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## PENN-UPRH Partnership for Research and Education in Materials

# Program

PREM Annual Meeting  
December 7<sup>th</sup>, 2018

University of Puerto Rico at Humacao  
Call Box 860, Humacao, PR 00791  
(787) 850-0000, ext. 9027



Sheraton Old San Juan Hotel  
100 Brumbaugh Street  
San Juan, Puerto Rico



## Abbreviations

<b>UPRH</b>	University of Puerto Rico at Humacao
<b>UPRC</b>	University of Puerto Rico at Cayey
<b>UPRB</b>	University of Puerto Rico at Bayamón
<b>RPGHS</b>	Ramón Power and Giralt High School, Humacao
<b>PENN</b>	University of Pennsylvania
<b>LRSM</b>	Laboratory for Research on the Structure of Matter
<b>USP</b>	University of the Sciences in Philadelphia
<b>CMU</b>	Carnegie Mellon University
<b>UFPR</b>	Universidade Federal do Parana, Brasil

## Notes

### Legend:

Names of undergraduates and high school students: Underlined

**Names of PREM faculty**: bold

**P-18** “Low Cost Starch-based Supercapacitors: Process Development”, Fangqiong Yang<sup>1</sup>, Jorge J. **Santiago-Avilés**<sup>1</sup>, Idalia **Ramos**<sup>2</sup>, Cyro Ketzer Saul<sup>1,3</sup>, <sup>1</sup>PENN, <sup>2</sup>UPRH, <sup>3</sup>UFPR

Over the last two decades, the need for electric power sources and storage systems has increased rapidly due to the miniaturization and portability of electronic devices. The public is worried of carbon input during manufacture, disposal and safety during use. In this work we present results on a work in progress related to the development of high surface area carbons for low cost, wearable safe supercapacitors using hydrothermal carbonization (HTC). The final objective of this research is to build EDLC with capacitance near or in excess of 100 F/g from the electrodes. The methodology involves, a uniform mixture of 0.8 M starch and distilled water transferred into a stainless-steel autoclave, heated at 200 °C for both 4 h and 6 h in an isotherm oven, and cooled to room temperature. Part of the black precipitate was thermally annealed at 800 °C with a heating rate of 20 °C/min and 2.5 h activation time under constant flow of nitrogen (N<sub>2</sub>) in a tube furnace. Further procedures to activate the carbon spheres are underway. Starch in acetic acid has the highest yield comparing to starch in distilled water, phosphoric acid, or sulfuric acid. Reason for this are being explored.

## Program

Friday December 7<sup>th</sup>, 2018  
Sheraton Old San Juan, San Juan, Puerto Rico

- 2:00 PM** Registration and Refreshments  
**Room: La Puntilla**
- 3:00 PM** Welcome
  - Idalia **Ramos**, UPRH
  - Arjun **Yodh**, PENN
- 3:10 PM** *Overview of PREM* (workforce development/ management /successes/plans )
  - Idalia Ramos
- 3:40 PM** *Overview of PREM Research /Q&A*  
  
 3:40 PM: **IRG-1: Multifunctional Nanodevices from Optoelectronic Devices**, Nicholas Pinto, UPRH  
  
 4:10 PM: **IRG-2: Nanoscale Interactions of Macromolecules at Soft and Hard Interfaces**, Ezio Fasoli, UPRH
- 4:40 PM** *Overview of PREM Education*, Gilda **Jiménez**, UPRH
- 5:10 PM** Coffee Break
- 5:20 PM** Group Discussion (enhancing collaborations and productivity)
- 6:30 PM** Working Dinner (continue discussion)
- 8:00 PM** Poster Session  
**Room: La Garita**
- 9:00 PM** Advisory Board meets to finish report.
- 10:00 PM** Closing

## Poster Presentations

(Abstracts, page 5)

- P-1** "Interaction of Brilliant Cresyl Blue with Gold Nanoparticles Modified with  $\beta$ -Cyclodextrin as a Sensor for Warfarin", Nicole M. González<sup>1</sup>, Amee L. López<sup>2</sup> & Rolando **Oyola**<sup>1</sup>, <sup>1</sup>UPRH, <sup>2</sup>RPGHS
- P-2** "Crystal Structure Editor for Molecular Dynamics Simulations of Metals ", Paola A. Alicea-Román, José O. **Sotero- Esteva** & Rolando **Oyola-Martínez**, UPRH
- P-3** "Understanding the Effects of Ligand Density on Protein Capture by Affinity Membranes", Edgardo Sánchez- Rivas<sup>1</sup>, Ivan D. **Dmochowski**<sup>2</sup>, Ezio **Fasoli**<sup>3</sup> & Vibha **Bansal**<sup>1</sup>, <sup>1</sup>UPRC, <sup>2</sup>PENN, <sup>3</sup>UPRH
- P-4** "In situ analysis and imaging of aromatic amidine in solid phase", Adaliz Torres-Rosado<sup>1</sup>, Christian Ortiz<sup>1</sup>, Adriana Santiago<sup>2,3</sup>, Ivan **Dmochowski**<sup>3</sup>, Sean Yeldell<sup>3</sup>, Rolando **Oyola**<sup>1</sup>, José **Sotero**<sup>1</sup>, Vibha **Bansal**<sup>2</sup> & Ezio **Fasoli**<sup>1</sup>, <sup>1</sup>UPRH, <sup>2</sup>UPRC, <sup>3</sup>PENN
- P-5** "Affinity membrane model for testing correction of confocal laser microscopy images", Jomarie Jiménez-González<sup>1</sup>, Ezio **Fasoli**<sup>1</sup>, José O. Sotero **Esteva**<sup>1</sup>, Junellie L. Cruz Lebrón<sup>1</sup>, Adaliz Torres-Rosado<sup>1</sup> & Ivan **Dmoschowski**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN
- P-6** "Confocal Laser Microscope for the determination of ligand density and protein binding using affinity membranes", Junellie Cruz-Lebrón<sup>1</sup>, Sean Yeldell<sup>2</sup>, José **Sotero**<sup>1</sup>, Vibha **Bansal**<sup>3</sup>, Ivan **Dmoschowski**<sup>2</sup> & Ezio **Fasoli**<sup>1</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN, <sup>3</sup>UPRC

- P-17** "Exploring Nano: a successful education & outreach PREM program", Junellie L. Cruz-Lebrón, Kelotchi Figueroa & Gilda **Jiménez**, UPRH

The UPRH-PREM education and outreach program for the Fall 2018 semester included activities for different ages and school levels: visits to schools, hands-on demonstrations, and laboratory tours for K-12 students and teachers, and seminars for the college community. We visited elementary schools to motivate children into studying science with hands-on demonstrations. Some of the demos included *Measure yourself, Smelly balloon and Hydrogels, produced by the NSF-funded NISEnet*. Demonstrations for middle schools included *Kinetic sand, UV bracelets, Sunblock, & ferrofluids* (also from NISEnet). HS students participated in open houses and were introduced to materials research with talks and demonstrations. We also integrated alumni from our Summer Research Program for HS students, Experimenta con PREM (ECP) to research for Science Fair with PREM faculty. All these events were organized by the PREM Student Education Representatives and the PREM Outreach Coordinator. Dozens of PREM students, faculty and other volunteers collaborated with in these outreach activities. Future plans include visiting new schools with hands on demonstrations, recruit students for ECP 2019, and bring materials science demonstrations and talks to communities.

**P-16** “Electronic transport in CVD-grown WSe<sub>2</sub>” Ahmad Matar Abed, Anamaris Meléndez, Nicholas J. **Pinto** & Idalia **Ramos**, UPRH

Two-dimensional transition metal dichalcogenides have attracted great attention due to their potential applications in optoelectronics. Of these, tungsten diselenide (WSe<sub>2</sub>) is a semiconductor with a trigonal structure, and a small bandgap ~1.6eV. Here we report electronic transport measurements of CVD-grown large area WSe<sub>2</sub> samples, provided by the 2D Crystal Consortium at Penn State University. The devices studied were a Schottky diode and a Field Effect Transistor (FET). To prepare them, the WSe<sub>2</sub> films were transferred onto a doped Si/SiO<sub>2</sub> wafer with pre-patterned gold electrodes over the oxide surface. The diode parameters were analyzed using the standard thermionic emission model of a Schottky junction. Results obtained at room temperature include a forward turn-on voltage of ~0.46 V, ON to OFF current ratio at ± 1 V of ~1100, barrier height of 0.41 eV and an ideality parameter of n~1.3. The device was tested as a half-wave rectifier showing a rectification ratio of 1150 with an output/input voltage ratio of 46.3%. In the FET, the bottom-gated device shows a 2D VRH transport mechanism in the temperature range from 300 K to 50 K. Ongoing work includes studying the temperature-dependent transport mechanisms of the Schottky diode.

**P-7** “A Novel Colorimetric and Fluorescent Assay for Aromatic Aldehydes Detection”, Andrea Marcano-Delgado & Ezio **Fasoli**, UPRH

**P-8** “Electrospun PEDOT:PSS nanoribbon field effect transistor with a ferroelectric polymer gate insulator”, Alondra Rosario-Soto & Nicholas J. **Pinto**, UPRH

**P-9** “Electrospun Carbon Nanotube-PEDOT:PSS Hydrogel Nanofibers”, Angelo Porcu-Madau<sup>1</sup>, Ahmad Matar<sup>1</sup>, Anamaris Melendez<sup>1</sup>, Idalia **Ramos**<sup>1</sup> & Mohammad **Islam**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

**P-10** “Synthesis of New Organic Borazine Compounds derived from 1-Amino-2-Naphthol and 3-Amino-2-Naphthol, and Characterization by their Chemical and Physical Properties”, José L. Rosario-Collazo, Yareslie Cruz, Melvin De Jesús & Margarita **Ortiz-Marciales**, UPRH

**P-11** “Synthesis of Organic Borazine Derived from Norephedrine for the Application in Electronic Devices and Electrochemistry”, Yareslie Cruz-Rivera, Christian Ortiz-Huertas, José L. Rosario, Melvin De Jesús, Anamaris Meléndez, Idalia **Ramos**, Nicholas **Pinto** & Margarita **Ortiz**, UPRH

**P-12** “Sucrose-based graphene oxide field effect transistor”, José Pérez-Gordillo, Ahmad Matar, Anamaris Meléndez, Nicholas **Pinto** & Idalia **Ramos**, UPRH

**P-13** “A Schottky diode fabricated by crossing MoS<sub>2</sub> with an electro-spun PEDOT-PSS nano-ribbon”, Kelotchi Figueroa Nieves<sup>1</sup>, José L. Pérez<sup>1</sup>, Ahmad Matar<sup>1</sup>, Idalia **Ramos**<sup>1</sup>, Nicholas J. **Pinto**<sup>1</sup>, Meng-Qiang Zhao<sup>2</sup> & A.T. Charlie **Johnson**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

- P-14** “Synthesis of Acetoxy-1-ferrocenyl-1-ethanol as a Building Block in the Functionalization of Graphene”, Naomi M. Rivera-Martínez, Margarita **Ortiz-Marciales**, Luis E. Piñero-Santiago, Anamaris Meléndez-Zambrana & Idalia **Ramos-Colón**, UPRH
- P-15** “Effect of varying the gate voltage scan rate in a MoS<sub>2</sub>/ferroelectric polymer field effect transistor”, Luis M. Rijos<sup>1</sup>, Nicholas J. **Pinto**<sup>1</sup>, Meng-Qiang Zhao<sup>2</sup>, William M. Parkin<sup>2</sup> & A.T. Charlie **Johnson**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN
- P-16** “Electronic transport in CVD-grown WSe<sub>2</sub>”, Ahmad Matar Abed, Anamaris Meléndez, Nicholas J. **Pinto** & Idalia **Ramos**, UPRH
- P-17** “Exploring Nano: a successful education & outreach UPRH-PREM program”, Junellie L. Cruz-Lebrón, Kelotchi Figueroa & Gilda **Jiménez**, UPRH
- P-18** “Low Cost Starch-based Supercapacitors: Process Development”, Fangqiong Yang<sup>1</sup>, Jorge J. **Santiago-Avilés**<sup>1</sup>, Idalia **Ramos**<sup>2</sup>, Cyro Ketzer Saul<sup>1,3</sup>, <sup>1</sup>PENN, <sup>2</sup>UPRH, <sup>3</sup>UFPR

- P-15** “Effect of varying the gate voltage scan rate in a MoS<sub>2</sub>/ferroelectric polymer field effect transistor”, Luis M. Rijos<sup>1</sup>, Nicholas J. **Pinto**<sup>1</sup>, Meng-Qiang Zhao<sup>2</sup>, William M. Parkin<sup>2</sup> & A.T. Charlie **Johnson**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

A ferroelectric field effect transistor (FE-FET) using chemical vapor deposition (CVD) grown monolayer MoS<sub>2</sub> as the semiconductor was fabricated and tested at room temperature. Ferroelectric poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE was used as the gate insulator, and the effects of varying the gate voltage scan rate from 200 mV/s to 4 mV/s on device performance were investigated. Prior to the device switching on, a negative trans-conductance was observed for all scan rates. It was followed by a rapid increase in the channel current to the on state, corresponding to the polarized down configuration of the FE. This effect was independent of the drain-source voltage. Our results revealed a narrowing in the memory window width, an increase in the mobility ( $\mu$ ) from 0.02 – 10 cm<sup>2</sup>/V-s, and a decrease in the sub-threshold voltage swing (SS) as the scan rate was lowered. These parameters appeared to stabilize at slower scan rates suggesting an asymptotic limit to their values. A model based on nucleation and unrestricted domain growth was used to explain these results. By lowering the gate voltage scan rate, the performance of polymer based FE-FET's can therefore be improved.

- P-14** "Synthesis of Acetoxy-1-ferrocenyl-1-ethanol as a Building Block in the Functionalization of Graphene", Naomi M. Rivera Martínez, Margarita **Ortiz-Marciales**, Luis E. Piñero-**Santiago**, Anamaris Meléndez-Zambrana & Idalia **Ramos-Colón**, UPRH

Ferrocene is an organometallic compound that due to its electronic properties, stability, and its easy functionalization has many applications in materials science as sensors, catalysts, and electroactive materials. Moreover, ferrocenyl compounds have the potential to undergo reversible oxidation providing suitable conditions for electrochemical sensor applications. Graphene is a well-known carbon material with  $sp^2$  hybridization that is closely packed in hexagonal lattice structures with electrical conductivity, high thermal conductivity, and elasticity. We are presently interested in developing key ferrocenyl compounds that when chemically bound to graphene can enhance conductivity properties for advanced electronic applications. Initially, 1-ferrocenyl-1-ethanol was prepared in 82% crude yield by the reduction of acetyl ferrocene with  $NaBH_4$  in methanol. Then, the 1-acetoxyethyl ferrocene was prepared by the acetylation of the alcohol with acetic anhydride, dimethylaminopyridine (DMAP), and triethylamine in  $CH_2Cl_2$  with an 83% crude yield. In addition, the 1-acetoxyethyl group was successfully displaced by  $NaN_3$  obtaining the 1-azido ferrocenyl ethane in 43% purified yield. These results have significant implications for the understanding of the behavior of ferrocenyl compounds to find the appropriate conditions for its functionalization. The prepared compounds were characterized by FT-IR and  $^1H$  and  $^{13}C$ -NMR. Presently, we are developing new methods to chemically bind the prepared ferrocenyl compounds to graphene oxide.

## Abstracts

## Poster Presentations

**P-13** “A Schottky diode fabricated by crossing MoS<sub>2</sub> with an electro-spun PEDOT-PSS nano-ribbon”, Kelotchi Figueroa-Nieves<sup>1</sup>, José L. Pérez<sup>1</sup>, Ahmad Matar<sup>1</sup>, Idalia **Ramos**<sup>1</sup>, Nicholas J. **Pinto**<sup>1</sup>, Meng-Qiang Zhao<sup>2</sup> & A.T. Charlie **Johnson**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

Monolayer MoS<sub>2</sub> was grown via chemical vapor deposition while PEDOT-PSS nanoribbons were fabricated via electrospinning. Each of these materials was electrically characterized separately in a field effect transistor configuration using SiO<sub>2</sub> as the gate dielectric. MoS<sub>2</sub> exhibited n-type behavior while PEDOT-PSS showed an Ohmic response. By crossing MoS<sub>2</sub> with a PEDOT-PSS nanoribbon, the current-voltage curve across the junction was non-linear and similar to that of a diode. When a positive (negative) voltage was applied to PEDOT-PSS (MoS<sub>2</sub>), the device turned on in the first quadrant of the I-V curve. Reversing the external connections resulted in the diode turning on in the third quadrant. The rectification ratio was 625 and the turn-on voltage was 0.1V. The device output data was analyzed using the standard thermionic emission model of a Schottky junction yielding an ideality parameter of 1.9 and a barrier height of 0.18eV.

A low turn voltage from our diode makes it better for small signal detection and has the advantages of having a higher ac rectification efficiency and a lower power loss compared to standard p-n diodes.

This work was supported by NSF under grants: RUI (1800262) and PREM (DMR-1523463).



**P-12** “Sucrose-based graphene oxide field effect transistor”,  
José Pérez-Gordillo, Anamaris Meléndez, Ahmad Matar,  
Idalia **Ramos** & Nicholas **Pinto**, UPRH

Graphene Oxide (GO) is a versatile material for applications ranging from optoelectronic devices to drug delivery. GO films were produced by hydrothermal carbonization of a 0.6 M sucrose solution, for 2 h at 200°C. The materials and methods used make these films easy to fabricate, inexpensive and environmentally friendly. The films were subjected to a pyrolysis treatment under N<sub>2</sub> at 800°C to reduce oxygen content and improve their electrical conductivity. Their structure, morphology and composition were characterized using XRD, SEM and EDS. A back-gated Field Effect Transistor was constructed by transferring a film onto a Si/SiO<sub>2</sub> substrate and evaporating gold contacts over it. The GO FET shows enhanced p-type behavior in vacuum, with On/Off ratio of 57 and a carrier mobility of  $9.1 \times 10^{-3} \text{ cm}^2/\text{V-s}$  and a charge density of  $4.14 \times 10^{11} \text{ electrons/cm}^2$ .

**P-1** “Interaction of Brilliant Cresyl Blue with Gold Nanoparticles modified with  $\beta$ -Cyclodextrin as a Sensor for Warfarin”, Nicole González-Vélez<sup>1</sup>, Amee L. López<sup>2</sup> & Rolando **Oyola**<sup>1</sup>, <sup>1</sup>UPRH, <sup>2</sup>RPGHS

Nanoparticles are essential tool for chemical sensing. Warfarin is a well-known anticoagulant with high affinity to human serum albumin and its concentration varies with dosage. In this work, we propose a chemical sensor for warfarin based on the interaction of Brilliant Cresyl Blue (BCB) with gold nanoparticles modified with  $\beta$ -cyclodextrin ( $\beta$ CDAuNP). BCB is a fluorescent dye that binds in a 1:1 ratio to  $\beta$ -cyclodextrin. In the BCB–AuNP assembly, NIR fluorescent BCB molecules act as fluorophores and are used for signal transduction, while AuNPs act as quenchers to quench the nearby fluorescent BCB molecules. In the presence of warfarin, fluorescent BCB molecules detached from AuNPs and restored their fluorescence. Warfarin concentrations of micromolar to nanomolar can be detected with this sensor. This sensor shows advantages of NIR fluorescence such as less interference due to inner filter effects, lower detection limit, and higher sensitivity. This work is supported by NSF-UPRH Penn-PREM Program (NSF-DMR-1523463).

**P-2** “Crystal Structure Editor for Molecular Dynamics Simulations of Metals”, Paola Alicea Román, José O. **Sotero-Esteve** & Rolando **Oyola-Martínez**, UPRH

The stacking arrangement of atoms in a particular way creates crystals. There are different structures systems, for each atom there is a specific volume, distance and position. In close packed structures there is presence of a small unoccupied space or hole between the atoms, while in non-close packed structure this room is much bigger. These areas are important, because other atoms or ions can fill them. Most metal crystals are arranged in a close packed structure, such as a face-centered. Also, in a body-centered structure which is not closed packed, but it is part of the cubic system. Metals, whose atoms arrange forming crystal structures are strong, function as good electricity conductors, and are malleable and ductile. They also have polymorphism phases where certain temperatures will affect their structure.

The aim of this project was to make computer programs with the appropriated stacking arrangements of atoms and their distance for the creation of metal crystal structures. This to study the relations between metal particles and peptides. As a first step we added a crystal editor to our molecular dynamic simulator. Molecular Dynamics studies the physical relations of atoms and molecules. The system used is cubic crystals, that includes Body-centered and Face-centered structures. The programs were written in Python and were added to Wolffia, which is an open source program developed for molecular dynamics simulations created by our Computational Group. Further goals include analyzing if a metal can modulate the amylin polymerization process.

**P-11** “Synthesis of Organic Borazine Derived from Norephedrine for the Application in Electronic Devices and Electrochemistry”, Yareslie Cruz-Rivera, Christian Ortiz-Huertas, José L. Rosario, Melvin De Jesús, Anamaris Meléndez, Idalia **Ramos**, Nicholas **Pinto** & Margarita **Ortiz**, UPRH

Organoborane reagents, such as oxazaborolidine, are well known compounds used as Lewis acid catalyst in many organic reactions, however the trimerization to prepare new organic borazine compounds is less known. The basic inorganic borazine molecule has a planar hexagonal structure of six alternating boron nitrogen atoms. Its polymeric material is used in semi-conductive boron nitride (BN) ceramics. However, borazines containing organic fragment are less well-known. Previously, our research group has been able to synthesize diverse organic borazines compounds. Presently, we first synthesized the oxazaborolidine derived from norephedrine using  $\text{BH}_3\cdot\text{DMS}$  and characterized by  $^{11}\text{B}$ -NMR. After heating the oxazaborolidine under nitrogen over  $170^\circ\text{C}$ , a trimerization took place forming the corresponding borazine, that was characterized by IR and NMR. Cyclic voltammetry analysis indicated that this compound shows an oxidation-reduction reaction. Also, the compound was pyrolyzed at  $900^\circ\text{C}$ . The result was the formation of a new BCNO material and the I-V analysis indicated that the material was conductive under a vacuum atmosphere. Exposure to long UV radiation waves, this BCNO material indicated an increase in current. The new material can be used for the formation of an electronic device, more specifically a diode that can measure a current in the scale of  $\mu\text{A}$ .

**P-10** “Synthesis of New Organic Borazine Compounds derived from 1-Amino-2-Naphthol and 3-Amino-2-Naphthol, and Characterization by their Chemical and Physical Properties”, José L. Rosario-Collazo, Yareslie Cruz, Melvin De Jesús & Margarita **Ortiz-Marciales**, UPRH

Borazines are compounds containing a six membered ring of alternating B and N atoms that can be used for hydrogen storage and new materials with optoelectrical properties. Presently, the synthesis of new organic borazines, that can display a strong local dipole moments, is an area of great interest for the development of semi-conductive materials. Our research group is highly interested in the synthesis of novel oxazaborolidine compounds derived from 2-amino-3-naphthol hydrochloride and 3-amino-2-naphthol as starting material to obtain the desired borazine. Initially, the synthesis of novel 2,3-dihydronaphtho[2,3-d][1,3,2]oxazaborole derived from 3-amino-2-naphthol was carried out in THF using  $\text{BH}_3 \cdot \text{DMS}$  (5.5 equiv). The reaction mixture was left stirring for 3 h at room temperature and the solvent was removed under reduced pressure. The corresponding crude oxazaborolidine was obtained as a white solid in 93% yield and analyzed by IR and  $^{11}\text{B}$ -NMR. The desired 2,3-dihydronaphtho[2,3-d][1,3,2]oxazaborole showed a doublet at 28 ppm in  $^{11}\text{B}$ -NMR, corresponding to the BH signal. Presently, the synthesis of the new borazine derived from 2,3-dihydronaphtho[2,3-d][1,3,2]oxazaborole is under study. In the future, the synthesis of the novel oxazaborolidine derived from 2-amino-3-naphthol hydrochloride and its corresponding borazine will be of interest to study its chemical and physic properties.

**P-3** “Understanding the Effects of Ligand Density on Protein Capture by Affinity Membranes”, Edgardo Sánchez-Rivas<sup>1</sup>, Ivan D. **Dmochowski**<sup>2</sup>, Ezio **Fasoli**<sup>3</sup>, Vibha **Bansal**<sup>1</sup>, <sup>1</sup>UPRC, <sup>2</sup>PENN, <sup>3</sup>UPRH

Ligand density is an important determinant of the protein binding capacity of a selective protein capture device. The optimal ligand density is, in turn, dependent on the size of target protein with respect to the size of ligand. A difference in the size of proteins will lead to varying degrees of steric hindrance to the binding of multiple protein molecules in regions of high ligand density. The objective of this project is to determine the effect of ligand density on protein binding capacity of para-aminobenzamidine (pABA) linked cellulose membranes using tissue-type plasminogen activator as the target protein. pABA is a known inhibitor and affinity ligand of trypsin-like serine proteases. Were modified membranes with para-aminobenzamidine through epichlorohydrin links between the hydroxyl groups on membrane and the para-amino groups of pABA molecules. Using varying amounts of epichlorohydrin allowed preparation of membranes with varying pABA densities on the surface. Then, pABA densities were quantified with the glyoxal method developed in our laboratory. The tPA was then labeled with FTIC to follow the protein during the binding experiment. Finally, the membranes with different ligand densities (X, X/2, X/4, X/10, X/12.5, and X/25) were used for fluorescently labeled tPA (fl-tPA) binding. Results indicated that the protein binding was directly proportional to ligand density under the conditions used. However, the ligand utilization efficiency, decreased with increasing ligand density. Protein binding experiments are being done using multicomponent protein solutions to determine the effect of ligand density on the selectivity of the pABA membranes for target protein.

**P-4** “In situ analysis and imaging of aromatic amidine in solid phase”, Adaliz Torres-Rosado<sup>1</sup>, Christian Ortiz<sup>1</sup>, Adriana Santiago<sup>2,3</sup>, Ivan **Dmochowski**<sup>3</sup>, Sean Yeldell<sup>3</sup>, Rolando **Oyola**<sup>1</sup>, José **Sotero**<sup>1</sup>, Vibha **Bansal**<sup>2</sup> & Ezio **Fasoli**<sup>1</sup>,  
<sup>1</sup>UPRH, <sup>2</sup>UPRC, <sup>3</sup>PENN

We show the development of a fast and accurate fluorescence-based assay for amidine determination in solid phase. The assay is founded on the glyoxal reaction, which involves a reaction of amidine group with glyoxal and an aromatic aldehyde, leading to the formation of a fluorophore that can be analyzed and quantified by fluorescence spectroscopy and Confocal Laser Scanning Microscopy imaging. While the assay has been reported previously for aromatic amidine estimation in solution phase, here we describe its adaptation and application to amidine linked to diverse forms of solid matrices, particularly benzamidine-linked cellulose membranes. These functionalized porous matrices find important application in purification of serine proteases. The efficacy of a protein separation device is determined by, among other factors, the ligand (amidine) density. Switching the aromatic aldehyde used in the glyoxal reaction from benzaldehyde to fluorene-2-carboxaldehyde led to the formation of a new fluorescent probe with different excitation and emission maxima, which expands the potential applications of this method. Finally, we show how this fluorescent labeling (glyoxal) method can provide a tool for imaging membranes and ligand distribution through confocal laser scanning microscopy.

**P-9** “Electrospun Carbon Nanotube-PEDOT:PSS Hydrogel Nanofibers”, Angelo Porcu-Madau<sup>1</sup>, Ahmad Matar<sup>1</sup>, Anamaris Meléndez<sup>1</sup>, Idalia **Ramos**<sup>1</sup> & Mohammad **Islam**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

Single-Walled Carbon Nanotubes (SWCNTs) gels have important properties for device applications including good electrical conductivity, high strength, light weight, and elasticity. In the form of fibers, they have higher surface-area-to-volume that make them attractive for electronic devices and sensors. In this project, gel fibers of SWCNT and a conductive polymer, Poly(3,4-ethylenedioxythiophene): Poly(styrene sulfonate) (PEDOT:PSS), were prepared using electrospinning. The SWCNTs hydrogel was prepared using a method previously reported (Islam et. al., Nano Energy 2015, 15). After the formation of a free-standing hydrogel was confirmed, the material was tip sonicated to recover the wet-gel solution. The precursor for electrospinning was prepared by adding a polymeric solution of 0-3% PEO in PEDOT:PSS to the gel, at a 1:2 volume ratio. No fibers were produced with 0% and almost none with 1% PEO. Fibers in the form of belts, with micrometric diameters and nanometric heights, were produced for 2wt% and 3wt%. SEM images show gel-like structures inside the fibers. The electrical conductivity of single fibers was measured by depositing them on Si/SiO<sub>2</sub> substrates with gold electrodes. Results show fibers with average conductivities of 270 S/cm for 2%, and 100 S/cm for 3% PEO. Current work includes tuning the electrical and mechanical properties of the composite fibers with PEDOT:PSS concentration.

**P-8** “Electrospun PEDOT:PSS nanoribbon field effect transistor with a ferroelectric polymer gate insulator”, Alondra Rosario-Soto & Nicholas J. **Pinto**, UPRH

Poly(3,4-ethylenedioxythiophene) doped with poly (styrene sulfonic acid) – PEDOT:PSS was electro-spun to produce high aspect ratio nanoribbons. The ribbons of varying thicknesses were electrically characterized in a field effect transistor (FET) configuration with ferroelectric (FE) poly (vinylidene fluoride-trifluoroethylene)-PVD F-TrFE as the top gate insulator. The devices exhibited p-type behavior consistent with hole charge transport in PEDOT-PSS and a memory window characteristic of a FE-FET. Such a memory effect has not been observed before in PEDOT-PSS. Thinner films exhibited stronger field effect with a change in the channel current of 104% in the on and off states. The charge mobility reached a maximum of 3 cm<sup>2</sup>/V-s for the 300nm thick nanoribbon. Thicker films did not show any field effect, suggesting that it is an effect confined to the polymer/gate insulator interface and does not penetrate deep into the bulk of the polymer film.

**P-5** “Affinity membrane model for testing correction of confocal laser microscopy images”, Jomarie Jiménez González<sup>1</sup>, Ezio **Fasoli**<sup>1</sup>, José O. **Sotero Esteva**<sup>1</sup>, Junellie L. Cruz-Lebrón<sup>1</sup>, Adaliz Torres Rosado<sup>1</sup> & Ivan **Dmoschowski**<sup>2</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN

A Confocal Laser Scanning Microscopy (CLSM) produces high-resolution Z stack images obtained from within a sample. Z stack images of cellulose membranes carrying para-aminobenzamidine (pABA) and following protein binding were analyzed in this project. A problem observed with CLSM images is that there is a loss of brightness at increasing depth, known as attenuation. To fix this issue, software was developed to correct attenuation using a histogram stretch method.

In order to test this procedure, control images were created to simulate affinity membranes. Attenuation was added in both channels of the image and the membrane was programmed to have a cylindrical shape, to represent the actual membranes more realistically. The simulated Z stacks were manipulated further, adding patches to resemble the distribution of fluorescent dyes in certain image levels, and occasionally turning off some pixels, as well as adding other types of noise.

The simulated membrane images can help observe how different issues such as noise affect numerically the intensity levels. This information is key for improving the written code and fixing the Z stacks so that the images show the membrane clearly in its entirety. Once the images are corrected, the composition of the membranes can be studied more efficiently to determine the effectiveness of the functionalized membranes and protein binding.



**P-6** “Confocal Laser Microscope for the determination of ligand density and protein binding using affinity membranes”, Junellie Cruz-Lebrón<sup>1</sup>, Sean Yeldell<sup>2</sup>, José **Sotero**<sup>1</sup>, Vihba **Bansal**<sup>3</sup>, Ivan **Dmoschowski**<sup>2</sup> & Ezio **Fasoli**<sup>1</sup>, <sup>1</sup>UPRH, <sup>2</sup>PENN, <sup>3</sup>UPRC

Affinity membrane purification is an advantageous technique which allows separation of proteins through binding between an affinity ligand linked to a membrane and the target molecules. The quantitative analysis of the ligand density and protein binding using a laser scanning confocal microscope (LSCM), were pursued in this research. LSCM is an instrument of choice for imaging solid phases with a fluorescent probe.

Affinity cellulose membranes were synthesized as follows: Cellulose acetate membranes with a pore size of 3  $\mu\text{m}$  (Sterlitech) were deacetylated in basic conditions, reacted with the 5 atom spacer arm, epichlorohydrine and further functionalized with para-aminobenzamidine (pABA), an affinity ligand for serine proteases in the cellulose acetate membranes.

In order to visualize the membranes structure and porosity under LSCM, the chemically modified membranes were dyed with a fluorescent probe Rhodamine B (ex. 545 nm, em. 580 nm). The PABA affinity ligands were reacted with glyoxal and Fluorene-2-carboxaldehyde leading to a fluorescent probe with  $\text{ex}_{\text{max}}$  488 nm and  $\text{em}_{\text{max}}$  530 nm. Finally the serine protease *Subtilisin carlsberg* from *Bacillus licheniformis*, was fluorescently labeled with Fluorescein isothiocyanate (ex. 480 nm, em. 520 nm) and used as model protein to study protein binding on chemically modified affinity membranes.

Different images of membrane carrying different ligand density, and protein concentration were taken using the LSCM. Analysis of images was done using an algorithm which allows through pixel counting to determine: the degree of membrane functionalized with the affinity ligand and the amount of protein bound to the ligand.

**P-7** “A Novel Colorimetric and Fluorescent Assay for Aromatic Aldehydes Detection”, Andrea Marcano-Delgado & Ezio **Fasoli**, UPRH

Aromatic aldehydes like benzaldehyde, vanillin, and cinnamaldehyde are widely used as solvents, flavoring materials in foodstuffs, fragrance industry and in the organic synthesis as precursors of a plethora of compounds. In the pharmaceutical industry, benzaldehyde is a toxic oxidation product of benzyl alcohol, a co-solvent used as a preservative in injectable formulations. Vanillin and cinnamaldehyde have long been of high demand because of the expense and shortage of natural extracts, representing millions of dollars annually in the food industry. Our research group is interested in the development of a simple, fast and sensitive colorimetric and fluorogenic assay for the detection of aromatic aldehydes at nanomolar concentrations. The assay is based on the reaction of an aromatic aldehyde with benzamidine and glyoxal to form the fluorescent benzyl imidazolone. The fluorophore formed was characterized by NMR, UV-VIS and fluorescence spectroscopy. The limit of detection was 79 nM, and the limit of quantification was 263 nM. Our work extends to apply our assay in different flavoring agents and injectable formulations to probe the sensitivity of the analytical method.