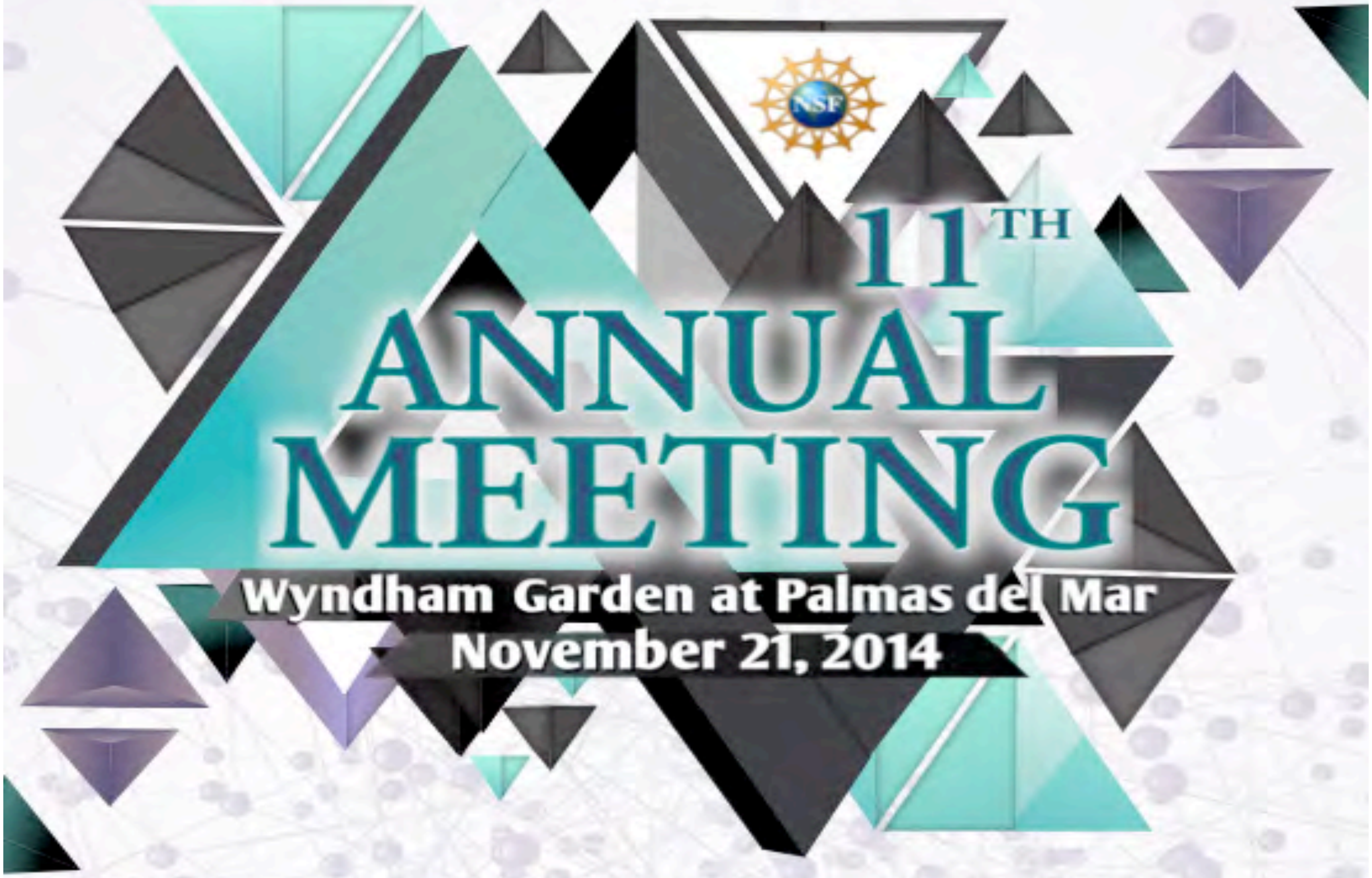


# 11TH ANNUAL MEETING

Wyndham Garden at Palmas del Mar
November 21, 2014

# PREM

PARTNERSHIP FOR RESEARCH & EDUCATION IN MATERIALS

**9:00 - 10:00 AM** **REGISTRATION & BREAKFAST**

**10:00 - 10:10 AM** **WELCOME MESSAGES**

**10:10 - 10:30 AM** **PREM UPDATE**

**Idalia Ramos**, UPRH, PREM PI

**Arjun Yodh**, PREM Co-PI and Director PENN MRSEC

**Andrew McGhie**, Associate Director PENN MRSEC

**10:30- 10:50 AM**

New organic materials with potential semiconducting and optoelectronic properties

**Margarita Ortiz-Marciales**, UPR-Humacao

**10:50- 11:10 AM**

Organic and Ferrocene Devivatives Synthesis and Study of their Properties

**Mirna Rivera**, Jorge Castillo-Ramirez[1], Marianela Pérez-Torres[2]
[1]UPR-Humacao, [2]UPR-RCM

**11:10 - 11:30 AM**

Electrochemistry as a Tool for the Understanding and Synthesis of Electrochemically Active Molecules for the Development of Energy Storage Materials

**Rocío del A. Cardona Couvertier**[1], Jorge Santiago Avilés[2]
[1] UPR-Bayamón [2] PENN

**11:30 - 11:50 AM**

Energy minimizing configurations in finite molecular arrays

**Pablo V. Negrón Marrero**[1], Melissa López Serrano[2], José O. Sotero Esteva[1] and Frances Martínez Miranda[1]
[1]UPR Humacao, [2]UPR Rio Piedras

**11:50 - 12:00 PM** **BREAK**

**12:00 - 1:30 PM** **WORKING LUNCH (Seats Assigned)**

**1:30 - 1:50 PM**

EFFECT OF SPACER ARM LENGTH ON PROTEIN BINDING CAPACITY OF AN AFFINITY MEMBRANE

Vibha Bansal[1] and **Ezio Fasoli**[2]
[1]UPR-Cayey, [2]UPR-Humacao

**1:50 - 2:10 PM**

AFM CHARACTERIZATION OF CONDUCTIVE ORGANIC POLYMERS TO PROBE THEIR MORPHOLOGY AND ELECTRICAL PROPERTIES ON THE NANOSCALE FOR IMPROVED ORGANIC – BASED DEVICES

**Josee Vedrine,** UPR-Humacao

**2:10 - 2:30 PM**

FACILE FABRICATION OF A $MoS_2$/p-Si JUNCTION DIODE

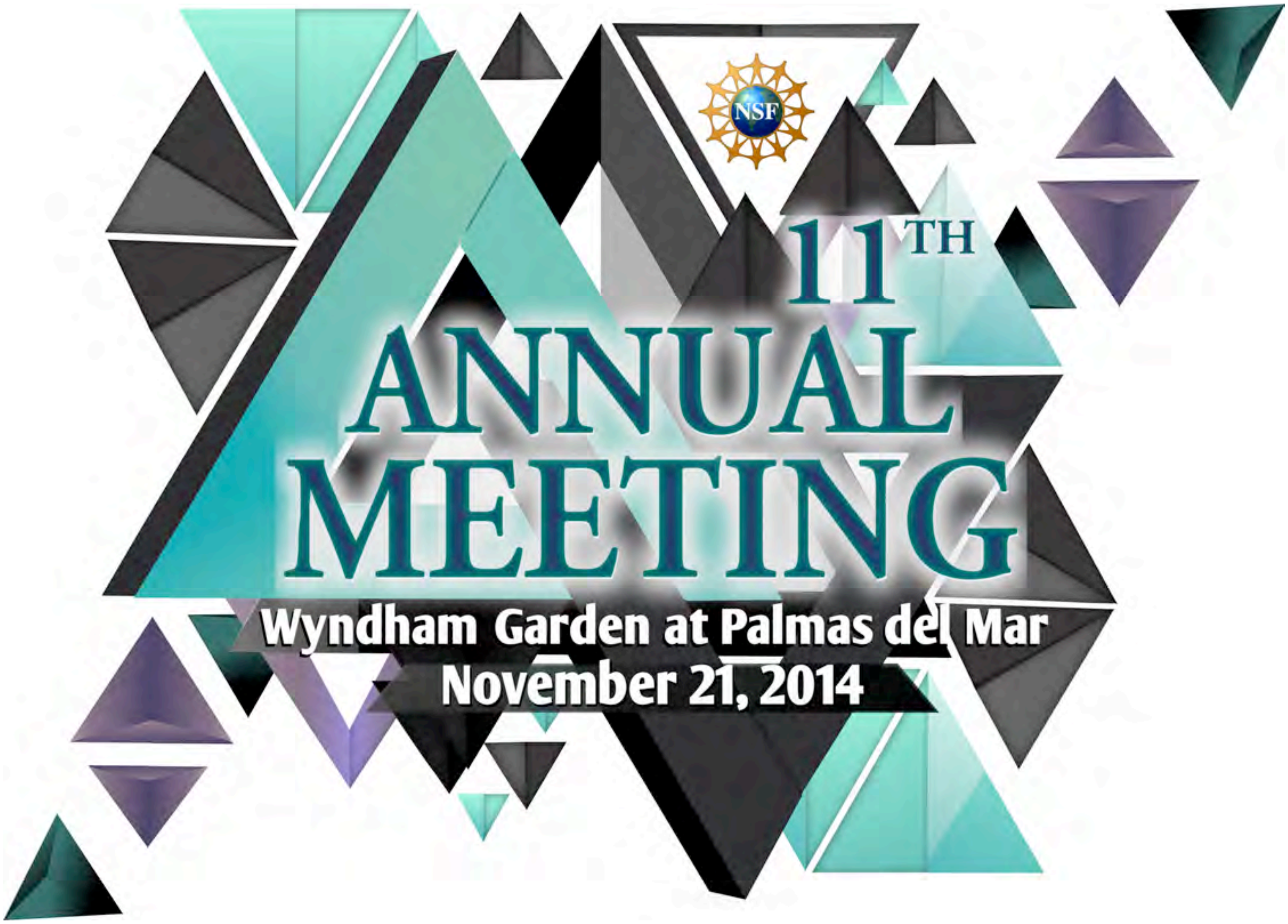
**Nicholas J. Pinto**[1]**,** Alan T. Johnson Jr.[2]
[1]UPR-Humacao, [2]PENN

**2:30 – 3:00 PM** **COFFEE BREAK & POSTER SETUP**

**3:00 - 4:30 PM** **STUDENT POSTER PRESENTATIONS & RECEPTION**

**4:30 - 5:30 PM** **ADVISORY COMMITTEE MEETS TO WRITE REPORT**

**5:30 PM** **CLOSING**



# Oral Research Presentations

# New organic materials with potential semiconducting and optoelectronic properties

Margarita Ortiz-Marciales
UPR-Humacao

The main goal of our proposal is to develop novel organic synthetic methodologies for the preparation of new materials with potential semiconducting and optoelectronic properties. Previously, we have developed new methods for the synthesis of borazines and for the photochemical doping of polyaniline. Thus, we plan to explore these methods to prepare new materials with possible important applications.

In general, our work will focus on the following aims: 1) continue studying our method for the photochemical doping of polyaniline previously developed in collaboration with Dr. MacDiarmid, and study other supporting material to optimize their physical and conductive properties. This project will be in collaboration with Dr. Pinto; 2) to develop new borazine compounds by our previous developed methodology using the reaction of amino alcohols with borane and study their photochemical properties. In addition, we will explore the potential of these materials as semiconductors with Dr. Pinto. This project will be carried out in collaboration with Dr. Gary Molander from UPENN and Dr. Rolando Oyola, who will collaborate in the photochemical studies. 3) To strengthens the educational background of our undergraduate students so that they can succeed in graduate school. Besides, this interdisciplinary project will strengthens our research capability in the search of novel materials and that can open new avenues for a future NSF proposal.

# Organic and Ferrocene derivatives synthesis and study of their properties

Mirna Rivera-Claudio[1] Jorge Castillo-Ramirez[1], Marianela Pérez-Torres[2]
[1]UPR-Humacao, [2]UPR-RCM

Our group has synthesized new chiral ferrocene acetals and used them to modify gold surfaces using self-assembly monolayers (SAMs). SAMs have been extensively used for solid surface modification because they provide a simple route to define the chemical composition of a surface with a highly ordered structure. They have been used for molecular recognition, electron transfer studies, electrocatalysis, immobilization of biomolecules, energy storage systems, and lithium insertion devices. The synthesis and characterization of the ferrocene acetals using FT-IR, NMR, GC-MS and UV/Vis will be presented, as well as results from the surface analysis of the gold surfaces and the evaluation of their anti-cancer properties in vitro. Other ferrocene derivatives has been study using UV/Vis, electrochemistry and Atomic Force Microscopy (AFM).

S

# Electrochemistry as a Tool for the Understanding and Synthesis of Electrochemically Active Molecules for the Development of Energy Storage Materials

Rocío del A. Cardona Couvertier[1], Jorge Santiago Avilés[2]
[1] UPR-Bayamón [2] PENN

Our generation has seen more technological changes than our predecessors. Cellphones, cameras, tablets, and computers have advanced greatly in the last decade, but none the less we still dealing with how to power these devices efficiently. To take advantage of the qualities of these equipment's we need to match their potential with energy storage devices that performed for longer time, without the necessity of been constantly recharged. These devices must also be light, small, and safe for use and have a low environmental impact. Polymer chemistry seems to be an answer. Polymers provide several advantages in the development of electronic devices. For instance, well designed polymers can serve both as electrode material and as separator membrane. They can be synthesized through different routes, including electrochemically methods, which would reduce dramatically the use of solvents and oxidizing agents in compound preparation, which would reducing environmental hazards while also diminishing production costs. We have interested in exploring the electrochemical and chemical synthesis of conducting co-polymers and the preparation of new blends of selected co-polymers with carbon composites such as activated carbon and carbon-derived carbons. This would contribute to enhance research in this area by introducing and characterizing new materials of potential use in sensor chemistry, batteries and permeable membranes development. Thru this presentation we will review the use of electrochemical methods for the synthesis and characterization of molecules as well as the proposed strategies for the synthesis of new electrochemically active co-polymers and their use in energy storage applications.

# Energy minimizing configurations in finite molecular arrays

Pablo V. Negrón Marrero[1], Melissa López Serrano[2],
José O. Sotero Esteva[1], Frances Martínez Miranda[1]

[1]UPR Humacao, [2]UPR Rio Piedras

It has been observed both in laboratory experiments and molecular dynamics simulations, that as the density of a fluid is progressively lowered (keeping the temperature constant), there is a certain ``critical'' density such that if density of the fluid is lower than this critical density, then bubbles or regions with very low density appear within the fluid. To study this phenomena we used a simple molecular model based on the Lennard—Jones potential. We consider finite molecular arrays with no periodicity boundary conditions and try to characterize the ``homogeneity'' of the energy minimizing configurations of such an array. For an array of three molecules and for a tetrahedron (four molecules) we found that there is a critical area and a critical volume respectively, such that if the area or volume of the array is greater than the corresponding critical value, then the uniform configuration of the array is no longer a minimizer of the energy functional for the system. For larger arrays we discuss a procedure for computing local densities in the fluid using Delaunay or Voronoi diagrams, which can be used to visualize regions of lower density in the fluid. Using this technique we analyze an actual molecular dynamics simulation of a fluid that was performed in our Computational Mathematics Laboratory.

# Effect of spacer arm length on protein binding capacity of an affinity membrane

Vibha Bansal[1], Ezio Fasoli[2]
[1]UPR-Cayey, [2]UPR-Humacao

Modification of membranes with ligands that have affinity and selectivity for the target protein provides a very effective tool for the separation of proteins that belong to a narrow size range. In the process of making available new membranes for separation processes, several things need to be considered, such as, the type of membrane, the length of spacer arm (SA), the type of ligand, membrane pore size, and last but not the least the ligand density on the surface of resulting affinity membrane. In our previous studies we demonstrated the need for optimization of spacer arm length for any given membrane based separation using regenerated cellulose (RC) membranes as the templates. We are now trying to determine a relation between ligand size and optimal spacer arm length while targeting the same protein. To this end, two different affinity ligands for plasminogen activator, L-lysine and para-aminobenzamidine were linked to the RC membrane through spacer arms of different lengths and tested for their ability to bind plasminogen activator. Results demonstrated that the optimal spacer arm length depended on ligand size even if the membrane template and protein involved in the separation were the same. The ligand density was also found to be a strong determinant of the protein binding capacity of the membranes.

# AFM Characterization of conductive organic polymers to probe their morphology and electrical properties on the nanoscale for improved organic –based devices.

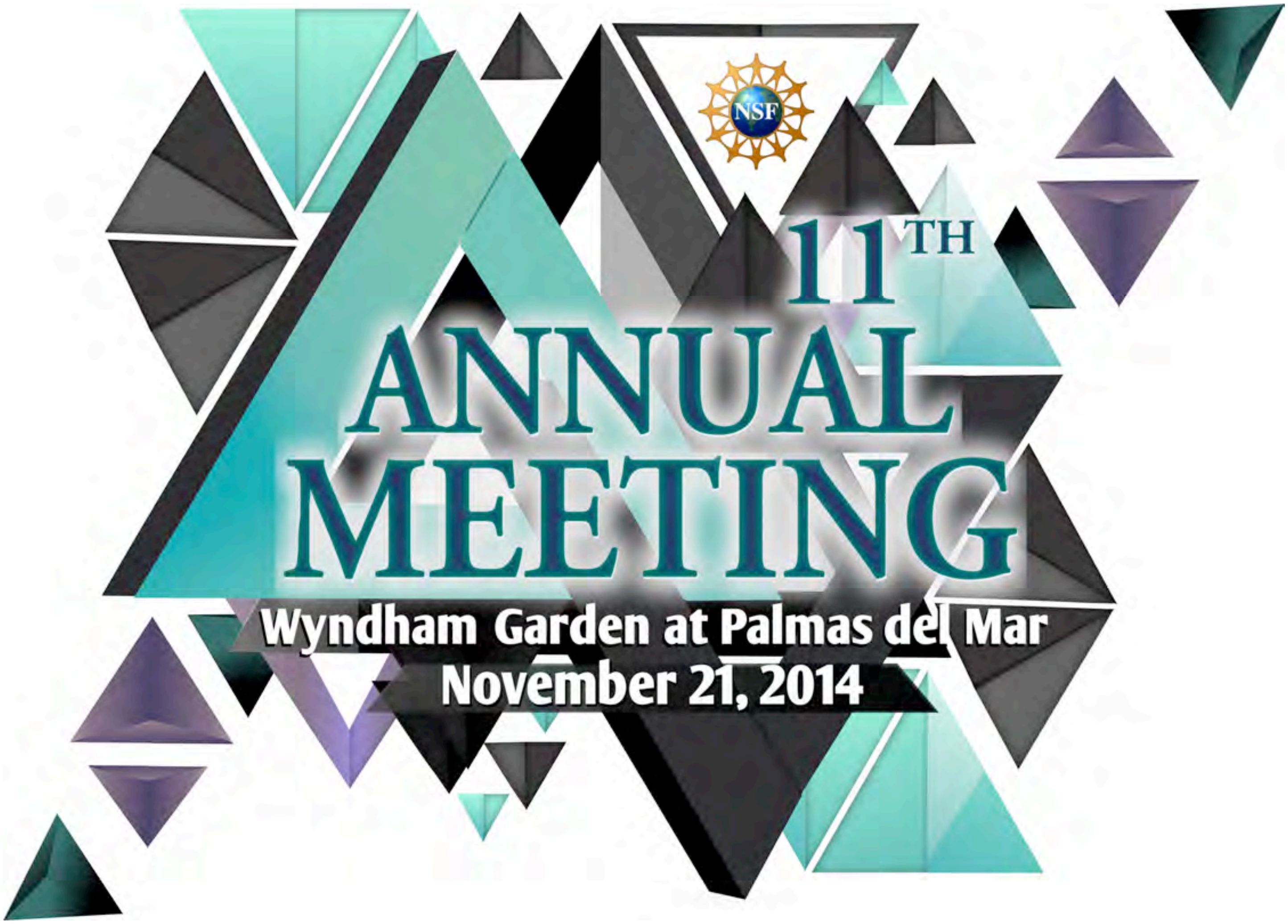
Josee Vedrine
UPR-Humacao

The properties of the organic bulk heterojunction used in device electronics have major implications on device performance. Our work presents the morphology of thermal annealed BHJ thin films *before* deposition of the cathode layer using atomic force microscopy (AFM). Although the driving force that contributes to the aggregation of the P3HT fibril network is not well understood, the contributing factors due to higher temperature annealing either *before* or *after* encapsulation of these networks have a dominant effect on overall device performance. We also present preliminary results of the conductive properties of P3HT thin films annealed for a fixed temperature and varying time. The present work is to better understand optimization parameters for flexible organic based devices, such as solar cells.

# Facile fabrication of a $MoS_2$/*p*-Si junction diode

Nicholas J. Pinto[1], Alan T. Johnson Jr.[2]
[1]UPR-Humacao, [2]PENN

Molybdenum disulfide is a transition metal dichalcogenide with strong covalently bonded S-Mo-S in-plane structures and weak van der Waals bonding between planes. In its bulk form, $MoS_2$ exhibits *n*-type behavior with an indirect band-gap of 1.2eV, while monolayer $MoS_2$ has a direct band gap. Monolayer $MoS_2$ crystals were grown via chemical vapor deposition on Si/$SiO_2$ substrates. These crystals were then transferred to a p-doped Si/$SiO_2$ wafer and formed a diode at the intersection of $MoS_2$ and the substrate. Under normal operation the majority carriers are electrons. The diode operates in air and in vacuum with a turn-on voltage of ~1.5V and a rectification ratio of ~80 at ±2V. Under UV illumination, the diode on-state current increases and this effect is reversible when annealed in air at 70C for a few minutes. UV light is believed to remove electron trapping species thereby increasing the current. A simple circuit connecting the diode to a series resistor was used to test it as an AC signal rectifier. Current was allowed to pass in the positive cycle but significant clipping was observed in the negative cycle demonstrating that this device can be used to generate DC signals that drive most hand-held electronic equipment. The ability to detect UV light and rectify AC signals makes this diode truly multifunctional in addition to consuming low power.



# Poster Presentations

## Fabrication of a glucose sensor using a polyaniline thin film

**P1**

Mereliz Fuertes, Nicholas Pinto
UPR-Humacao

With time science has uncovered the great influence that polymers have had on the technological world making our planet more advanced. The manufacture of sensors using polymers has helped reduce the fabrication cost. In this work we employ the use of a conductive polymer *polyaniline* (PANI) for the fabrication of a Glucose Sensor. For the preparation of the sensor we drop cast a PANI film on a substrate with pre-patterned gold electrodes. The PANI used was doped with *camphoruwulfonic* acid (CSA). Prior to application, this polymer was dissolved in *chloroform* (CHCl3) and filtered. Two types of glucose ($C_6H_{12}O_6$) concentrations (0.1M and 1M) where used for the application to the sensor. After letting the polymer dry, a gold wire connection is made to each end of the electrode with a drop of silver-*polyepoxide* taking care that the two contacts do not touch each other. Our sensor is on a sample holder that is connected to the electrometer which will provide a voltage and also measure the current through the sensor while the application of the glucose is done. We observed that during the application of 0.1M glucose concentration response obtained was faster, while the response that was obtained from 1M was slower and more durable, also its sensitivity is larger than the 0.1M. These results demonstrate that the current which can transmit 1M glucose concentration is greater than 0.1M due to the larger glucose concentration. This conductive polymer polyaniline (PANI) could help in the fabrication of glucose test strips for diabetes patients which would be more lightweight, flexible, and could detect more accurately the amount of glucose in the blood.

## Characterization of Activated Carbon/Polystyrene/PEDOT:PSS electrodes for Electrical Double Layer Capacitors

**P2**

Génesis Ayala, Idalia Ramos
UPR-Humacao

Electrochemical double layer capacitors (EDLCs), are one of the most promising energy-storing devices due to their environmental friendliness, high power density, rapid charging/discharging ability, and long cycle life. In EDLCs, two electrodes are placed in an electrolyte and a voltage is applied between them, forming an electrochemical double layer on both electrodes. They have the high storage capacity of batteries and the fast charging characteristics of capacitors. The capacitance of these devices is determined by the specific surface area and electrical conductivity of electrode materials. Activated Carbon (AC) has been used as the main electrode material in EDLCs due to its extensive surface area, high surface reactivity, pore size distribution, and low cost. The purpose of this research is to prepare and characterize electrodes composed of AC, Poly(3,4-ethylenedioxythiophene-poly(styrenesulfonate) (PEDOT:PSS) and Polystyrene (PS) for EDLCs or super-capacitors. The properties of the electrodes were analyzed using Scanning Electron Microcopy (SEM), Electrical Conductivity Measurements, Energy-dispersive X-ray Spectroscopy (EDS), and X-ray Diffraction (XRD). Carbide Derived Carbon (CDC) will also be studied as a material for electrodes. CDC samples treated with Chloride and Hydrogen for 2h-3h at 200 C, 300 C, 500 C and 600 C were analyzed using SEM, EDS, and XRD.

## P3 Preparation and Characterization of GaN/Chitosan Nanofibers.

Gabriela Nieves, Idalia Ramos
UPR-Humacao

Chitosan(CS) /Poly(vinyl)alcohol (PVA) nanofibers containing gallium nitride (GaN) nanoparticles were fabricated using the electrospinning method. Highly crystalline GaN nanoparticles were produced using a combustion technique with ammonia gas ([Chen.et.al.2011]. Appl.Phys A.). The particles were sonicated for an hour at a frequency of 40kHz and centrifuged at a speed of 3,200 rpm to obtain smaller and dispersed particles, then added to a 60/40 CS/PVA polymeric solution, before electrospinning. The GaN nanoparticles and composite nanofibers were characterized using X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM)/Energy Dispersive Spectroscopy (EDS), and Photoluminescence (PL). The photoluminescence emission spectra of GaN nanoparticles and composite nanofibers were obtain upon 325nm excitation wavelength at room temperature. Results show that the emission peeks range from deep UV (310nm) to the visible light (600nm). In the future, we plan to enhance the PL properties of the nanofibers by using doped GaN and other nanoparticles, and to study their use for optical applications.

## P4 Synthesis and Luminescence Properties of BCNO Phosphors

Joshua L. Robles-García, Anamaris Meléndez Zambrana, Idalia Ramos
UPR-Humacao

Boron carbon oxynitride (BCNO) phosphors have been widely investigated due to their great properties such as been a rare earth free phosphor, inexpensive raw materials, high emission yield, and multi color photoluminescence properties. BCNO has potential applications in lightning (white LEDs), optoelectronics, sensors, and medical applications.The emission wavelength of BCNO can be tuned by changing the ratio of the raw materials and adjusting the sintering conditions. In this work we fully synthesized BCNO using boric acid (BA), urea and polyethylene glycol (PEG) at a mass ratio of 1:2.5:0.3 (BA:Urea:PEG). The raw materials were dissolved in deionized water (DI water) at 85°C until a homogeneous and clear solution was obtained. Then, the temperature was increased to over 100°C to evaporate the water and obtain a white precipitate. The obtained precipitate was grinded and sintered in air from 200°C to 400°C for 45 minutes. X-Ray Diffraction (XRD), Energy Dispersive Spectroscopy (EDS), and Photoluminescence (PL) were used to characterized the phosphors. We have studied how synthesis temperature affects the crystal structure and PL performance of BCNO phosphor nanoparticles. We observed that the PL peak shifts from blue to green when the sintering temperature increases.

## Facile fabrication of a MoS2/p-Si junction diode

P5

William Serrano[1], Nicholas J. Pinto[1], Alan T. Johnson Jr.[2],
Carl Naylor[2], Nicholas Kybert[2]
[1]UPR-Humacao, [2]PENN

A p-n junction diode and field-effect transistor of the transition metal dichalcogenide Molybdenum disulfide (n-doped) and Silicon (p-doped) were characterized. Bulk MoS2 has an n-type behavior with an indirect band-gap of 1.2eV. A monolayer MoS2 has a direct band gap, much bigger than the bulk band-gap. Single layers of MoS2 crystals were grown via CVD technique directly on Si/SiO2 substrates. These crystals were then transferred to the cleaved corner of a p-doped Si/SiO2 substrate forming the p-n heterojunction. The diode operates in air and in vacuum with a turn-on voltage of ~1.5V and a rectification ratio of ~80 at ±2V. Under UV light the diode on-state current increases, this effect is reversible when annealed in air at 70C for a few minutes. The rectifier is characterized connecting the p-n junction in series to a resistor to test the rectification of an AC signal. Current was allowed to pass in the positive cycle but a significant clipping was observed in the negative cycle demonstrating that this device can be used to generate DC signals that drive most hand-held electronic equipment. The ability to detect UV light and rectify AC signals makes this diode truly multifunctional in addition to consuming low power.

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## A two dimensional nonlinear wave equation to model wavefronts indrosophila embryos

P6

Josean Velázquez, Pablo Negrón
UPR-Humacao

In early embryos of many species, including Drosophila, mitosis progresses as a wavefront through the embryo. The speed of the wavefront slows down with cycle. Such signaling is generally assumed to be biochemical but there is evidence of a mechanical component due to displacements during division of the nuclei on the membrane. In this paper we study a model for this phenomena for a two dimensional plane membrane. The model is based on a wave equation with friction in which the speed of propagation and the frictional coefficient depend on the nuclei density. The model equation also includes a nonlinear forcing term that emulates the external (dipole type) forces due to the activation of the nuclei during division. We present some finite element computer simulations using the proposed model and estimate the wavefront speed as a function of the number of nuclei on the membrane.

**P7**

## Computational methods for the detection of nucleation sites in finite molecular arrays

Melissa López, Frances Martínez, Pablo Negrón, José Sotero
UPR-Humacao

Subjecting liquids or gels to low pressures is a method often used to induce cavities. When sonicating a mixture, the nucleation process of a gas bubble occurs at the low pressure region of sonic waves and expands during several high-low pressure oscilations. Understanding the process of nucleation is important to understand the effect of nucleation in materials. When using discrete models of materials such as those used in Molecular Dynamics (MD) simulations distinguishing between regions where there is liquid from those that are gas is not obvious since one is dealing escentially with a set of points.

We propose a method to detect and characterize nucleation sites when a local cavity starts to form by means of Delaunay triangulation and Voronoi diagrams. Using a Voronoi diagram we defined local densities. With those densities we produced 3D density profiles and polytopes that visually represent areas with relatively very low densities. Graphs of the distribution of Voronoi cells volumes where also plotted.

A case study has been done using a molecular simulation of chloroform with and without carbon nanotubes (CNT). The 3D density profiles and polytope representation of low density regions show how nucleation occurs at low pressures. In the presence of CNT it occurs close to the CNT.

**P8**

## Asymmetric Synthesis of β-Azido and β-Amino Alcohols via Optically Pure Epoxides

Hai-Yang Wang, Kun Wang, Melvin de Jesús,
Sandraliz Espinosa, Rosely Quiñones, Margarita Ortiz-Marciales

UPR-Humacao

A highly efficient method for the regio- and stereoselective ring-opening of enantiopure monosubstituted epoxides was developed. Aromatic and aliphatic nonracemic epoxides were obtained in good yield via borane reduction of 2-haloketones catalyzed by the spiroaminoborate ester **1.** The nucleophilic ring-opening reaction by sodium azide in hot water takes place mainly at the most substituted α position of the oxiranes with complete inversion of configuration producing the nonracemic 2-azido-2-substituted ethanols in high yield. In addition, the enantiopure 1,2-azido ethanols were reduced with $PPh_3$ in water/THF to obtain the desired (*R*)-2-amino ethanols with inversion of configuration at the stereogenic center.

## In the search of diamond like carbon

**P9**

Aixa de Jesús Espinosa, José O. Sotero-Esteva
UPR-Humacao

Carbon is the sixth most abundant element in the universe, and its considered unusual in the number of its allotropic structures and the diversity of structural forms, as well as in its broad range of physical properties. It is found free in nature in three allotropic forms: amorphous, graphite, and diamond, whose properties span a range of extremes. In its various forms, is the most extensively examined and widely utilized electrode material in supercapacitors, energy storage devices with high power density that stores electrical charge on high-surface-area conducting materials. Amorphous carbon, which does not have any clear shape, form or crystalline structure, have been used as electrode for supercapacitors. Diamond-like carbon (DLC) is a metastable form of amorphous carbon containing a significant fraction of $sp^3$ bonds. It is the amorphous carbon films combination of Graphite-Like Bond or $sp^2$ and Diamond-Like Bond or $sp^3$. Using Wolffia, Classical Molecular Dynamics Simulations at high temperatures (700 °C) would be conducted, in wich, starting from a well organized diamond structure, a DLC assemblage would be derived eliminating bonds in the original diamond structure, where the bond length surpass the natural distance between atoms.

## Molecular dynamics simulation of adsorption of ionic liquids on porous carbon

**P10**

Jordan Caraballo, José Sotero
UPR-Humacao

The development of new energy storage devices have increased based on their great need and wide range of applications. Supercapacitors have transformed the perspective of what common electrical devices are thanks to their long cycle life, high power capability, and environmentally friendliness. They are electrical devices composed by two electrodes and a dielectric material, best known for their high storage capacity of batteries, and fast charging characteristics of capacitors. An approach to make such devices smaller while preserving the capacity to hold significant amounts of charges depends on the use of materials for electrodes that provide a large surface area for the adsorption of electrolytes. Previous work developed a model for molecular dynamics simulations of carbon nano-onions (CNO) in order to test how well electrodes increased the effective surface area on which Sulfuric Acid ions with water, as electrolytes, were adsorbed. Unlike Sulfuric Acid, ionic liquids (IL) have emerged as promising electrolytes thanks to their interesting and unusual physical properties. The favorable solvation behavior, high ionic mobility, and high thermal stability make IL an interesting electrolyte to work with. CNO electrodes were solvated with $[BMIM][PF_6]$ IL and simulated with controlled presure (1 atm) at room temperature in order to observe and quantify the adsorbtion of cations and anions. The amount of ions adsorbed onto the onions was counted as a measure of effective area. It was found that nano-onions had enough binding energy to stay bundled in plain water as well as in the presence of electrolytes. The effective adsorption area is greater than in a planar electrode. Ions easily penetrate crevice and holes based on their size.

## P11

# Dual input logic AND gate using exfoliated MoS2

Luis M. Martínez[1], Nicholas J. Pinto[1], Alan T. Johnson[2]
[1]UPR-Humacao, [2]PENN

A split-gate field effect transistor (SG-FET) on a Si/SiO2 substrate was fabricated with exfoliated MoS2 (molybdenum disulfide) layers. We applied the MoS2 using the scotch-tape method to place the exfoliated MoS2 between the source and drain contacts of the SG-FET. Using this compound we were able to functionalize the device to act as a dual input logic AND gate. The drain-to-source voltage would be held constant at 1V and the voltages on both gates would be combinations of either 20V or -20V. Here 20V is a logic 1(input) and -20V is a logic 0(input). When 20V are applied to both gates (VG1 and VG2 ), the device would become conductive and the maximum channel current found was 95.7mA. We varied both gate voltages ({2}VG1=20V and VG2=-20V, {3}VG1=-20V and VG2=20V, {4}VG1=-20V and VG2=-20V) to find that the FET would become more resistive i.e. less channel currents, demonstrating the off state of the logic AND gate. This is first study where exfoliated MoS2 is used as a dual input logic AND gate.

## P12

# Fabrication of Organic Bulk Heterojunction Solar Cells on Flexible Substrates

Gabriel Calderón Ortiz[1], Milzaida Merced Sanabria[1], Josee Vedrine-Pauléus[1,2]
[1]UPR-Humacao, [2]Institute of Functional Nanomaterials

The active layer for the organic solar cells fabricated on this project is composed of P3HT:PCBM, poly(3-hexylthiophene) (P3HT) as the electron donor and phenyl-C61-butyric acid methyl ester (PCBM) as the electron acceptor. These polymers were used due to their promising characteristics for devices such as bulk heterojunction solar devices. As substrates we used polyethylene terephthalate (PET), a highly flexible plastic, with indium tin oxide (ITO) as the transparent conducting anode for the device. We use UV lithography technique patterned the ITO substrates on PET; this is to facilitate multiple devices on a single substrate. The fabrication process for pattern transfer incorporates developing and etching processes. We diluted the HCl and D.I. water of 0.5:1 ratio to etch out the ITO. The passivation of PEDOT:PSS and active layer of P3HT:PCBM were deposited on (3.0 sq-cm) of patterned ITO/PET by spin coating method at 5000 rpm and 600 rpm, respectively. The cathode was thermally evaporated with 90 nm Al. The characterization of the device was made using a Keithley 2400 sourcemeter. We also simulated portions of the device using PET on graphene. The virtual model was created using COMSOL Multiphysics software that allows simulation and modeling of physical phenomena of the real world using differential equations. We analyzed the electrical conductivity; we added the electrical currents equations and the contact impedance equations to the model. Our experimental and computational data are preliminary work. As future work, we intend to fabricate cells with distinct parameters using as a guide the ideal conditions of the computational model.

## Synthesis of Affinity Membranes for the purification of plasminogen activators

**P13**

Junellie Cruz[1], Osiris Martínez[1], Christian López[1], Krizia Perez[1],
Vibha Bansal[2,], Ezio Fasoli[1]
[1]UPR-Humacao, [2]UPR-Cayey

Plasminogen activators (PAs) are important therapeutic proteins used as emergency thrombolytic agents for the treatment of thrombovascular disorders such as myocardial infarction and stroke. The separation and purification of these proteins from complex mixtures of cell cultures is a challenging task due to the lack of efficient and suitable processes available. In order to develop a new efficient method for the purification of plasminogen activators, our research was directed towards the development of an effective and accessible affinity membrane-based isolation process that could selectively bind the molecule of interest in a single filtration step. Regenerated cellulose (RC) membranes were chemically modified with spacer arms carrying epoxide or aldehyde moiety which reacted with the hydroxyl moiety of cellulose membrane. Spacer arms of different length (5, 7 and 14 atoms) were tested in order to optimize the process. The spacers were further reacted with two different selective ligands for PAs (para-aminobenzamidine (pABA) and L-Lysine). The modified membranes were characterized in term of epoxide content, ligand density and further used for the purification process. Results showed a 40-fold purification in a single step separation of PA from cell lines HEK-293 conditioned media using these affinity membranes, irrespective of the length of the spacer arm. The system also showed to be very stable and could be reused several times achieving 90% of the PA binding capacity of the membranes even after five cycles of use.

## Synthesis of Chiral Oxetanes via the Enantioselective Reduction of Prochiral 2-Halogenated Ketones

**P14**

Blanca Quiñones, Jennifer García, Rebecca Laguna Carrillo, Ileanne Martínez, Kiara Santiago, Irisbel Guzmán, Viatcheslav Stepanenko, Margarita Ortiz-Marciales
UPR-Humacao

The enantioselective reduction of prochiral 2-halogenated ketones is a practical and effective way to synthesize nonracemic γ-halogenated alcohols, which can be transformed into enantiopure oxetanes. The ring opening of oxetanes with amino compounds can produce a variety of optically active amino alcohols, which are key precursors in the synthesis of biological active compounds, particularly, for the treatment of neurological diseases, such as depression and anxiety. Our work is based on the asymmetric borane–mediated reduction of prochiral β-halogenated aryl ketones to their corresponding optically active alcohols using as catalyst the spiroaminoborate ester derived from ethylene glycol, triisopropyl borate and (*S*)-(-)-diphenyl-2-pyrrolidinemethanol. The enantiopure alcohols were purified by column chromatography with silica gel and characterized by $^{1}$H NMR, $^{13}$C NMR, IR, GC/Chiral Column and GC/MS. The cyclization of the nonracemic alcohols to form the oxetane was successfully achieved using 3 equivalents of potassium *tert*-butoxide as base, obtaining the oxetane in excellent yield.

**P15**

## Influence of the $O_2$:Ar ratio on the physical properties of ZnO thin films grown by the reactive pulsed DC magnetron sputtering technique

Adrián Camacho-Berrios[1], Víctor Pantojas[2], Carlos Ortiz[2],
Wilfredo Otaño[2]
[1]UPR-Río Piedras, [2]UPR-Cayey

The physical properties of ZnO have made this material suitable for many applications. Areas of applications include optoelectronics, UV photodetectors, photovoltaic cells, gas sensors and much more. Some of the properties that make ZnO attractive for these applications are better understood than others. This is the case with the magnetic properties. In the last decade it has been reported that when ZnO is doped with transition metals, it exhibits ferromagnetic ordering above room temperature. In recent years, it has also been reported that room temperature ferromagnetism is achieved when ZnO is doped with rare earth elements. Other groups claim that undoped ZnO can exhibit ferromagnetism due to point defects (oxygen vacancies and zinc interstitial). Lastly, the intercalation of layers of zinc and ZnO has been used to produce a ferromagnetic response. The mechanism for the ferromagnetic ordering is still unclear for ZnO. For this reason, ZnO thin films have been deposited by the reactive magnetron sputtering technique to study how defects influence their magnetic properties. Low sputtering powers and high substrate temperatures have been used to increase adatom mobility during deposition while oxygen to argon ratio and deposition pressure are expected to produce changes in oxygen vacancies, zinc interstitials and properties such as stress and densification. The deposited samples were studied using XRD, AFM, UV-VIS, VSM and MPMS. The results of these studies will be presented and the dependence of several film properties such as roughness, optical band gap and magnetic response on plasma processing parameters will be discussed.

**P16**

## Dielectric Characterization of The N-Doped Polymer [P(NID2OD-T2)]

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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 materials that have a high dielectric constant and low loss tangent are important for device applications our goal was to characterize the dielectric properties of this polymer. 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. Knowing the geometrical capacitance of the sample, the polymer complex dielectric permittivity ($\varepsilon^* = \varepsilon' - i\varepsilon''$) was then calculated. At high frequencies, $\varepsilon'$ 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. Exposure to UV light however caused a decrease in the impedance and an increase in its relaxation time. Our results show that [P(ND12OD-T2)]n is a good candidate for use in electronic devices in a limited temperature range.

**P17**

## Pyrrole/Pyrrole-3-carboxylic Acid Copolymer Matrix for the Development of Metal Ion Sensors

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Conducting polymers are an attractive matrix for electrode surface modifications. These materials, not only can improve the electron transfer kinetics between redox species and the electrode surface, they can be prepared by electropolymerization or chemical methods. The accessibility of monomers with different functional groups allow their chemical derivatization for the covalent attachment of a diversity of molecules that could act as recognition centers for sensing applications. Our experiments are focused toward the development of an electrochemical sensor using an electrode modified with poly (pyrrole-co-pyrrole-3-carboxylic acid) films for the detection of $Fe^{2+}$ and $Fe^{3+}$ ions in biological samples. In this first stage, we have synthesized these films by applying a constant and oxidative potential to a solution of varying monomers molar ratio. Different variables such as as electrolyte solution, applied potential, and monomers concentration were tested. Fourier Transform Infrared Spectroscopy (FT-IR), Chronocoulometry (CC), Cyclic Voltammetry (CV), Square Wave Voltammetry (SWV) were employed to characterize the films. Our next step is the modification of these films with two distinct ferrocene-ligand conjugates that will make possible the selective electrochemical detection of $Fe^{2+}$ and $Fe^{3+}$ in biological samples. Currently, we are working in the synthesis of these conjugates. We will present results on the films preparation and characterization.

**P18**

## Development of An Electrochemical Biosensor for Detecting the ADP-Ribosylation of Proteins by Pathogen Toxins

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*Pseudomonas aeruginosa* (*Pa*) is a gram-negative bacterium that infects an immunocompromised host on the production of virulence factors like the ADP-ribosylating toxin, Exotoxin A (Exo A). This toxin catalyzes the transfer of the ADP-ribose from ß-$NAD^+$ to the eukaryotic elongation factor 2 (eEF-2) affecting its protein activity and as consequence inhibiting the synthesis of important proteins. We are interesting in the construction of an electrochemical biosensor for the detection of *Pa*. We have synthesized and fully characterized seven copolymers of poly-(Sty-co-NAS) as anchoring platforms in the construction of the biosensor. Preliminary results indicated that the highest sensitivity in the electrical response for the communication between the redox biomolecule and the electrode surface was achieved when using the 50:50 poly-(Sty-co-NAS) copolymer. The ADP-ribosylation reaction will be monitored *in vitro* using a ferrocene-labeled NAAD cofactor (Fc-NAAD). The chemical synthesis of Fc-NAAD was done through the reductive amination of the primary amine in the adenine moiety of NAAD using Fc-COH and $NaCNBH_3$. OSWV analysis showed a decrease in the anodic potential of Fc-NAAD (292 mV) when compared with the anodic potential of Fc-COH (508 mV). Fc-NAAD shows chemical reversibility (Ipa/Ipc = 1.087 uA at 200 mV/s) and electrochemical quasi-reversibility. We are currently studying various clinical strains of *Pa* isolates to detect the presence of Exo A and determine if the protein is able of ADP-ribosylating the eEF-2 in the presence of Fc-NAAD. Concurrently we are optimizing the attachment of Fc-NAAD to the electrode surface and began the work for the sensor testing the post-translational modification of eEF-2.

## P19 Synthesis of 1- Benzazepines as Nicotinic Acetylcholine Agonist

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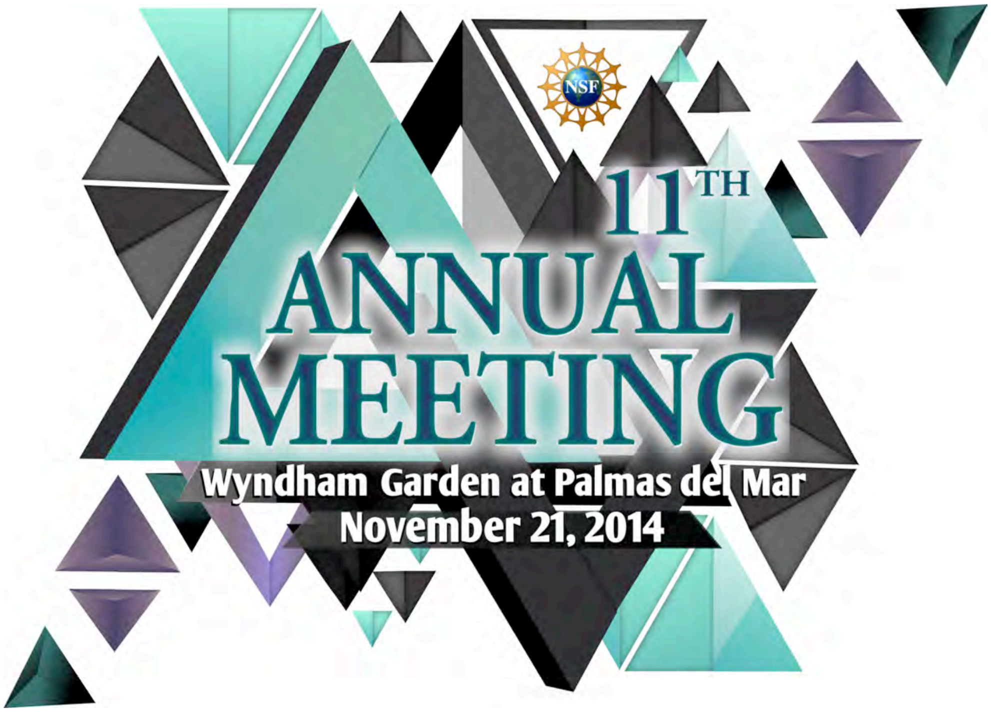
Cyclic and acyclic anilines are very important organic compounds that are used as intermediates for the synthesis of a variety of pharmaceutical products. Aniline derivatives, such as benzazepines have been recently studied as a relevant compound in biological systems. The benzazepines has important biological activity for the treatment of degenerative neurological diseases, such as Alzheimer's and Parkinson. In this investigation we are trying to synthesize analogues of 1-benzazepine to use them as nicotinic acetylcholine agonist using a method developed in our laboratory. The development of the new efficient method of our laboratory to re-arrange O- silylated oximes on reduction of boron triflouride/ borane system. In this project we are synthesizing 7-methoxy-2,4,5-tetrahydro-1-Benzazepine and 7,8-dimethoxy-2,4,5-tetrahydro-1-benzazepine to be study and analyzed his biological activity and toxicology.

# Notes



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