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UPR-PENN PREM

University of Puerto Rico at Humacao
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Partnership for Research & Education in Materials

17th PREM Annual Meeting

December 16, 2022

Program

Wyndham Palmas Beach & Golf Resort
170 Candelero Drive, Palmas de Mar
Humacao, Puerto Rico 00791

Abbreviations

UPRH	University of Puerto Rico at Humacao
UPRC	University of Puerto Rico at Cayey
UPRM	University of Puerto Rico at Mayagüez
EBA	Especializada Bellas Artes Anita Otero High School, Humacao
PENN	University of Pennsylvania
LRSM	Laboratory for Research on the Structure of Matter
DREXEL	Drexel University
TU	Temple University
USF	University of South Florida
SJU	Saint Joseph's University

Legend:

Names of undergraduates and high school students: Underlined

Names of PREM faculty: bold

NOTES

P-20 "Detection of aromatic aldehydes via a paper-based sensor", Yelisbeth Santa, Bianca K. Ríos, Gabriela Villafañe & Ezio **Fasoli**, UPRH

A rapid, simple, and sensitive chromogenic and fluorogenic assay was developed for the qualitative and quantitative detection of aromatic aldehydes in a solid phase. The assay consists of the immobilization of para-amino benzamidine (pABA) on cellulose filter paper. The paper is then reacted with glyoxal bisulfite and an aromatic aldehyde such as benzaldehyde, furfural, vanillin, or cinnamaldehyde. The reaction leads to the formation of a fluorescent benzyl imidazolone, which is visible on the paper sensor. For the quantitative analysis, the concentrations used were: 25 to 1,000 µM for benzaldehyde and 25 to 250 µM for furfural. In addition to this, using a Fluorescence Spectrophotometer the wavelength of excitation was 375 nm and the wavelength of emission was 500 to 600 nm. Also, the assay was implemented as a workshop for Experimenta con PREM where students were exposed to the topic of sensors and were able to recognize the different aldehydes given to them. Students also were exposed to fluorescence spectroscopy analyzing their results with fluorimeter.

Program

Friday December 16, 2022

Rooms: Ópalo and Rubí

8:30 AM **Registration and Breakfast**

9:30 AM Welcome Messages

Progress Report: IRG-1. Charge dynamics in transition metal and carbon-based materials

9:40 AM O-1 "Graphene, carbon nanotubes and conducting polymers", Nicholas J. **Pinto**, UPRH

10:00 AM O-2 "Input-output studies of Fabri-Perot cavities within the strong coupling regime", Natalya A. **Zimbovskaya**, UPRH

10:15 AM O-3 **"**Carbon-based nanomaterials", Idalia **Ramos**, UPRH

10:35 AM O-4 "Controlling the ordering of oxygen vacancy channel in brownmillerite $SrFeO_{2.5}$/$SrCoO_{2.5}$ superlattices", Juan **Santana**, UPRC

Progress Report: IRG-2. Surface-functionalized nanomaterials for sensing applications

10:55 AM O-5 "Magnetron sputtering physical vapor deposition for low-cost, large-area, ultra-sensitive and ultra-selective surface-enhanced Raman sensors", Francisco **Bezares**, UPRM

11:15 AM Break

11:30 AM O-6 "Alternative platforms for enzyme activity assay", Vibha **Bansal**, UPRC

11:50 AM O-7 “Sampling conformation of patterned polymeric brushes and an app for cellulose-based plates analysis”, José O. **Sotero Esteva**, UPRH

12:10 PM O-8 “Nanomaterials for potential applications associated to biomedicine and chemical analysis”, Rolando **Oyola**, UPRH

12:30 PM O-9 “Chemically modified cellulose matrix for development of sensors and purification devices”, Ezio **Fasoli**, UPRH

Group Photo & Lunch

12:50 PM Group Photo, Hotel Lobby

1:00 PM Working Lunch

PENN & Education

2:30 PM “Future directions for the Laboratory for Research on the Structure of Matter”, Eric **Stach**, PENN

3:00 PM O-10 “Increasing LatinX representation in STEM through Science Communication & Mentoring”, Kevin **Alicea**, UPRH

Poster Session, Advisory Board Meeting, and Closing

3:15 PM Poster Session

4:30 PM Advisory Board Meeting with PIs

5:00 PM Closing

P-19 “Cellulose-bound hemicryptophane for removal of fluoride in potable water”, Fabián González[1], Aria Fodness[2], Ezio **Fasoli**[1] & Ivan **Dmochowski**[2], [1]UPRH, [2]PENN

Fluoride polluted drinking water can lead to damaging conditions in human health like arthritis, joint related problems, kidney and liver damage. If fluoride levels reach up to 1.5 gm/L removal methods are needed, but due to the high solubility of fluoride in aqueous media the removal can become challenging. Various fluoride adsorbents such as activated carbon, activated alumina and rare earth oxides have been reported. In this work we present the synthesis of hemicryptophane molecular cages capable of trapping fluoride and its immobilization on cellulose paper filters for the removal of fluoride from drinkable water. The cage for fluoride was synthesized by linking cyclotriveratrylene CTV cap and tris(2-aminoethyl)amine (tren) as the anion binding site forming tren-hemicryptophane. Cellulose acetate filters commercially available from Sterlitech were deacetylated, functionalized with epichlorohydrin and linked to the tren-hemicryptophane. The fluoride binding to the device was followed by 19F NMR.

P-18 "Pillararene cellulose matrix for the removal of heavy metals from potable water", Grace M. Sánchez, Jubetzy L. Crespo, Fabián González & Ezio **Fasoli**, UPRH

Pillararenes (PAs) are a new class of macrocycles for supramolecular chemistry composed of repeating hydroquinone units. These novel compounds are capable of forming host-guest complexes, and their role as host molecules has attracted researcher's interest. PAs have been studied for their ability to encapsulate heavy metals and organic molecules within their cavities. The immobilization of PAs on cellulose matrix has been studied in our laboratory with the aim of developing new chemical sensors and purification devices for the detection and removal of water contaminants (heavy metals and/or organic molecules).

Oral Reports

O-1 "Graphene, carbon nanotubes and conducting polymers", Nicholas J. **Pinto**, UPRH

We present results on charge transport in these electrically conducting materials using a field effect transistor platform, as a function of temperature and gate voltage. Charge activation or charge hopping are some of the mechanisms observed in our experiments on charge transport in these materials. While graphene is ambipolar, the CNT's are p-type while the conducting polymer studied here (poly[benzimidazobenzophenanthroline]-BBL) is n-type. By working with a single material or by combining them in series we look at the possibility of fabricating devices and sensors. Back-gating with SiO_2 as the gate material and ionic liquid gating are two methods used to change the carrier charge concentration. This presentation will include a brief overview of the experiments the students have worked on since the last PREM meeting. Charge transport in electrostatically doped BBL films, ionic liquid gating of graphene and fabricating and testing BBL/CNT and BBL/p-Si diodes are some of the experiments that will be discussed in this talk.

O-2 "Input -Output studies of Fabri-Perot cavities within the strong coupling regime", Natalya A. **Zimbovskaya**, UPRH

We present a theoretical analysis of the dissipative dynamics of an optical Fabri-Perot (FP) cavity. The analysis is carried on assuming that the molecules in the cavity could be treated as identical harmonic oscillators strongly coupled to the coming photons. Strong light-matter interactions in such systems results in appearing of collective excitations called polaritons. We study the response of the molecules to the light using two different approaches. Within the first approach we consider optical properties of the FP cavity as a problem of classical electrodynamics. Within the second approach we treat the response of the cavity molecules to the light as a scattering problem based on quantum-mechanical treatment of the system. Within both approaches we get results for main optical characteristics of the considered FP cavity.

P-17 "Dynamic light scattering studies of gallium nanoparticles", Alondra Y. Feliciano, Anamaris Meléndez, Idalia **Ramos** & Rolando **Oyola**, UPRH

Nanoparticles shows potential as drug-delivery in medicine. In this work, we synthesized β-cyclodextrin (βCD)-modified gallium nanoparticles (GaNPs) to function as a drug delivery. The antibiotic amoxicillin (Amox) was used as a drug model. The objective of this work is the characterization of GaNPs by scanning electron microscopy (SEM), dynamic light scattering (DLS), and zeta potential (ZP). DLS and ZP were determined in the presence of Amox, human serum albumin (HSA), and GaNPs in water. The results showed that the size of these GaNPs on average is within 412 nm and as the concentration of the antibiotic or protein increases, this value changes. As future work, we seek to modify the surface of the GaNPs with a fluorescence probe.

P-16 "Fluorescence study of the complex formation between amoxicillin and gallium Nanoparticles (GaNP)", Nicole M. De Jesús-Lozada & Rolando **Oyola Martínez**, UPRH

Amoxicillin, antibacterial agent, reacts with lysine amino acids present in human serum albumin (HSA) triggering an immune response and liver injury during medical treatment. The use of cyclodextrins in pharmaceutical drug delivery is well-known approach to modulate the solubility, bioavailability, and chemical stability, among others, of the drugs. Here in, we proposed to modify the surface of gallium nanoparticles with β-cyclodextrin (GaCDNP) with the objectives to protect amoxicillin from HSA and to increase the loading capacity of the delivery. The binding constant (Kb) of Amox/GaCDNP was follow by the antibacterial emission increase upon addition of GaCDNP. Confirmation of the binding between Amox and β-CD modified GaNP was proof by NP surface modification with hydroxyl groups (Ga(OH)NP) were drug's emission remains constant with increasing amounts of Ga(OH)NP.

O-3 **"**Carbon-based nanomaterials", Paola Del Pozo[1], José L. Pérez-Gordillo[1], Daniel Rivera[1], Melvin De Jesús[1], Anamaris Meléndez[1], Idalia **Ramos**[1], Arjun **Yodh**[2], Mohammad **Islam**[3] & Jorge **Santiago**[2], [1]UPRH, [2]PENN, [3]CMU

We present an overview of research performed by undergraduate students on the preparation, characterization, and device fabrication using carbon-based nanomaterials. In one project, we analyzed the properties of reduced graphene oxide (rGO) obtained from hydrothermal carbonization of sucrose. A rGO/n-Si heterojunction was fabricated and tested as a self-powered UV photodetector. In another project, we prepared conductive aerogels using single-walled carbon nanotubes (SWCNT) coated with camphor sulfonic acid (CSA)-doped polyaniline (PANI). We will present results from the aerogel properties analyzed using high resolution scanning electron microscopy (HR-SEM), Raman Spectroscopy, and electrical conductivity measurements. Finally, we will discuss the integration of research topics into education and outreach activities. In the Summer 2022, high school research students visiting our laboratory prepared rGO/cellulose membranes and analyzed their electrical conductivity and microstructure using current-voltage measurements and SEM. We also designed two modules to introduce students and public to nanofibers preparation using electrospinning and to measure the electrical conductivity of nanomaterial thin films. The modules were fabricated using 3D-printed parts integrated with hardware and electronics. The modules have been tested in several visits to local schools.

O-4 **"**Controlling the ordering of oxygen vacancy channel in brownmillerite SrFeO2.5/SrCoO2.5 superlattices", Juan A. **Santana**[1] & Yalexander Sánchez-Navarro[1], Gabriela A. Marrero-Hernández[1], David Bugallo[2], Steve **May**[2], Alexander **Gray**[3], Eric A. **Stach**[4] & Andrew M. **Rappe**[4], [1]UPRC, [2]DREXEL, [3]TU, [4]PENN

Controlling oxygen vacancy channels (OVCs) ordering can be an effective path for engineering oxide materials for multiple applications and exploring fundamental questions in materials science. Brownmillerite oxides (BOs) have atomically ordered one-dimensional OVCs. Previous works show that the orientation of the OVCs can be controlled by epitaxial strain, e.g., growing it as a thin film. OVCs of a BO such as $SrCoO_{2.5}$ can be orientated parallel, while for a BO like $SrFeO_{2.5}$, OVCs are perpendicular on a given substrate. An exciting and unexplored possibility is the orientation of OVCs at the interface of superlattices of these BOs, such as $(SrCoO_{2.5})n/(SrFeO_{2.5})m$. We perform density functional theory calculations and grow these superlattices by MBE to study their OVCs ordering. PBE+U calculations show that OVCs in $SrFeO_{2.5}$ will be perpendicular under compressive strain (apc < 3.87 Å) and parallel under tensile (apc > 3.92 Å). In $SrCoO_{2.5}$, OVCs will be perpendicular under compressive strain (apc < 3.82 Å) and parallel under tensile (apc > 3.90 Å). Thin films of $SrCoO_{2.5}$, $SrFeO_{2.5}$, and superlattices comprising repetitions of those materials were grown on LSAT (001) substrates (a = 3.868 Å). The ratio between the thickness of both materials, the thickness of each repetition unit, and total thickness was varied. XRD data shows half-order peaks in 00l scans for $SrCoO_{2.5}$ and superlattices but not for $SrFeO_{2.5}$. Results suggest OVCs are perpendicular to the substrate in $SrFeO_{2.5}$ and parallel in both $SrCoO_{2.5}$ and the superlattices. Interestingly, this happens independently of the first material grown, or the relative ratio of Co/Fe in the superlattices explored.

P-15 "Fluorescence spectroscopy for the quantitative determination of PTAA in electro-spun nanofibers", Nitza V. Falcón-Cruz[1], Alejandro J. Cruz-Arzón[1], William Serrano-García[2], Rolando **Oyola**[1] & Nicholas J. **Pinto**[1], [1]UPRH, [2]USF

Biodegradable and biocompatible electroactive polymers are important for medical applications, such as healthcare devices and wearable electronics. Poly(lactic acid) (PLA)/ poly(triarylamine) (PTAA) nanofibers were fabricated at low PLA concentrations using the electrospinning method. However, the resulting conductivity of the nanofibers shows a maximum efficiency at 5 wt%- PLA/PTAA. The goal of this study is to quantitatively determine PTAA in precursor solution and in the fiber to test its incorporation into the nanofiber. Fluorescence spectroscopy was used following the emission of PTAA using chloroform as solvent. A PTAA standard calibration curve was performed, and fluorescence spectra were taken from the precursor solutions with different wt%-PLA/PTAA. Formed nanofibers for each precursor solution were dissolved in chloroform and the emission was measured. Results show that PTAA concentration in precursor solutions is constant within error. However, a higher amount of PTAA is found in fibers made from 5 wt%-PLA/PTAA precursor solution. These results suggest that PTAA is better incorporated into the fibers at 5 wt%-PLA/PTAA and, thus, correlates with the conductivity response.

P-14 "Gallium nanoparticles interactions with Aβ40 in the presence of membranes", Alondra Brito-Pérez & Rolando **Oyola**, UPRH

Alzheimer's disease is a progressive neurological disorder which pathology and cellular toxicity has been linked to aggregation of oligomeric species of amyloid-β (Aβ), such as Aβ40, at the membrane interface of neurons. It has been implicated that cellular membranes can catalyze amyloid aggregation, which is proposed to lead to interactions that disrupt and permeabilize neuron membranes, thus affecting normal neuronal function. There are small molecular compounds capable of suppressing amyloid aggregation and cellular toxicity, except when the presence of a lipid membrane interferes with their inhibitory abilities. Few compounds that can act as membrane active inhibitors and affect formation of membrane-assisted Aβ40 aggregates have been identified. Although the use of Gallium nanoparticles as an amyloid peptide formation inhibitor has not been thoroughly explored, it has recently been shown that gallium nitride nanoparticles (GaN NP) intervene on oligomeric nucleus formation of the Aβ40 peptide. The purpose of this research project is to study the inhibition of oligomerization by GaN NP in the presence of DOPC membranes. Through the use of biophysical approaches, such as Thioflavin T fluorescence, it will be possible to gain insights into how the presence of membranes impact GaN NPs inhibition mechanism, by measuring and monitoring Aβ40 aggregation kinetics, fibril formation and intermolecular interactions.

O-5 "Magnetron sputtering physical vapor deposition for low-cost, large-area, ultra-sensitive and ultra-selective surface-enhanced Raman Sensors", Edgard Díaz[2], Gabriel García[2], Camila Negrón[1], Lorena Reyes[1], Adam Alfieri[3], Joshua Chaparro[1], Wanda Rivera[2], Luis Vázquez[2], Erich **Stach**[3], Deep **Jariwala**[3], Ezio **Fasoli**[4] & Francisco **Bezares**[1], [1]UPRM, [2]UPRC, [3]PENN, [4]UPRH

Magnetron Sputtering Physical Vapor Deposition (MSPVD) is a reliable and inexpensive technique for depositing different materials onto substrates which, makes it amenable fabrication technique for commercial applications. Our discussion will describe experiments in which MSPVD was utilized for the fabrication of Ag nanoparticles onto SiO_2 substrates for the optimization of Surface-enhanced Raman Scattering (SERS) sensors. Temperatures and deposition times were varied during fabrication to study their effects on nanoparticle size, nanoparticle separation, and morphology. SEM measurements demonstrate that the relationship between these parameters within the studied ranges on our experiments is not monotonic and thus, suggests the optimization of parameters for maximization of SERS intensities. Our SEM results also offer valuable insights into the nanoparticle growth dynamics at play. TEM measurements confirmed SEM results in addition to demonstrating the presence of multiple distributions of particle sizes in our samples, as well as crystallinity. SERS measurements showed very consistent results over relatively large areas (~cm^2) with Raman signal enhancement factors comparable to other more expensive and time-consuming methods. Possible approaches for improved future results will also be discussed.

O-6 "Alternative platforms for enzymatic assays", Vibha **Bansal**[1], Daeyeon **Lee**[2], Rolando Albarracín[1], Gabriela B. Gomez-Dopazo[1], Renis J. Agosto Nieves[1], Daniel Rivera Nazario[3] & Idalia **Ramos**[3], [1]UPRC, [2]PENN, [3]UPRH

Membrane discs have emerged as attractive alternatives to micro bead-based chromatography columns. The poor economy and performance-related problems associated with chromatographic separations add significantly to the cost of the final protein product, particularly in case of clinical applications. Membranes, on the other hand, offer higher accessible surface area, lower diffusional resistance, and pressure drop problems. The goal of this project is to develop affinity membranes for protein capture from biological mixtures. Towards this end, the study being reported here focused on understanding: i) the effect of chemical modification on the structural integrity of the membranes; and ii) the effect of ligand density on the protein binding capacity of the affinity membranes. Commercially available cellulose acetate membranes were chemically modified to obtain amidine as the end group, using protocols previously established in our laboratory. The pore size of modified membranes, as determined using a gravity driven water flow through the membranes, was observed to decrease with increase in ligand density. SEM analysis indicated that the membranes' structural integrity was not affected adversely by the modification process. The model proteins chosen for protein binding experiments included Trypsin and Tissue type Plasminogen Activator (tPA), both trypsin type serine proteases. The proteins were fluorescently labeled to facilitate the protein monitoring during binding experiments. Experiments performed using membranes in ligand density range of 0- 5.0 µmol per ml showed that protein binding increases with increase in ligand density up to amidine concentration of 4.0 µmol per ml. After this point a saturation effect was observed.

P-13 "Conditional generative adversarial network for self-avoiding walk generation", Michael J. Rivera Lazú, Adalis Castro Santiago & José O. **Sotero Esteva**, UPRH

In the last PREM symposium, we presented the results of an implementation of a Generative Adversarial Network (GAN)(Goodfellow et.al, 2014) to generate grafted self-avoiding walks (SAWs) which could be used to model surface-linked polymers. Although a general agreement between the distributions was hinted at by the resulting diagrams, a lack of uniformity of the grid nodes used by the generator network was also noticeable. To gain more from a GAN model, in this work we tested a newer development called a Conditional Generative Adversarial Network (cGAN) (Isola et.al., 2018). As in the previous model, training is based on a competition between a generative network and a discriminator network. In cGAN the input of the generative network replaces noise with a conditional input image, a kind of approximation of the desired result. These structures of the networks also differ. cGAN was designed to manage general RGB pictures. Therefore, modifications were needed to adapt it to or representation of SAWs. Preliminary results of the cGAN show a better agreement with expected distributions.

P-12 "Computer application for the analysis of cellulose-based well plate images", Emmanuel Rosa Delgado[1], José O. **Sotero Esteva**[1], Vibha **Bansal**[2] & Gabriela B. Gómez Dopazo[2], [1]UPRH, [2]UPRC

Enzyme activity assays can be made through paper-based plates that replace other materials which ultimately benefits the environment. Currently we are working in a collaboration with Professor Bansal and her group at UPR-Cayey which are designing paper-based plates. Through this project we designed a computer application prototype which is able to work in an efficient way towards the analysis of enzyme activity assay in paper-plates. This app, which runs in computers as well as in cell phones, aims to replace expensive analysis equipment and allow measurements in the field. It utilizes digital image processing techniques to perform image segmentation in order to gather information from the pixels of the images. Following this, the edges of the plate are identified with the help of filters. Afterwards, the wells of the plate are found with a projective mapping of a CAD (Computer Aided Design) of a micro-well plate. A keystone effect correction is applied to the CAD which leads to the deformation where the polygons are displayed over the wells of the plate. Upon obtaining the pixels in the wells, the user uploads or specifies using the app a protocol that classifies the wells as blanks, positive and negative controls and samples. A comparison based on singular value decomposition is made between the wells which contain a sample and the ones that don't in order to achieve the intensities of each well which are displayed along with a calibration graph which can be downloaded for further use.

O-7 **"**Sampling conformation of patterned polymeric brushes and an app for cellulose-based plates analysis", José O. **Sotero Esteva[1]**, Michael J. Rivera Lazú[1], Emmanuel Rosa Delgado[1], Génesis N. Pérez Gonzalez[1], Preston **Moore**[2], Vibha **Bansal**[3] & Gabriela B. Gómez Dopazo[3], [1]UPRH, [2]SJU, [3]UPRC

Self avoiding walks (SAW) over grids provide an alternative to extend the quantity of feasible conformations of polymer brushes in studied by molecular dynamics simulations. Adversarial convolutional generating networks (GAN) were used first to generate large quantities of long SAWs with limited success since they suffer from mode collapse. We report on a variation of Cycle-Consistent Adversarial Networks (cCAN) that translate short SAWs to walks of twice the length that does not suffer from mode collapse. A novel approach in which neural networks operate with members of finite fields instead of real numbers was also developed. Gradients used in regular networks were replaced by a combination of genetic algorithms and Metropolis-type modifications. A network was trained to determine if a SAW passes through a given set of points on a grid reached accuracies of 70%. Finally, we report on the development of a prototype of a web application to analyze cellulose-based 96-wells plates for analytical research being developed by V. Bansal's group at the UPR-Cayey. The app can be used from computers, tablets and cell phones. It accepts images or allows the user to take the photo of the plate using the phone camera. The app produces estimates of the concentrations of the analytes present in the plate, statistical analysis and a calibration curve.

O-8 "Nanomaterials for potential applications associated to biomedicine and chemical analysis", Rolando **Oyola**[1], Nitza V. Falcón-Cruz[1], Alondra Brito[1], Nicole De Jesús[1], Alondra Y. Feliciano[1], Alondra T. Martínez[1] & Kamillie Díaz-Dávila[2], [1]UPRH, [2]EBA

Gallium nitride nanoparticles (GaN NP) derivatives have received increased attention for their potential use in different biomedical areas. Our research laboratory focuses on using Ga NP for different purposes, such as Abeta(1-40) and IAPP aggregation inhibitor during amyloidosis, drug transport and interaction with human serum albumin. Our results show that the lag phase of Abeta(1-40) aggregation kinetics is significantly retarded by GaN NP. However, for IAPP, GaN NP increase the lag phase but in a lower magnitude, indicative of GaN higher peptide selective inhibition. As for drug delivery, the GaN NP' surface were modified with beta-cyclodextrin (CD). Amoxicillin (Amox), an antibacterial drug, was used as a model for drug delivery and characterized by fluorescence spectroscopy. GaN NP interaction with human serum albumin (HSA) were studied by the intrinsic protein tryptophan fluorescence where it was shown that GaN NP affinity towards HSA is lower than for gold nanoparticles. In relation of quantitative detection and sensing, we explored of the use of thin-film deposition of PEDOT:PSS and PEDOT:PSS with carbon microspheres (CS) over glassy carbon electrode (GCE) with the aim of increasing analytical sensitivity. We tested the system using chiral acetal (2R,5R)-2-ferrocenyl-5-methyl-4,4-diphenyl-1,3-dioxalene and ferrocene. In terms of education, our laboratory was also involved in new experiments where a simple 3D-printed fluorescence spectrometer was proposed to determine 8-Hydroxypyrene-1,3,6-trisulfonic acid trisodium salt present in pen highlighter.

P-11 "Automatic classification of samples on a cellulose-based well plate image", Génesis N. Pérez González[1], José O. **Sotero Esteva**[1] & Vibha **Bansal**[2], [1]UPRH, [2]UPRC

Recently, cellulose-based plates have been designed by Professor Vibha Bansal and her group at the University of Puerto Rico at Cayey with the purpose of eventually replacing plastic plates for enzyme assays. Currently, our group is working in collaboration with Professor Bansal on developing a computer application prototype which aims to analyze samples on these cellulose-based well plates. At this moment, the app requires the well plate image once the samples were deposited, and the user needs to specify a protocol identifying: sample wells, positive control wells, negative control wells and blank wells. Our main goal was to design an automatic classification technique, so the user doesn't need to upload a protocol for each well plate to be analyzed. The developed strategy applies principal component analysis (PCA) and clustering algorithms to representations of the pixel's colors on each well. The PCA is used for analyzing big datasets while preserving the maximum amount of information and visualizing it, while the clustering algorithms aim to divide and organize these data. Some tests have been done so far and the technique has demonstrated that it efficiently identifies the sample wells but is less efficient in identifying negative control wells. Even though we have started seeing some positive results on our road to the automatic classification of samples, this work needs more testing on images with different illumination conditions so our results can be validated.

P-10 "Silane grafted silica particles based liquid marbles as microreactors for colorimetric reactions", Renis J. Agosto Nieves[1], Gabriela B. Gomez-Dopazo[1], Joseph Rosenfeld[2], **Daeyeon** Lee[2] & Vibha **Bansal**[1], [1]UPRC, [2]PENN

Liquid marbles (LM) offer a promising vehicle for the evolution of innovative enzymatic assay techniques. LM form when particles assemble on the air-liquid interface, stabilizing a droplet of liquid. Once formed, they offer a closed system wherein reactions can occur between the entrapped reagents, or alternatively, additional reagents injected into the LM. The main objective of this project is to modify silica particles (SP) with different silanes, with the purpose of designing a robust and transparent LM to perform colorimetric assays for quantification of enzyme activity. The LM in this project were modified by a base catalyzed hydrolysis followed by a condensation reaction to covalently link the silanes on the surface of the SP. Robustness of the LM is measured by subjecting the system to various mechanical stresses. In addition, contact angle studies were performed to quantitatively determine hydrophobicity of each sample, which is directly related to the mechanical strength of the system. Enzymatic assays, using Alkaline Phosphatase, α-Chymotrypsin, and Bicinchoninic acid (BCA), were carried out as applications for the system. These results were analyzed with a conventional spectrometer and a smart phone application. Consequently, the results with the smart phone app proved to have considerable linearity when compared to the conventional method; indicating that LM can be successfully used as microreactors for enzymatic assays.

O-9 "Chemically modified cellulose matrix for development of sensors and purification devices", Ezio **Fasoli**, UPRH

Paper has been used as a solid matrix for many applications in purification, PoC diagnostics and sensors. Cellulose offers several advantages as it can be tuned with various molecules for the development of sensors and purification devices. In this work we present the development of Pillararenes (PAs) and Hemicryptophane cellulose matrix for the removal of heavy metals and fluorides from potable water and the use of para-amino benzamidine (pABA) cellulose-based sensor for the detection of aromatic aldehydes. The PAs project was mainly developed at UPRH: Cellulose matrix were functionalized with propargyl bromide and epichlorohydrin to create a linker for attachment of PAs. The synthesis 1,4-dimethoxypillar[5]arene (DMPA) was achieved by reacting 1,4-dimethoxybenzene and paraformaldehyde in the presence of trifluoroacetic acid as catalyst. The linking of The PAs to the paper matrix is under optimization. During Summer 2022, in collaboration with the Dmochowski's group at PENN, we focused on the synthesis of hemicryptophane molecular cages capable of trapping fluoride followed by their immobilization on cellulose discs with a similar approach as with PAs. Finally, we present the development of a rapid, simple, and sensitive chromogenic and fluorogenic assay for the qualitative and quantitative detection of aromatic aldehydes. pABA was immobilized on cellulose and then reacted with glyoxal bisulfite, and an aromatic aldehyde leading to a fluorescent signal. This assay was implemented as a workshop for Experimenta con PREM where students were exposed to the topic of sensors, fluorescence spectroscopy and were able to recognize and quantify the different aldehydes given to them.

O-10 **"**Increasing LatinX representation in STEM through Science Communication & Mentoring", Kevin **Alicea-Torres**[1], Mark **Licurse**[2], Ashley **Wallace**[2], Daniel Rivera-Nazario[1], Anamaris Meléndez-Zambrana[1] & Idalia **Ramos Colón**[1], [1]UPRH, [2]PENN

Science communication (SciComm) educates society about science-related topics or shares stories of scientists and their successful scientific careers. Unfortunately, SciComm initiatives are not always inclusive and do not represent a diverse community, impeding students' awareness of LatinX role models in science, technology, engineering, and mathematics (STEM), including in materials research. Therefore, increasing the presence of LatinX materials scientists in the classroom, public events, or media using SciComm platforms would allow them to serve as role models and inspire young minds to pursue their dreams in STEM. In addition to SciComm, mentoring significantly increases science diversity and supports future scientists and leaders. Our UPR-Penn Partnership for Research and Education (PREM) program has: 1) increased the visibility of materials scientists in the media, schools, and public events; 2) created a blog and a podcast called "Qué hacen en el Lab"; and 3) developed a mentoring program that prepares senior undergraduates on future careers and decision-making in STEM. Through these initiatives, we have impacted over 5,736 students and teachers, of which 55% were females, and 45% were males of ages 5 to 61 from over 60 municipalities in Puerto Rico. In addition, our blog and science news articles have an estimated reach of more than 12,753 people on social media. All this has involved more than 12 PREM student volunteers and mentees. Our analysis highlights the importance of SciComm and mentoring experiences, which can contribute to increased public engagement with STEM education and the development of future science leaders.

P-9 "Fabrication and scanning electron microscopy characterization of paper microwell plates", Gabriela B. Gómez-Dopazo[1], Daniel Rivera[2], Idalia **Ramos**[2] & Vibha **Bansal**[1], [1]UPRC, [2]UPRH

Analytical methods for quantification of enzyme activity in the laboratory typically involve colorimetric/fluorimetric assays performed in commercially available microwell plates made from a variety of polymers. Despite the convenience this system offers, it requires availability of microplate readers that are expensive and inaccessible in non-laboratory setup or in laboratories with scarce resources. Paper-based analytical devices (PADs) have become of great interest during the past years due to their compliance with the ASSURED principles established by the World Health Organization. In this work, 3D paper microwell (96-well) plates were fabricated as cost-effective and ecofriendly alternatives to the commercially available microwell plates and were studied using Scanning Electron Microscopy (SEM). The paper microwell plates were fabricated in 96-wells format as a proof of concept. Mold design was modified to make wells of different shapes: conical and round bottomed, similar to those available in polystyrene plates. Paper plates were prepared using a cellulose acetate solution and a series of post treatments performed. This included impermeabilizing the well surface using a commercially available product. Subsequently, the plates were exposed to different solvents to study the coating's resistance to these. SEM analysis indicated the pores to be in the range of 6 µm – 287 µm and a uniform distribution of the impermeabilizing agent on the plate surface. The paper plates fabricated in this study were found to be a robust and eco-friendly alternative to traditionally used polystyrene plates. The fabrication process is simple and does not require advance skills or instruments.

P-8 **"**TEM and SEM of Ag via magnetron sputtering physical vapor deposition for photonic sensing devices" Edgard O. Díaz[1], Gabriel García[1], Camila Negrón[2], Lorena C. Reyes[2] & Francisco **Bezares**[2], [1]UPRC, [2]UPRM

Magnetron sputtering physical vapor deposition (MSPVD) is a very powerful materials deposition technique, widely-used in academia as well as in industry due to its relative low costs, reliability, precision, as well as its flexibility. In addition, it allows for the deposition of a great diversity of materials, whether in the form of nanoparticles or thin films. In particular, our experiments focus on this technique for the fabrication of large- area (wafer scale), ultra-sensitive and highly reproducible Surface-enhanced Raman spectroscopy (SERS) sensors. Here, we will show the results of systematic studies in which the physical deposition parameters of MSPVD of Ag nanoparticles, well below the melting temperature of Ag, are correlated to the SERS enhancement of the devices. TEM and SEM measurements provide great insight into the physical mechanisms underlying the deposition of the Ag nanoparticles. For example, the TEM images in particular, clearly demonstrate that more than one nanoparticle size distribution can result, depending on deposition time and/or temperature. A simple model for the prediction of the Ag nanoparticles topography, size and shapes will be presented.

PREM

Poster Presentations

P-1 "Effect of the gate voltage scan rate on charge transport in graphene that is gated with an ionic liquid", Elvin Cordero[1], Nicholas J. **Pinto**[2], Chengyu Wen[2] & A.T. Charlie **Johnson**[2], [1]UPRH, [2]PENN

P-2 "Temperature dependent charge transport in electrostatically doped BBL thin films", Alejandro J. Cruz-Arzón[1], William Serrano-Gracía[2], Nicholas J. **Pinto**[1], Nikita Gupta[3] & Alan T. Charlie **Johnson**[3], [1]UPRH, [2]USF, [3]PENN

P-3 "Fabrication and electrical characterization of a p-n diode using an n-type polymer and a p-doped Si/SiO2 substrate", Alexander Real-Quiñones, Alejandro Cruz-Arzón & Nicholas J. **Pinto**, UPRH

P-4 "Self-powered photoresponse in reduced graphene oxide/silicon p-n heterojunction", José L. Pérez Gordillo[1], Daniel Rivera[1], Anamaris Meléndez[1], Idalia **Ramos**[1], Nicholas **Pinto**[1] & Jorge J. **Santiago**[2], [1]UPRH, [2]PENN

P-5 "Preparation and characterization of PANI-coated SWCNT aerogels", Paola Del Pozo[1], Anamaris Meléndez[1], Arjun **Yodh**[2], Mohammad **Islam**[3] & Idalia **Ramos**[2], [1]UPRH, [2]PENN, [3]CMU.

P-6 "DFT calculations of brownmillerites: bulk $SrFeO_{2.5}$ and $SrCoO_{2.5}$ and the superlattice $SrFeO_{2.5}/SrCoO_{2.5}$", Yalexander Sánchez-Navarro, Gabriela A. Marrero-Hernández & Juan A. **Santana**, UPRC

P-7 "Optical studies of magnetron sputtering physical vapor deposition of Ag for ultra-sensitive, large-area plasmonic sensors", Camila Negrón[1], Lorena C. Reyes[1], Edgard O. Díaz[2], Gabriel García[2] & Francisco **Bezares**[1], [1]UPRM, [2]UPRC

P-8 **"**TEM and SEM of Ag via magnetron sputtering physical vapor deposition for photonic sensing devices" Edgard O. Díaz[1], Gabriel García[1], Camila Negrón[2], Lorena C. Reyes[2], & Francisco **Bezares**[2], [1]UPRC, [2]UPRM

P-9 "Fabrication and scanning electron microscopy characterization of paper microwell plates", Gabriela B. Gómez-Dopazo[1], Daniel Rivera[2], Idalia **Ramos**[2] & Vibha **Bansal**[1], [1]UPRC, [2]UPRH

P-10 "Silane grafted silica particles based Liquid marbles as microreactors for colorimetric reactions", Renis J. Agosto Nieves[1], Gabriela B. Gómez-Dopazo[1], Joseph Rosenfeld[2], Daeyeon **Lee**[2] & Vibha **Bansal**[1], [1]UPRC, [2]PENN

P-11 "Automatic classification of samples on a cellulose-based well plate image", Génesis N. Pérez González[1], José O. **Sotero Esteva**[1] & Vibha **Bansal**[2], [1]UPRH, [2]UPRC

P-12 "Computer application for the analysis of cellulose-based well plate images", Emmanuel Rosa Delgado[1], José O. **Sotero Esteva**[1], Vibha **Bansal**[2] & Gabriela B. Gómez Dopazo[2], [1]UPRH, [2]UPRC

P-13 "Conditional generative adversarial network for self-avoiding walk generation", Michael J. Rivera Lazú, Adalis Castro Santiago & José O. **Sotero Esteva**, UPRH

P-14 "Gallium nanoparticles interactions with Aβ40 in the presence of membranes", Alondra Brito-Pérez & Rolando **Oyola**, UPRH

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P-7 "Optical studies of magnetron sputtering physical vapor deposition of Ag for ultra-sensitive, large-area plasmonic sensors", Camila Negrón[1], Lorena C. Reyes[1], Edgard O. Díaz[2], Gabriel García[2] & Francisco **Bezares**[1] , [1]UPRM, [2]UPRC

Surface-enhanced Raman spectroscopy (SERS) is a very promising technique for the development of novel chemical and biological sensors and has received a lot of attention by the scientific community in recent decades. However, despite such efforts, the commercial development of these sensors has been slow due to challenges imposed by fabrication costs, reliability and reproducibility. Here, results from optical studies of large-area (wafer scale), ultra-sensitive and highly reproducible SERS sensor will be presented. We will show that the magnetron sputtering physical vapor deposition of Ag allows for flexibility, uniformity, tunability, consistency and very high SERS enhancements over large areas. Optical far-field studies such as Raman, Reflectance and Photoluminescence spectroscopic techniques will be presented. As such, optical far-field studies will be compared to the optical near-field measurements of Tip- enhanced Raman spectroscopy on these sensors.

P-6 "DFT calculations of brownmillerites: bulk $SrFeO_{2.5}$ and $SrCoO_{2.5}$ and the superlattice $SrFeO_{2.5}/SrCoO_{2.5}$", Yalexander Sánchez-Navarro, Gabriela A. Marrero-Hernández & Juan A. **Santana**, UPRC

Brownmillerite oxides (BOs) are materials with atomically ordered one-dimensional oxygen vacancy channels (OVCs). The orientation of OVCs can be controlled by epitaxial strain. We have performed density functional theory calculations (DFT) of bulk $SrFeO_{2.5}$ and $SrCoO_{2.5}$ and the superlattice form from growing these two BOs to study their OVCs ordering. The results from PBE+U show that OVCs in $SrFeO_{2.5}$ will have perpendicular orientation under compressive strain (apc < 3.87 Å) and parallel under tensile (apc > 3.92 Å). In the case of $SrCoO_{2.5}$, OVCs will be perpendicular to the substrate under compressive strain (apc < 3.82 Å) and parallel under tensile (apc > 3.90 Å).

P-15 "Fluorescence spectroscopy for the quantitative determination of PTAA in electro-spun nanofibers", Nitza V. Falcón-Cruz[1], Alejandro J. Cruz-Arzón[1], William Serrano-García[2], Rolando **Oyola**[1] & Nicholas J. **Pinto**[1], [1]UPRH, [2]USF

P-16 "Fluorescence study of the complex formation between amoxicillin and gallium nanoparticles (GaNP)", Nicole M. De Jesús-Lozada & Rolando **Oyola Martínez**, UPRH

P-17 "Dynamic light scattering studies of gallium nanoparticles", Alondra Y. Feliciano, Anamaris Meléndez, Idalia **Ramos** & Rolando **Oyola**, UPRH

P-18 "Pillararene cellulose matrix for the removal of heavy metals from potable water", Grace M. Sánchez, Jubetzy L. Crespo, Fabián González & Ezio **Fasoli**, UPRH

P-19 "Cellulose-bound hemicryptophane for removal of fluoride in potable water", Fabian González[1], Aria Fodness[2], Ezio **Fasoli**[1] & Ivan **Dmochowski**[2], [1]UPRH, [2]PENN

P-20 "Detection of aromatic aldehydes via a paper-based sensor", Yelisbeth Santa, Bianca K. Ríos, Gabriela Villafañe & Ezio **Fasoli**, UPRH

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ABSTRACTS

Poster Presentations

PREM

P-5 "Preparation and characterization of PANI-coated SWCNT aerogels", Paola Del Pozo[1], Anamaris Meléndez[1], Arjun **Yodh**[2], Mohammad **Islam**[3] & Idalia **Ramos**[1], [1]UPRH, [2]PENN, [3]CMU

Lightweight, flexible, and electrically conductive aerogels are important for energy storage and wearable sensors. We report the preparation and characterization of aerogels composed of single-walled carbon nanotubes (SWCNT) and the conducting polymer polyaniline (PANI). A SWCNT hydrogel was first prepared and then coated with camphor sulfonic acid (CSA)-doped polyaniline (PANI). After gelation, the samples were soaked in increasing concentrations of ethanol up to 100%. Samples were then soaked in baths of 0.3, 0.6, and 0.9 wt% PANI solutions and then placed in 100% ethanol. Finally, all the hydrogels were dried using critical drying point method. The aerogels obtained are lightweight, free standing, and mechanically robust. The samples with 0.3 wt% PANI concentration were analyzed at PENN using high resolution scanning electron microscopy (HR-SEM) and Raman spectroscopy. HR-SEM shows networks with filamentous structures and high porosity, with polymer wrapping around nanotubes. Raman analysis confirmed the integration of PANI into the aerogel. The electrical conductivity of all the gels was obtained using two-probe current-voltage measurements. The conductivity for SWCNT aerogels is ~60 S/m and decreases with the addition of the polymer. The physical structure of the aerogels appears to be reinforced with PANI. Ongoing experiments include changing solvents and stress-strain tests to determine optimal conductivity and mechanical properties.

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P-4 "Self-Powered photoresponse in reduced graphene oxide/silicon p-n heterojunction", José L. Pérez Gordillo[1], Daniel Rivera[1], Anamaris Meléndez[1] Idalia **Ramos**[1], Nicholas **Pinto**[1] & Jorge **Santiago**[2], [1]UPRH, [2]PENN

Graphene Oxide (GO) films are prepared from the hydrothermal carbonization of sucrose at a 0.1 M concentration. The GO films are continuous, have few layers, and with subsequent annealing their electrical properties are improved. For the annealing process the films are put under nitrogen at 600°C in a tube furnace to achieve an oxygen content of ~15% and produce reduced graphene oxide (rGO). EDS, and Raman analysis show the graphitic properties and confirm the desired nature of our samples. HR-SEM and AFM show the morphology and thickness of the films. The rGO films are then cleaved over a n-type SiO_2 substrate to form p-n heterojunction diodes. The diodes have photodetection capabilities under ultraviolet and visible light at room temperature and 0 V bias. Photoconduction results show that the sensor has responsivities of up to 223 mA/W, and response and recovery times in the order of milliseconds. These parameters are comparable to other photosensors reported in literature produced via more expensive methods.

PREM

P-1 "Effect of the gate voltage scan rate on charge transport in graphene that is gated with an ionic liquid", Elvin Cordero[1], Nicholas J. **Pinto**[2], Chengyu Wen[2] & A.T. Charlie **Johnson**[2], [1]UPRH, [2]PENN

Charge transport in CVD graphene was investigated at room temperature using a field effect transistor platform with an ionic liquid (IL) as the gate material. Using an IL lowers the gate voltage needed for device operation due to its high specific capacitance. Impurity charges adsorbed on the graphene surface during growth and post processing act as dopants and influence charge transport. Applying a voltage to the IL (V_G) changed this impurity charge concentration and shifted the charge neutrality point (CP) in graphene. In this work we varied the gate voltage scan rates from 100 mV/s to 1 mV/s and examined its effect on the channel current (I). Lowering the scan rate led to the following observations in the I-V_G plots: (i) a non-linear shift in gate voltage at the CP voltage from a positive value toward V_G = 0 (i.e. n-doping), (ii) an increase in the electron and hole mobilities and (iii) a narrowing of the spread in the current near the CP. We believe that a slower scan rate helped create a more uniform electric double layer at the graphene/IL interface which could neutralize impurity charges. The result was a homogeneous redistribution of un-neutralized impurity charges and a reduction in charge scattering of carrier charges. By using an IL that selectively absorbs gas species, our device can also be used as a gas sensor. The low applied voltages in combination with transistor operation make this device multifunctional and suitable in battery powered electronics.

P-2 "Temperature dependent charge transport in electrostatically doped poly[benzimidazobenzophenanthroline] (BBL) thin films", Alejandro J. Cruz-Arzón[1], William Serrano-García[2], Nicholas J. **Pinto**[1], Nikita Gupta[3] & Alan T. Charlie **Johnson**[3], [1]UPRH, [2]USF, [3]PENN

Charge transport in electrostatically doped BBL, poly-[benzimidazobenzophenanthroline], thin films in a field-effect transistor geometry were investigated in the temperature range 150K < T < 370K. At low temperatures activation and hopping transport mechanisms dominated, while phonon scattering dominated at high temperatures. The activation energies (EA) were found to lie in the range 140meV < EA < 400meV implying the existence of deep traps within the polymer bandgap of 1.8eV. Two quasi-linear dependencies of EA on the gate voltage (Vg) were observed with EA decreasing as Vg increased. An unexpected "metallic-like" transport characteristic appeared for T > 335K which depended on Vg. Enhanced electron delocalization combined with increased carrier density could be responsible for this "metallic-like" behavior. Our results show that the existence of deep traps with multiple energy distributions, combined with increased carrier density led to the unusual temperature dependence of charge transport observed in BBL.

P-3 "Fabrication and electrical characterization of a p-n diode using an n-type polymer and a p-doped Si/SiO2 substrate", Alexander Real-Quiñones, Alejandro Cruz-Arzón & Nicholas J. **Pinto**, UPRH

Electronic solid-state devices contain at least one interface between a p-type and an n-type semiconductor. Such hetero junctions form the basic building block in logic circuits that are at the heart of microprocessors and are typically fabricated from all inorganic Si based materials. Here we present a technique to fabricate a hybrid p-n diode using a p-doped Si/SiO2 substrate and an n-type organic polymer film. The n-type polymer used was commercially available poly[benzimidazobenzophenanthrolin](BBL). Thin films of the polymer were prepared by sandwiching a drop of BBL dissolved in methane sulfonic acid between two coverslips and submerged in DI water for 72 hours. The films were then thermally annealed and placed along the cleaved edge of a p-Si/SiO_2 wafer forming a p-n junction diode at the interface of the film/p-Si substrate. The I-V curves across the junction were asymmetric with current increasing in the first quadrant with increasing voltage, but with limited current flowing in the third quadrant. In this poster we will present our data analysis of the diode where we calculate the diode turn-on voltage, the diode rectification ratio and the diode ideality parameter. Our goal is to make the diode tunable by controlling the semiconducting properties of the materials using an external gate voltage.