1</sup>, Gabriel Calderon<sup>1</sup>, Josee Vedrine<sup>1</sup>, Nicholas J. Pinto<sup>1</sup>, G. Hee<sup>2</sup> and A.T. Johnson Jr.<sup>2</sup> <sup>1</sup>UPR-Humacao, <sup>2</sup>UPENN

Graphene is a mono-layer of sp2 bonded carbon atoms arranged in a honeycomb pattern. Our research has focused on the charge transport in CVD graphene as a function of temperature. The device transconductance was measured as a function of temperature and the channel resistance at the Dirac point calculated at each measured temperature. The device was then exposed to UV irradiation and once again characterized as a function of temperature. UV irradiation is seen to slightly increase the resistance as temperature is lowered. The device was then removed from the vacuum chamber and coated with 1nm of Ag in a thermal evaporator and once again electrically characterized as a function of temperature. Coating graphene with Ag led to reduced mobility and weaker dependence of R as a function of temperature. The results of these series of experiments will be presented in this poster.



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Notes



# Partnership for Research and Education in

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CUH STATION 100<sup>TH</sup>, 908 RD. HUMACAO, Puerto Rico 00791-4300 (787) 850-0000, ext. 9027 Web Page: <u>prem.uprh.edu</u> **NSF-DMR-0934195** 

