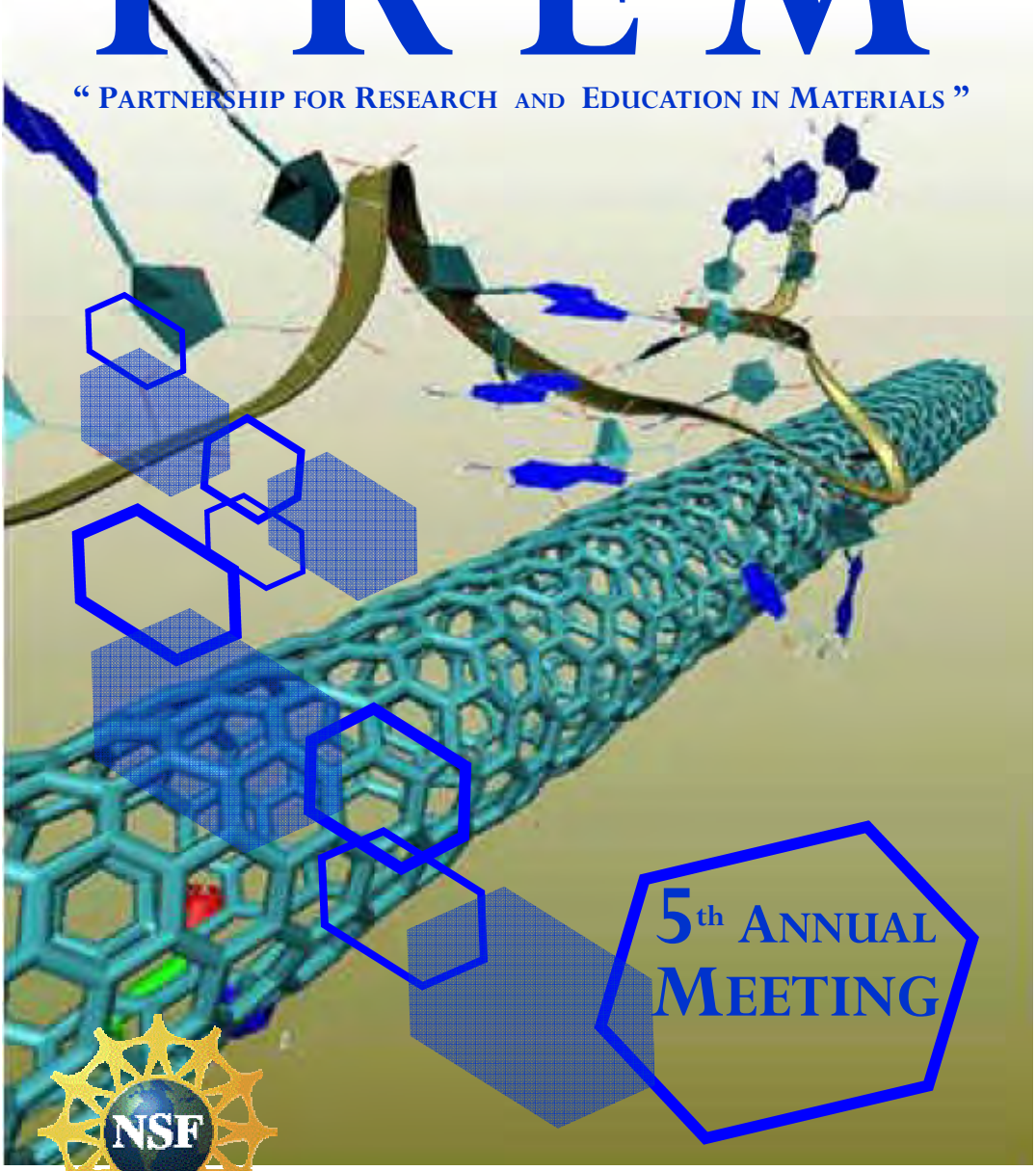
PREM

"Partnership for Research and Education in Materials"



Palmas del Mar- Humacao

November 7, 2008

PROGRAM

Friday November 7, 2008

Four Points by Sheraton Hotel,
Palmas del Mar, Humacao, PR

9:00 - 9:30 AM	Registration & Breakfast
9:30 - 9:40 AM	Welcome Messages
9:40 - 10:30 AM	Presentation and Discussion: ***PREM Program Report: NSF Reverse Site Visit,*** **Idalia Ramos**, UPRH.
10:30 - 12:00 PM	**Oral Presentations**
10:30 - 11:00 AM	***Inelastic and charging energy effects on the electron transport though molecular junctions*** (See **Abstract O1)**, **Natalya Zimbovskaya,** UPRH
11:00 - 11:30 AM	***FEM simulations of a thin film capacitor, combinatorics, and molecular dynamics simulations*** (See **Abstract O2**), **José O. Sotero Esteva**, UPRH
11:30 - 12:00PM	***Electrical characterization of cro sed nanofibers of polyaniline and SnO_2 prepared via electros pinning*** (See **Abstract O3**), **Nicholas Pinto**, UPRH

12:00 - 1:30 PM	**Working Lunch:** Research and Education teams discuss future of collaborative activities
1:30 - 3:00 PM	**Oral Presentations**
1:30 - 2:00PM	***Variation of morphology and crystalline parameters in palladium nanostructures and their applications in hydrogen technology (***See **Abstract O4**), Wilfredo Otaño, UPRC
2:00 - 2:30 PM	***Development of an Eletrochemical Biosensor for Salmonella Detection*** (See **Abstract O5**), **Ana Guadalupe**, UPRRP
2:30 - 3:00 PM	***PREM Outreach Activities*** (See Abstract **O6**), **Ramón Rivera Ocasio**, UPRH
3:00 - 4:30 PM	**Students Posters Presentations**
4:30 - 5:30 PM	Advisory Committee Meets to write Report
5:30 PM	Closing

Oral Presentations

O1: Inelastic and charging energy effects on the electron transport though molecular junctions

Natalya Zimbovskaya
Dept. of Physics and Electronics, UPRH

We consider the effects of stochastic nuclear motions on the electron transport through molecular junctions. We treat a molecule sandwiched between metal electrodes as a quantum dot, and we represent the thermal environment as a phonon both directly or indirectly coupled to the latter. The electron transmission is computedusing the Buttiker model within the scattering matrix formalism. This approach is further developed, and the dephasing parameter is expressed in terms of relevant energies including the thermal energy. Temperature dependencies of current and conductance are analyzed, and the results are applied to study electron transport in conducting polymers. We trace the transition from the Coulomb blockade regime to Kondo regime in the electron transport through the quantum dot occuring when we gradually strengthen the coupling of the dot to the charge reservoirs. The current-voltage (I-V) characteristics are calculated using the equations of motion approach within the nonequilibrium Green's functions formalism (NEGF) beyond the Hartree-Fock approximation. The results are consistent with the results obtained by means of the transition rate equations.

O2: FEM simulations of a thin film capacitor, combinatorics, and molecular dynamics simulations

José O. Sotero[a], Mariem Rosario[b], Preethi Gopu[c], Jorge J.Santiago[b], Preston Moore[c], Myrna Merced[a], DesiréeVelázquez[a], John E. Morales [a], Axel Y. Rivera[a], Melissa López[a], Elizabeth Rivera[a], Francheska Lebrón[d]

[a]Dept. Of Mathematics, UPRH; [b]Dept. of Electrical and Systems Engineering, PENN: [c]Dept. of Chemistry and Biochemistry, USiP; [d]Petra Mercado Bougart High School.

A progress report will be presented on three continuing projects,computer analysis of devices, graphical user interfaces for molecular dynamics (MD) simulations, and combinatorial modeling of polymers, and on a new collaboration started this summer on coarse grain MD simulations.

Finite Element Simulations (FEM) using COMSOL are being carried out to simulate and analyze a thin film type I redox capacitor. The electrodecouples consist of oxidized PProDOT films electrochemically deposited on platinum collectors separated by a sheet of polypropylene porous membrane impregnated with an electrolyte. A combination of 1D domains and 2D domains was used in the FEM simulation of this device to obtain thermal and stress profiles at different scales.

During this year the MOSDAS-GUI VMD plugin graphical user interface (GUI) prototype for constructing polymer-CNT hybrids for MD simulations has evolved into a GUI, now called NT-Poly, that aims to integrate the whole process of preparation, remote execution and analysis of the simulations. On the other hand, The study of purely combinatorial objects applicable to the study of polymer conformations have beencontinued obtaining a formula for counting self avoiding polygons on lattices. Finally, we report about the first preliminary results on a new project that aims to develop a fast and spacial local estimates of the interaction, particularly when water is represented in Coarse grain systems.

O3: Electrical characterization of crossed nanofibers of polyaniline and SnO_2 prepared via electrospinning

Nicholas J. Pinto[a], Katherine Carasquillo[a] and Ritesh Agarwal[b]

[a] Dept. of Physics and Electronics, UPRH

[b] Dept. of Materials Science and Engineering, PENN

Using a simple electrospinning technique, nanofibers of polyaniline and of SnO_2 were prepared in air and within seconds. In the preparation of SnO_2, the only time consuming step was annealing the fibers in air at 600 C for one hour. Polyaniline is an organic conducting polymer which is p-type doped while SnO_2 is an n-doped semiconductor. The junction of these two crossed polymers is expected to reveal interesting properties due to the heterogeneous nature of charge carriers on either side of the junction. Initial studies show that in some samples, the junction behaves as a Schottky diode when measured in air while in others the junction is Ohmic. In the presence of NH_3, the measured currents are reduced due to the de-doping of polyaniline with a concomitant reduction in the device rectification ratio. Removal of NH_3 reproduces the Schottky behavior albeit with much reduced currents. Globally gating the device shows that the diode turn on voltage can be varied. In addition, one can explore many other possibilities of modulating the current in one arm of the device via extremely localized gating using the other arm or via UV/VIS light, making this a useful configuration to investigate charge transport in hetero-junctions at reduced dimensions in organic-inorganic systems.

O4: Variation of morphology and crystalline parameters in palladium nanostructures and their applications in hydrogen technology

Wilfredo Otaño[a], Víctor M. Pantojas[a], Carlos Ortiz-Rodríguez[a], Diego Rodriguez[b], Melvin Arias[a] and Jorge J. Santiago[c]

[a]Dept. of Physics-Mathematics, UPRC; [b]Dept. of Physics, UPRRP ; [c]Dept. of Electrical and System Engineering ,PENN

Nanoscale morphologies and nanocrystalline structures are being developed for hydrogen sensors and heterogeneous catalysis applications. In our group, it has been shown that electrospinning and dc sputtering are effective in the fabrication of such nanostructures. The formation of palladium nanostructures, with high surface area and high aspect ratio, prepared by coating thermally degradable templates of electrospun fibers using dc-magnetron sputtering will be briefly reviewed. It will be shown how the synthesis of these structures has been controlled to produce variations in morphology and crystalline parameters and how those are related to hydrogen sensing and storage. In a set of experiments designed to understand the effect of the plasma processing on the crystalline structure, palladium films were prepared by dc sputtering in an experimental configuration called the "metalhenge", where six substrates are concentrically positioned with respect to the target to minimize variations in deposition conditions. The substrates were at different inclinations with respect to the holder. As a result of that, the incoming palladium flux was deposited at different average angles with respect to the substrate normal of each sample. X-rays diffraction, scanning electron microscopy, transmission electron microscopy and scanning probe microscopy were used to study the nucleation and growth of the palladium crystals. The results obtained will be explained in terms of shadowing and competitive growth.

O5: Development of an Electrochemical Biosensor for Salmonella Detection

Ana Guadalupe
Dep. of Chemistry, UPRP

In this research, we report on the development of a NAB prototype using a polymer modified electrode surface together with an electroactive ferrocene (Fc) derivative. To test this prototype, we are using Salmonella as our target microorganism. Polystyrene (PS) films functionalized with nucleic acid sequences (probes) from the *Salmonella* genome are used to modify carbon electrode surfaces. The hybridization step is detected by looking at the Fc redox process in various schemes. For instance, we are using a Fc label and a water soluble Fc-PEG derivative to design different detection strategies. Our goal is to choose that configuration that affords the best response without the need for the target modification.We have synthesized several PS films and anchored nucleic acid sequences with different lengths at gold and carbon surfaces. The hybridization event is detected electrochemically with a Fc-COOH modified target and with a Fc-PEG conjugate. We observed a small current at the expected redox potential for both Fc compounds without signal amplification. Our experiments are now centered on the optimization of the PS surfaces in terms of probe surface density, PS molecular weight and morphology changes. In all cases, the Glucose Oxidase-Glucose enzyme system will be used to augment the electrochemical signal. Once the best conditions are found, we will concentrate our efforts to build the sensor and to determine its analytical characteristics and potential for real-world applications.

O6: PREM Outreach Activities

Ramón Rivera Ocasio
PREM Program, UPRH

UPRH PREM outreach program has its primary focus on providing educative and hands-on opportunities to kids, youth and adults on Material Science and Nanotechnology. Our education plan during these five years has included school visits, talks and workshops for k-12 students and teachers, summer research experience for high school students, museum collaboration, materials science exhibits, networking with other outreach programs and searching for additional funding to expand activities. Since 2004 PREM Outreach has impacted over 8,000 people: 5,700 in the Strange Matter Exhibition, 825 k-12 students and teachers in workshops, 1200 in open houses, 84 high school students in summer research program, 554 in NanoDays 2008, 15 high students in research with PREM faculty and 220 in opend houses for industry people.. As a result of our efforts PREM has increased its visibility for its compromise with science and education in and out UPRH Campus. During the past year we have increased collaboration with the community and industry. Due to the success on the Strange Matter Exhibit in 2007 we have been making efforts to find a place and funding to begin establishing science museum for the Puerto Rican community.

Students Posters

P1: Electrical characterization of crossed nanofibers of polyaniline and SnO_2 prepared via electrospinning

Katherine Carrasquillo[a], Nicholas Pinto[a] and Ritesh Argawal.[b]

[a]Dept. of Physics, UPRH; [b]Dept. of Materials Science and Engineering, PENN

Crossed nano-junctions of polyaniline and SnO_2 were prepared and electrically characterized in air and in vacuum. Some junctions behave as a Schottky diode in air but in vacuum the currents were too small to measure, while some junctions were Ohmic when measured in air or vacuum. By applying a global gate voltage in the range -30V to +30V we were able to change the diode turn-on voltage from 0.6V to 0.4V respectively. We have used the thermionic emission model of a Schottky junction to analyze the diode parameters. A single nanofiber of SnO_2 was also electrically characterized in a field effect transistor configuration. The fiber is seen to be n-type doped and the device I-V characteristics were analyzed using the standard model of a field effect transistor. The charge mobility (m) was calculated to be $2x10^{-2}$ $cm^2/V\text{-}s$.

P2: Dielectric permittivity of the anti-ferroelectric crystal NH_4H_2

Jean M. Cruz Maurás [a] **and Nicholas Pinto** [b]
[a]Petra Mercado Community High School
[b]Dept. of Physics, UPRH

We report on the anti-ferroelectric single crystal ammonium dihydrogen phosphate (NH_4 H_2 PO_4 - ADP). These crystals were grown from an aqueous solution via slow evaporation. When the solution supersaturates, tetragonal crystals of ADP are formed. A single crystal of ADP was cut and polished to give it a rectangular shape. Silver paint was applied to two opposite sides of the polished crystal to form a capacitor. Dielectric permittivity measurements where made using an impedance analyzer as a function of frequency and temperature. The purpose of this work is to study the phase transition that occurs as temperature is lowered. The ultimate goal is to fabricate ferroelectric capacitors capable of memory storage.

P3: Characterization of Electrospun Fibers using Scanning Probe Microscope

Norberto Hernández Ramos, Melvin Arias, Wilfredo Otaño, Yaritza Figueroa and Enitza Charriez
Dept. of Physics-Mathematics, UPRC

A new Veeco CP-II Scanning Probe Microscope was used to study zinc oxide doped with iron fibers and other morphologies (ZnO-Fe) using Atomic Force (AFM) and Magnetic Force (MFM) microscopy techniques. The AFM and MFM complement the scanning electron microscope (SEM) and EDS to obtain a complete characterization of the topographic and magnetic properties of the different morphologies. The MFM is used to study fibers with different percentages of Fe and the formation of ferromagnetic domains. The ZnO-Fe fibers were created using electrospinning techniques.

P4: TGA/DTA/DT Analysis and UV-VIs spe troscopic data on precursor EC/THF/ DMA/$SnCl_4$ solution for electrospinning SnO_2 nanofibres

Peter J. Rosado[a], T. Chavez-Gil[a], Idalia Ramos[b], Jetsenia Toro[b], Jorge J. Santiago-Aviles[c], Andrew R. McGhie[d]
[a]Interamerican University[b], Dept. of Physics, UPRH ; [c]Dept. of Electrical Engineering, PENN; [d]LRSM, PENN.

Tin oxide nanofibers have been extensively studied for a myriad of uses ranging from gas sensors to potential satellite applications as well as in nano-electronics. The purposes of these analyses were to conduct several thermogravimetrical and UV-Vis optical-spectroscopic tests upon a simple EC/THF/DMA/$SnCl_4$ precursor polymeric solution utilized for electrospinning SnO_2 nanofibres. Thermogravimetry analysis (TGA) and its corresponding derivative (DTG) as well as the temperature differential (DT) methods were conducted on the precursor solution for electrospinning, obtaining successful insights on the characteristics of the solution under thermal stress. Several endothermal and exothermal data concerning fast evaporation of solvents and the decomposition followed by consequent burning of the EC polymer were determined. Instant oxidation measurements of SnO_2 in the region of 400 - 800 ^oC are reported, with the possibility that the remaining residue is SnO_2 as deposited. UV-Vis absorbance spectroscopy was also conducted on the precursor solution in order to characterize their components and its absorption behavior. Results showed the presence of polymer (EC) and tin compound ($SnCl_4$) in solution, forming a possible non-covalent conjugate, as THF/ DMA was used as a background solvent. Further investigations will be followed by issuing an FT-IR profiling in order to determine the bond vibration aspects on the molecules involved in the current research.

P5: Construction of a gas sensor using a single tin oxide nanofiber

Lytzamed Santa [a], Maritza Reyna[a], Anamaris Meléndez[a], Jetsenia Toro[b] and Idalia Ramos[b],
[a]Petra Mercado Community High School
[b]Dept. of Physics, UPRH

A gas sensor of SnO_2 was constructed for the detection of Ethylene. SnO_2 nanofibers were fabricated using electrospinning and a precursor solution composed of Tin Chloride/ Propanol/ 2Propanol/ Ethyl- Cellulose/ Tetrahydrofuran and Dimethylacetamide. The electrospun fibers were collected on a Silicon wafer covered with a Silicon dioxide layer. Then, the fibers were sintered in air at 700°C for 1 hour. SEM/EDS analysis showed that the fibers have nanometric dimensions and are composed of SnO_2. The sensor was constructed by evaporating gold electrodes onto a single nanofiber. The sensing capability was tested by measuring the electrical current through the nanofiber with and without exposition to the gas. Results showed that the sensor is sensitive to the presence of the gas. The detection of Ethylene has important applications in the food industry. For example it can be used to monitor the ripeness of fruits and vegetables.

P6: Evaluation of Composite Electronic Materials based upon Single-Wall Carbon Nanotubes and Highly Charged Poly (aryleneethynylene)s for Supercapacitor Applications

Mariem Rosario[a], Pravas Deria[a], Michael J. Therien[b] and Jorge J. Santiago Aviles[c]

[a]Dept. of Chemistry, UPENN; [b]Dept. of Chemistry, Duke Univ.; [c]Dept. of Electrical and Systems Engineering, PENN

This work explores the use of rigid, polyanionic poly (aryleneethynylene)s that helically wrap single-wall carbon nanotubes (SWNTs) and provide unusual solubility and dispersion characteristics for the SWNTs in several solvents. The polymer-wrapped SWNTs were used to elaborate a variety of electronically active composites with the EAP poly (3,4-propylenedioxythiophene) (PProDOT) that can function as supercapacitor charge storage media. The performance of these composites was compared against that of established PProDOT-based anode and cathode material benchmarks. Results on the morphological, electrochemical as well as simulation studies that will provide insight about the thermo-mechanical properties, redox kinetics, and charge transport in these systems will be presented.

P7: Single-Wall Carbon Nanotube/Poly(p-Napthaleneethynylene) Composites as Electrode Materials for Electrical Double-Layer Capacitors

María Abreu[a], Mariem Rosario[b] and Jorge J. Santiago-Avilés[b]

[a]Dept. of Physics, UPRH

[b]Dept. of Electrical Engineering, UPENN

The objective of this research is prepare, characterize and test new electrode materials and composites based on electroactive polymers (EAPs) and carbon nanotubes for supercapacitor applications. We are preparing and testing new materials to use as electrodes, such as PNES/SWNT, *Single-Wall Carbon Nanotubes and Highly Charged Poly-(p-Napthaleneethynylene)*, and testing it in different electrolytics solutions as: organic media, 0.007M EMIBTI, 0.1M TbAP; and in non-organic media: 1M H_2SO_4, 6M KOH. The way we test it is assembling a double layer capacitor using two platinum modified electrodes suspension of PNES/SWNT in and Cyclic Voltammetry studies. From the obtained voltammograms, a I(mA) vs t (ms) plot is constructed and integrating the area above the curve we can obtain the charge on anode and cathode. Using any of this values, cathodic charge or anodic charge, the capacitance could be calculated by the equation C= Q/V ~ Farads. Results for the CV tests at n (scan rate) between 50 to 1000 mV/s of the prototype show that testing in the aqueous solutions 1.0 M H2SO4 and 6.0 M KOH resulted in CVs very similar in shape to the ideal capacitor behavior, an indication that good capacitance properties were obtained with the PNES/SWNT films in these media. On the other hand, the CV tests in the organic electrolytes resulted in non-symmetrical voltammograms for 0.077 M EMIBTI/PC and 0.10 M TBAP/PC.

P8: Development of a Nucleic Acid Biosensor for the Electrochemical Detection of Salmonella

Madeline Díaz Serrano[a], Dianichia Santana[b], José Ortiz[a], Arelys Rosado[a], Joselyn del Pilar[a], Esther Vega[b] and Ana R.Guadalupe[a]

[a]Dept. of Chemistry, UPRRP

[b]Dept. of Biology,UPRH

In this research, we report on the development of a NAB prototype using a polymer modified electrode surface together with electroactive ferrocene (Fc) derivative. To test this prototype, we are using a 158 bp PCR product of the OmpC gene from Salmonella as our probe. This PCR product has been modified to anchor it in a polystyrene-modified carbon surface as an electrode. The hybridization step is detected by looking at the Fc redox process in various schemes. For instance, we are using a cationic Fc-polymer, a Fc-Ruthenium bimetallic complex, and a water soluble Fc-PEG derivative to design different detection strategies. Our goal is to choose that configuration that affords the best response without the need for the target modification.

We have been able to synthesize several PS films and to anchor nucleic acid sequences with different lengths at gold and carbon surfaces. The hybridization event has been detected electrochemically by the conventional method, which is modifying the target with Fc-CCOH and with the Fc-PEG conjugate. We observed a small current at the potential for the Fc oxidation without signal amplification. Our experiments are now centered on testing the cationic polymer and the bimetallic complexes. We hypothesize that a Glucose Oxidase-Glucose enzyme system will augment the electrochemical signal. Once the best conditions are found, we will concentrate our efforts to build the sensor and to determine its analytical characteristics and potential for real-world applications.

P9: A recurrence equation for estimating self – avoiding cycles

Francheska I. Lebrón López[a] **and José O. Sotero Esteva**[b]

[a]Petra Mercado Bougart Community High School

[b]Dept. of Mathematics, UPRH

This work addresses the problem of determining the number self-avoiding cycles that can be drawn on a rectangular lattice. A rectangular lattice is an array of dots arranged in rows and columns. Segments that form the cycles without intersections connect adjacent points horizontally or vertically. These cycles are represented as a list of column state diagrams. Each column state diagram can be represented as the product transpositions. Then a digraph with vertexes labeled with state diagrams, which are connected by arrows indicating the direction they can take the routes is defined. Each route that you draw in the digraph corresponds to a cycle on the lattice and vice versa, and thus the length of the route in the digraph, will be the same length as the lattice. Therefore, counting paths of length W in the digraph is equivalent to counting cycles on a rectangular lattice of width W. A peculiar property of the digraph is that the digraph corresponding to a lattice of height H has copies of digraphs corresponding to smaller lattice heights. Based on this property we present a recurrence equation that counts a subset of all possible self-avoiding cycles .

P10: Study of *Gallium Nitride Nanofibers*

Anamaris Meléndez[a], Kristle Morales[a], Idalia Ramos[a], Nicholas Pinto[a], Eva Campo[b] and Jorge Santiago[c]

[a]Dept. of Physics, UPRH; [b]Centre Nacional de Microeléctronica, Barcelona, Spain; [c]Dept. of Electrical and Systems Engineering, PENN

Gallium Nitride (GaN) is known to have high thermal conductivity and a wide band gap, characteristics which make it a good material in the field of optoelectronics and in sensing applications. The use of GaN nanofibers is preferred instead of thin films and powders because its sensitivity is expected to increase as the exposed area increases. The simple and inexpensive technique of electrospinning is used in this experiment for the production of long GaN nanofibers. The fibers were made using a precursor solution composed of pure Gallium Nitrate dissolved in Dimethyl-Acetamide (DMA) and a viscous solution of Cellulose acetate dissolved in mixture of DMA and Acetone. Using a tube furnace, they were sintered under a Nitrogen atmosphere to decompose the polymer and to reduce Oxygen contamination. This process was followed by sintering under a NH_3 flow to complete the synthesis of GaN. Morphology analysis was done using a SEM and a profilometer . This analysis showed that the fibers were continuous with diameters ranging from 20 to few hundred nanometers, and lengths of up to a few centimeters. XRD, EDS, and FTIR analysis were used to verify the composition of the samples. Future work will include further composition analysis as well as conduction, sensing and photoluminescence tests.

P11: Interprocess communication for the remote execution of molecular dynamics simulations

Axel Y. Rivera Rodríguez, Desireé E. Velázquez Rios and John E. Morales García
Dept. of Mathematics, UPRH

NT-Pol is a molecular dynamics software coded in Python. It works as an extension of Visual Molecular Dynamics (VMD) software. As part of this project, NT-Pol has been enhanced to remotely execute simulations using NAnoscale Molecular Dynamics (NAMD) software. NT-Pol now takes the information given by the user and sends it to an NT-Pol module running at the server that will create the appropriate NAMD configuration files and execute the molecular dynamic simulation. A data structure based on the contents of a typical NAMD configuration file consisting physical and chemical parameter values was designed and implemented using Python dictionaries. Since the sockets for communication between processes used in the Python version 2.2 provided by VMD 1.8.6 are old and incompatible for this work, the source code of the VMD 1.8.6 was edited and recompiled to use the version 2.5 of Python. This version of VMD can use the modules of Python version 2.5 and the Python modules of VMD. A debian package was created for the distribution of this modified version of VMD. For easy access to the NT-Pol and new VMD binaries, a publicly available repository system using SVN was created.

P12: NT-Pol: an enhanced system for the simulation of nanotube-polymer hybrids

Myrna I. Merced Serrano, John E. Morales García, Melissa López Serrano, and José O. Sotero Esteva
Dept. of Mathematics, UPRH

Molecular dynamics (MD) simulations are commonly used to study different kinds of systems. The aim of this project is to develop a software that provides ease of use for the novice and that is going to be a powerful application for the expert researchers in the area of MD simulations. The first version of the MoSDAS-GUI was capable of setting up MD simulations of nanotube-polymer hybrids. MoSDAS-GUI version beta 2, now renamed as NT-Pol, has a better organized structure and new features. NT-Pol is closer to be an integrated environment for MD simulations of nanotube-polymer hybrids. NT-Pol now can be used to setup, run and see statistical analysis of the MD simulations as axial distribution and distances between the nanotube and the polymer.

Ongoing work on further enhancements to the existing user interface includes a revamping of the main window and the dialogs for specifying the molecules that are going to be constructed. The dialogs for constructing nanotubes and polymers will incorporate new user interface elements including entry fields, buttons, text fields and spinboxes. Furthermore, visual feedback will be provided by showing the molecule status during its formation.

The addition of a toolbox and tabs to the main window will give the user an experience closer to production software. The toolbox will simplify access to functions such as select, move, merge, center and align. By the addition of these features the GUI will be more effective and easier to use.

P13: Field effect devices and sensors based on electrospun polymer assisted tin oxide nanofibers

Richard Rojas[a], Anamaris Meléndez[a], Idalia Ramos[a], Jorge J. Santiago-Avilés [b] and Nicholas J. Pinto [a]
[a]Dept. of Physics, UPRH
[b]Dept. of Electrical and Systems Engineering, PENN

Electrospinning is presented as a facile method of preparing relatively long tin oxide (SnO_2) nanofibers that are robust and stable in air. Upon heat treatment, the fibers collapse into a ribbon-like structure with surfaces that are not smooth, rather, are marked with several interconnected pathways that increase the surface to volume ratio. These nanofibers were electrically characterized in a field effect transistor configuration in vacuum, with and without ultra violet (UV) light exposure. The resultant variable resistor device exhibits n-type behavior having an on/off ratio of ~ 6000. The devices show a direct response to UV with faster response times upon exposure to longer wavelength light. In the presence of UV, the device conductance and mobility increases, reaching a value ~ 2 cm^2/V-s for the 364 nm UV light source, comparable to amorphous Si.

P14: Schottky diodes based on electrospun polyaniline nanofibers: Effects of varying fiber diameter and doping level on device performance

Rut Rivera and Nicholas J. Pinto
Dept. of Physics, UPRH

Nanoscience and nanotechnology has great potential in enhancing the way we look at all of our present day electronic devices and sensors. If only part of this potential can be made into reality, the results will be phenomenal. Devices and sensors based on the use of p-conjugated conducting polymers are considered by many in the field to shape the next generation of cheap and disposable electronic inventions. We report on a simple method called electrospinning to fabricate in air, and within seconds, field effect transistors, Schottky nanodiodes and gas sensors using polyaniline and an inorganic semiconductor. In this talk, we will present our recent results on Schottky nanodiodes made from electrospun polyaniline nanofibers. By varying the fiber diameter and the doping level, we examine the role of surface states on barrier height, charge transport and device performance. The diode characteristics are analyzed using the standard thermionic emission model of a Schottky junction. Clear rectification is observed for diodes fabricated from thick fibers with significantly reduced rectification ratios for diodes fabricated from thinner fibers. Lowering the fiber doping also reduces the forward bias current and the diode rectification ratio. The surface states on the semiconductor exert a weaker influence on diodes fabricated from thinner fibers due to reduced junction area, and for the thinnest fiber, the analysis suggests a charge tunnelling mechanism rather than thermionic emission at the junction.

P15: Electrochemical and Spectroscopic Characterization of Ferrocene Charcones Derivatives

Kenneth Hernandez, Rocío del A. Cardona, Myrna Otaño, Ingrid Montes, Ana R. Guadalupe
Dept. of Chemistry, UPRRP

We will present the electrochemical and spectrophotochemical characterization of three Ferrocene chalcones derivatives by cyclic voltammetry and UV-Vis. These compounds have similar structures which differ only by the position of the nitrogen in the pyridine substitutients. We expect a difference in electrochemical and spectroscopic characteristics due to the nitrogen position. This difference will be useful in future applications as labels, since it will provide a tool for simultaneous detection. The electrochemical experiments were done using a three electrodes cell platinum as working electrode, Ag/AgCl (3M NaCl) and nichrome as reference and auxiliary electrodes respectively. The experiments were done in TBAP/acetonitrile under a nitrogen atmosphere. The data showed that all compounds exhibit a quasi-reversible electrochemical behavior and reversible chemical behavior as evidenced by ΔEp and Ipa/Ipc values. The formal potential for these compounds are: (774,733 and 762)mV for the o, m, p-pyridine derivatives, respectively. Also the number of electron transfer per mol and the diffusion coefficients were calculated using Ferrocene as internal standard. The diffusion coefficient for all compounds are on the order of 10-5cm2/s and the number of electrons transfer per mole is equal to one. The UV-Vis experiments were done in acetonitrile with different concentrations to calculate the molar extinction coefficients. The UV-vis spectra showed characteristic bands for aromatic systems in the UV region and band in the visible that are in accordance with p-extended systems. Our future work consists in the methylation of these compounds to use them as electroactive label to detect DNA hybridization by the electrostatic interactions of our compounds and DNA.

P16: Analytical Solution of a Toroidal Ion Channel with Circular Croos Section

Ramón Mundaray and Lesser Blum
Dept. of Physics, UPRRP

Ion channels are membrane protein complexes and their function is to facilitate the diffusion of ions across biological membranes. Understanding ion channels is still a very open problem, because of the many exquisite tuning details of real life channels.

Here we consider an ion channel of toroidal shape immersed in a conducting medium, confined to a 3-D space. The ions are charged hard spheres, and are treated using a scaling Mean Spherical Approximation (SMSA) and Perfect Screening Theorem (PST). We got the graphs of analytical solutions for radial distribution function the ions.

P17: Measurement of the contact angle of a water droplet on a flat surface

Uriel Vazquez[a], Chi-cheng Chiu[b], Wataru Shinoda[c],D. Vladimir Perez[d], Preston B Moore[e] [d]and Steven O. Nielsen[b]

[a]Centro de Investigacion en Matemáticas, Guanajuato, Mexico; [b]Dept. of Chemistry, The University of Texas at Dallas; [c]Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [d]Dept. of Chemistry and Biochemistry, West Center of Computational Chemistry and Drug Design, USiP.

The surface tension of an oil/water interface is recognized as having tremendous potential to control the organization and assembly of nanoparticles. However, there is no way to measure the surface tension at a nanoscale level directly. It is possible to relate the surface tension with the contact angle, but current theory is flawed and is not applicable to nanoparticles. We report on our progress to correct this theory, specifically inclusion of three-phase contributions to the line tension and the curvature dependent surface tension. We present a new method to measure the contact angle. The density profile of a liquid droplet computed in cylindrical coordinates. Then using the Gibbs dividing surface we get the radius as a function of the height from the surface. Finally, we fit this radius to an ellipse and determine the contact angle of the droplet. We show that the contact angle is size dependent consistent with the curvature dependence of the surface tension.

P18: A study of the distribution of water molecules in molecular dynamics simulations for the estimation of coulomb interactions

Elizabeth Rivera Cruz[a], José O. Sotero Esteva[a], Preston Moore[b]

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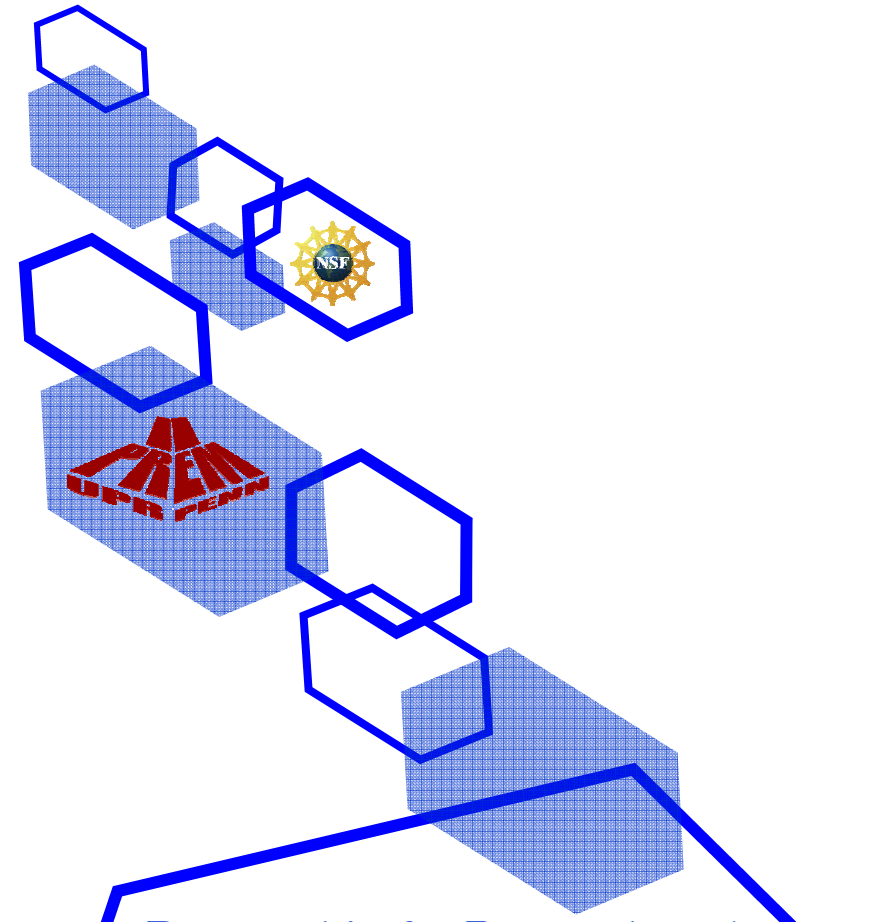
The Ewald sum is the standard algorithm used to compute electrostatic long range interactions energies in molecular dynamics simulations of periodic systems. The aim of this project is to develop a fast and spacial local estimates of the interaction, particularly when water is represented in Coarse grain systems. This could be important in interfaces and protein systems. A molecular dynamics code was modified to study a sample of the media and test the limitations of the new algorithm. This algorithm counts the amount of neighbors of each atom within a spheres of varying radii, considering the periodic boundary condition. A profile of the distribution of neighboring atoms was obtained. This helps to find out how many molecules of water will be between the atoms to be studied and screening effect it makes on charged particles. Eventually, it will help to estimate the screening between particles and replace the Ewald summation in coarse grain simulations.



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