



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

UPRH-PENN Partnership for Research & Education in Materials

18"ANNUAL MEETING













Abbreviations

UPRH University of Puerto Rico at Humacao

UPRC University of Puerto Rico at Cayey

UPRM University of Puerto Rico at Mayagüez

PENN University of Pennsylvania

Legend:

Names of students: Underlined

Names of PREM and NRT faculty: bold

P-23 "Multiferroic characteristics of hafnium-doped material for neuromorphic computing applications"

Eric Sánchez-Ayala¹, Cynthia Rodríguez-Cruz¹, María Rodríguez-Ortiz¹, and Danilo **Barrionuevo**²

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As medical technology advances, the potential of neuromorphic computing to transform medical diagnostics is being increasingly explored. This brain-inspired computing approach improves diagnostic speed and accuracy. Its applications range from image recognition to early disease detection, leveraging artificial neural networks to mimic the human brain's information processing. Examples include accurately diagnosing skin diseases by analyzing images of skin lesions in a fraction of the time taken by experts and enhancing the accuracy and efficiency of cancer diagnosis in mammograms, detecting otherwise unnoticed tumors. Neuromorphic computing also enables quick and precise detection and diagnosis of heart conditions like arrhythmia. A multiferroic tunnel junction offer the opportunity to get fourstate logic because of the ferromagnetic and ferroelectric components, electron and spin tunneling can be controlled, and a four-state resistance device can be realized by polarization and magnetization switching. We will use this material for our multiferroic tunnel junctions. A single-phase multiferroic material, $(Hf_{0.5}Zr_{0.5})_{0.90}(Fe_{0.5}Nb_{0.5})_{0.10}O_2$ (HZFN), shows promise as a tunnel barrier in multiferroic tunnel junctions. This discovery underscores the possibility of fine-tuning their properties at the nanometer scale, thereby opening new avenues for technological applications in nanoelectronics, particularly in the realm of multiferroic tunnel junctions for next-generation nonvolatile memory devices.

ORAL PRESENTATIONS Program

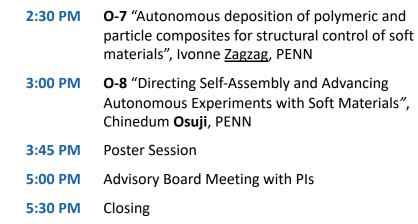
Friday December 8, 2023 **Rooms:** Ópalo-Rubí-Topacio

9:30 AM Welcome Messages

9:45 AM PREM Progress Report, Idalia Ramos, UPRH

UPR Faculty Progress Reports

- **10:00 AM O-1** "Ionic liquid gate tunable diodes based on monolayer MoSe₂", Nicholas J. **Pinto**, UPRH
- **10:15 AM O-2** "Alternative platforms for colorimetric measurements", Vibha **Bansal**, UPRC
- **10:30 AM O-3** "Encapsulation and release studies of sulindac in cubosomes nanoparticles using microfluidics", Rolando **Oyola**, UPRH
- **10:45 AM O-4** "Pillararene modified cellulose matrix for detection and removal of metals and organic molecules", Ezio **Fasoli**, UPRH
- **11:00 AM O-5** "Physical Vapor Deposition of Random Arrays of Ag Nanoparticles: Sensing Applications and Beyond", Francisco **Bezares**, UPRM
- **11:15 AM O-6** "Data Science applications to the study of polymers, colorimetry, and particle separation", José O. **Sotero-Esteva**, UPRH
- 11:30 AM *Panel:* "Best practices for recruiting, retaining, and supporting graduate students from MSIs", Andrea Marcano, MIT; Deliris Ortiz, UM-Ann Arbor; Idalia Ramos, UPRH; Kristin Field, PENN
- **12:45 PM** Group Photo, Hotel Lobby
- 1:00 PM Working Lunch



P-22 "Zinc oxide with silver nanoparticles for gas sensing applications"

Yasmarie Colón-Saez¹, Paola García-Polanco², Wilfredo Otaño³, and Danilo **Barrionuevo**³

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The monitoring of air quality holds paramount significance in our society for comprehending and enhancing public health. The adverse effects of outdoor air pollution, characterized by the presence of noxious gases such as NO2 and CO2, have been correlated with morbidity and mortality rates related to chronic obstructive pulmonary disease. The primary objective of this project is to develop cost-effective arrays of highly sensitive sensors tailored for NO2 monitoring. In the context of this project, our primary emphasis is on augmenting gas-sensing capabilities through the utilization of Zinc oxide (ZnO) thin film gas sensors. ZnO serves as the semiconductor material, while Silver (Ag) is selected as the metal for the nanoparticles. Furthermore, the fabrication process involves the use of a solution comprising 10% Polyvinylpyrrolidone (PVP) in Ethanol (EtOH) to produce electrospun SMO nanofibers. This fabrication process combines electrospinning with multiple cycles of sputtering. Electrospinning is a potent technique that yields nanofiber structures. Following the nanofiber deposition, a 30 nm ZnO layer is sputtered onto the substrate, and subsequently, Ag nanoparticles are deposited at 200 °C. The resulting sample exhibits a notable ability to detect NO2 at concentrations as low as 5 ppm (parts per million).

P-21 "Utilizing ferroelectric structures for energy storage applications"

Edward Hickey-Figueroa¹, Patricia Gierbolini-Santos² and Danilo **Barrionuevo**³

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The world efforts to reduce their dependency on fossil-based energy reserves, the successful production, distribution, and storage of electricity will form a basis for the development and growth of society and technology in the coming century. The advance of a high energy density electrical capacitor is much desirable as it has the potential to transform the field of power electronics, allowing for rapid miniaturization of modern electronic devices and improving the performance of electric vehicles, portable electronics, and medical devices. Our research is focused on performing the fundamental science needed to synthesize and modify the structure of promising solid-state superlattices (Hf_{0.5}Zr_{0.5}O₂ (HZO)/BaTiO₃(BTO)) dielectric material while preserving the good relaxor-ferroelectric properties and fabricated thin films for high power and energy density capacitor applications. The synthesis of HZO and BTO materials was completed. The structures of powder mixtures and the target were verified with the xrd equipment, these results obtained by the xrd verify the monoclinic structure of the HZO, they were worked at various temperatures during the investigation, but the optimum temperature was 1400 °C. For the preparation of the BTO target, the optimal temperature found was 1250 °C and the structure was tetragonal.

O-1 "lonic liquid gate tunable diodes based on monolayer MoSe₂"

Nicholas J. Pinto

Department of Physics and Electronics, University of Puerto Rico at Humacao, Humacao, PR 00791

CVD grown MoSe₂ monolayers were electrically characterized at room temperature in a field effect transistor (FET) configuration using an ionic liquid (IL) as the gate dielectric. The high specific capacitance (~7 mC/cm²) of the IL significantly reduced the operating voltages. The device exhibited ambipolar charge transport with holes (p-type) and electrons (n-type) as the majority charge carriers in the MoSe₂ channel depending on the sign of the gate voltage. This motivated us to fabricate and test devices fabricated from MoSe₂/Si heterojunctions. As grown MoSe₂ monolayers exhibited *n*-type behavior with standard backgating using a doped Si substrate. Heterojunctions of MoSe₂/p-Si and MoSe₂/n-Si should therefore exhibit current (I)-voltage (V) characteristics like that of a diode (asymmetric non-linear) or like that of a resistor (symmetric linear). While the device fabricated with the p-Si substrate operated as a diode as expected, it is not clear why the device fabricated with the n-Si substrate also showed diode-like I-V behavior. By gating the junction using an IL we were able to tune the I-V output characteristics. We are currently in the process of repeating these measurements to better understand the observed data.

This work was funded by NSF under grant: DMR-PREM-2122102.

O-2 "Alternative platforms for colorimetric measurements"

Vibha Bansal¹, Ezio Fasoli², José Sotero³, Idalia Ramos⁴, Ivan Dmochowski⁵, Daeyeon Lee⁶

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Colorimetric assays allow quantitation of various analytes in teaching, research, and healthcare settings. These assays are performed mostly in polystyrene microwell plates, which are rarely reused or recycled, contributing to massive plastic waste generation. The goal of this project is to develop platforms that can form viable and environmentally friendly alternatives to the plastic plates. We previously reported fabrication of opaque white cellulose acetate (CA) microwell plates, that can be used in combination with a smartphone app for these assays. In continuation of this work, we have been developing transparent CA plates with the goal of facilitating the CA plate usage with spectrophotometers. The evaporation of CA solution (in acetone) leads to a transparent film formation, but the film tends to shrink, bend, and suffer from bubble entrapment. CA disc formation is thus being optimized for improved transparency, elasticity, and overall texture. In the past, we have also reported fabrication of liquid marbles (LM) for colorimetric assays. Further study of these LM has allowed us to conclude that the stability of LM fabricated in this study is caused by the particle size of the silica gel particles in the coating rather than their hydrophobicity.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-20 "All-solid-state thin-film batteries with solid electrolytes for medical applications"

Carla Baez-Velázquez¹, Xavier Zayas-Rodríguez², Kyanelisse <u>Flores Morales</u>¹, R. S. Katiyar³, and D. **Barrionuevo**⁴

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All solid-state thin film batteries (ASSTFB) hold great promises for medical devices and implants, representing an exciting frontier for the healthcare industry. These batteries utilize solid electrolytes, offering advantages over traditional ones. Notably, they possess high energy density, enabling compact designs for medical devices like pacemakers, enhancing patient comfort and reducing complications. Furthermore, solid state batteries have long cycle lives, reducing the need for battery replacement surgeries and lowering healthcare costs. They also provide increased safety by avoiding leakage or swelling issues associated with liquid electrolytes. Solid state batteries are particularly valuable in the development of smart implants that can deliver targeted treatments. This project will focus on the development of high energy and power density devices, allowing the rapid miniaturization of modern electronic devices and improving the performance of wearable devices that are according with the broader impact. We propose to use LiCoO₂ (LCO) as cathode, LiPON as solid electrolyte and Lithium metal as anode. In this study, some of the main strategies to improve the energy and power density properties include: to study the interface performance between LCO/LiPON and LiPON/Li. We will use the sputtering technique for the fabrication of the ASSTFB.

P-19 "The effect of image equalization on colorimetric analysis using Smartphones"

Génesis N. <u>Pérez González</u>¹, Emmanuel <u>Rosa Delgado</u>¹, Ezio **Fasoli**², José O. **Sotero Esteva**¹

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A concern present in literature describing colorimetric analysis of chemical assays using smartphones is the effect of the image precessing that those devices perform in images with visual enhancement purposes that are often undisclosed to the public. An example of this kind of manipulation is the image equalization that aims to make the luminosity of all parts of the image more even. Thus, it is expected to alter the colors of the analyzed samples and impact the concentration estimates of the chemical compounds being studied.

In this work we are developing software with the aim of analyzing 96-wells plate assays using smartphones. One of the goals is the automatic detection of the wells in which samples are being placed and their classification according to composition and concentration. These functions are not present in existing plate-analysis apps. Principal component analysis and clustering techniques such as K-means are combined to achieve this goal.

The effect of image equalization on this method has been tested using different kinds of plates and analytes. Examples of instances where image equalization may have some impact on sample detection and classification will be presented.

This work was funded by NSF under grant: DMR-PREM-2122102.

O-3 "Encapsulation and release studies of sulindac in cubosomes nanoparticles using microfluidics"

Rolando **Oyola**¹, Daeyeon **Lee**², Roberto <u>Vaquero</u>¹, Yildeliz <u>Díaz</u>¹

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²Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA 19104

Sulindac (SD) is a Non-Steroidal Anti-Inflammatory Drug (NSAID) used to treat chronic inflammatory diseases such as rheumatoid arthritis and acute symptoms of inflammation. SD has also been of interest for more than a decade as a chemopreventive for adenomatous colorectal polyps and colon cancer. However, SD is associated with dangerous gastrointestinal, renal, and cardiovascular side effects. In general, SD is taken orally, has low solubility, low bioavailability and shows poor stability. Therefore, to overcome these problems, encapsulating the NSAIDs into polymeric carriers is a possible alternative. This work aims to test if cubosome nanoparticles encapsulate SD and can serve as a drug delivery system by studying the release profile in aqueous media. Cubosomes are a particular kind of biocompatible lipid nanovesicles (NVs) produced by dispersion of a bi-continuous cubic phase lyotropic liquid crystalline in water with sizes ranging from 100 to 300 nm. We propose using a microfluidic platform to self-assemble cubosomes and run the SD binding and release profile studies in a continuous fashion.

This work was funded by the NSF-DMR-2122102 program.

O-4 "Pillararene modified cellulose matrix for detection and removal of metals and organic molecules"

Ezio **Fasoli**

Department of Chemistry, University of Puerto Rico at Humacao, Humacao, PR 00791

Pillararenes (PA) are a new class of macrocycles with interesting host guest properties with a variety of inorganic and organic molecules. PA have been studied for their ability to encapsulate heavy metals and cationic organic molecules within their aromatic rings. The chemical structure of PA allows them to be chemically linked to solid material and to use their properties to trap water pollutants. The objective of this work is to functionalize a cheap, environment-friendly soft material (cellulose) with PA, for trapping and detecting potable water pollutants.

1,4-dimethoxypillar[5]arene (DMPA) was synthesized by reacting 1,4-dimethoxybenzene and paraformaldehyde in 1,2-dichloroethane in the presence of trifluoroacetic acid as a catalyst. The so formed DMPA was treated with BBr₃ to selectively remove one methoxy group. The so formed product was purified by column chromatography and characterized by LC-MS and NMR.

Cellulose filters were functionalized with epichlorohydrin to create a linker for attachment of the macrocycles. The chemically modified membranes were characterized by FT-IR spectroscopy and SEM microscopy.

As an alternative approach PA were mixed at different w/w ratios with cellulose nanofibrils and immobilized on membranes. The membranes were tested for their ability to trap P-nitrophenol.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-18 "Overview of Neural Network architectures for the study of polymers"

Michael J. <u>Rivera Lazú</u>¹, Sophia L. <u>Martínez Miranda</u>², Preston **Moore**³, José O. **Sotero Esteva**¹

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The rising popularity of Neural Networks has extended to applications in materials science and polymers. In this work, we show different architectures such as Convolutional Neural Networks, Generative Adversarial Networks (GANs), Cycle GANs, and a Neural Network that generated coordinates representing polymers that were trained with Lennard-Jones and Bond potential energy function as loss function parameters for the model. We will show the results obtained and what we learned from these methods such as strengths, weaknesses, what worked, and what could have been done differently. Additionally, a preview of the next step in this project will be shown, where we leverage what we have learned into a new way to tackle this problem which consists of Graph Networks for simulating polymers. GN has been used for simulating fluids, and we want to test this type of architecture for polymer applications. We also aim to implement attention mechanisms in the training of these networks, a popular technique that has been shown useful in the improvement of GN.

P-17 "Optimized 3D-printed fluidic devices for separation of carbon spheres"

Robert A. Rosario González¹, Kimberly M. Hernández Ferrer², Rolando Oyola³, Jorge J. Santiago Avilés⁴, José O. Sotero Esteva¹

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In this innovative study, we present a comprehensive analysis of two distinct fluidic models aimed at optimizing the separation of carbon spheres, utilizing advanced photo analysis techniques. First, we will be measuring the channels in the fluidic device so we can make sure it fits the requirements needed to create different methods of separation of the carbon spheres. Then, we will be working on two different models with different mechanisms to and structures to study the behavior of these spheres with photo analysis. The goal is to optimize the project so it can work on its own. One of the fluidic models has a spiral form, meaning it has one entry where we introduce the fluid and the solvent at the top and it goes down in a spiral form and ends in four different exits. The other model has only one entry and one exit and has a cubic form with the channels on the inside. The challenges we are facing currently are that we are using an 'Ender-3' 3D printer which is a very affordable printer and may bring limitations that may be negative for the outcome. We are making the channels as thin as possible, demonstrating we can create the channels with more control in the dimension want. We want to optimize the project so we can change the following parameters easily: how divided are the spheres, proportions of different solvents, velocity in which we inject the solvent to the device and the angles in which exit channels are placed.

This work was funded by NSF under grant: DMR-PREM-2122102.

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O-5 "Physical Vapor Deposition of Random Arrays of Ag Nanoparticles: Sensing Applications and Beyond"

Francisco Bezares

Department of Physics, University of Puerto Rico at Mayagüez, Mayagüez, PR 00681

Magnetron Sputtering Physical Vapor Deposition (MSPVD) of Ag nanoparticles is a promising technique for the fabrication of largearea, ultra-sensitive Surface-enhanced Raman Scattering sensors. However, to make this technology commercially amenable, the control of physical properties, such as morphology, nanoparticle sizes and interparticle distances, is key. In addition, an understanding of the effects of particle-to-particle interactions as well as contributions from the substrate may provide valuable insight that may lead to new capabilities and novel technologies. In this talk, we will present a comprehensive study of the physical and optical properties of random arrays of Ag nanoparticles, fabricated via MSPVD, and will show that they present a strong case for the development of sensing as well as other photonic applications. We will discuss how different components of the optical properties of these nanoparticles can be tuned or adjusted to better suit specific applications, according to their particular requirements, and how the random character of the nanoparticle arrays may offer exciting new possibilities for light control at the nanoscale.

This work was funded by NSF under grant: DMR-PREM-2122102.

O-6 "Data Science applications to the study of polymers, colorimetry, and particle separations"

José O. **Sotero Esteva**¹, Michael J. <u>Rivera Lazú</u>¹, Emmanuel <u>Rosa Delgado</u>¹, Génesis N. <u>Pérez González</u>¹, Frances J. <u>Martínez Miranda</u>¹, Robert A. <u>Rosario González</u>¹, Sophia L. <u>Martínez Miranda</u>², Kimberly M. <u>Hernández Ferrer</u>³, Preston **Moore**⁴, Ezio **Fasoli**⁵, Vibha **Bansal**⁶, Rolando **Oyola Martínez**⁵, Jorge J. **Santiago Avilés**⁷, Idalia **Ramos**⁸

¹Dept. Mathematics, UPRH, Humacao, PR 00791; ²Petra Mercado Bougart High School, Humacao, PR 00791; ³Ramón Quiñones Medina High School, Yabucoa, PR 00767; ⁴Dept. Chemistry & Biochemistry, Saint Joseph's University, Philadelphia, PA 19131; ⁵Dept. Chemistry, UPRH, Humacao, PR 00791; ⁶Dept. Chemistry, UPRC, Cayey, PR 00736; ⁷Dept. Electrical & Systems Eng., PENN, Philadelphia, PA 19104; ⁸Dept. Physics & Electronics, UPRH, Humacao, PR 00791

In this talk, we will present an overview of various applications of data science to materials research and education. One of the research projects involves studying the conformations of polymers grafted onto a surface in the presence of different solvents using coarsegrained molecular dynamics simulations. This study has led to the test of new ways to find better optima using different kinds of neural networks. Currently, generative graph neural networks are being tested. The coarse-grain model has also been used in materials science outreach in the Experimenta con PREM workshop, where high school students learn fundamental computer programming to generate initial conformations for molecular dynamics simulations. They then analyze these simulations using custom programs, spreadsheets, and VMD. In another project, novel image processing and automatic classification techniques are being used to perform colorimetric analysis of chemical assays on well-plates made with either standard rigid materials or flexible materials such as cellulose acetate. Application prototypes for plate analysis that can be used on computers as well as mobile devices have been made on open-source dashboard platforms as well as on the Microsoft Power App service. Finally, we are undertaking a new research path that will develop expertise applicable to autonomous experimentation projects. For this, they are proposing the design and semi-automatic optimization of fluidics methods using devices made with 3D printers for the separation of carbon spheres. This work was funded by NSF under grant: DMR-PREM-2122102.

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P-16 "Colorimetric assay analysis using Microsoft Power Platform"

Frances J. Martínez-Miranda, Emmanuel Rosa-Delgado, Génesis Pérez-González, José J. **Sotero-Esteva**

Department of Mathematics, University of Puerto Rico at Humacao, Humacao, PR 00791

We are developing a prototype of an application that aims to perform colorimetric analysis of 96-well plates using the Microsoft Power Platform. Previously our team had made a similar application, using Streamlit with Python. Some limitations of this application are the constant updates and the necessity to have a server running constantly for the application to function correctly, in addition to the extensive code and development time. Microsoft Power Platform is a low-code platform for rapidly building customized end-to end solutions using many products areas that are designed for a connected experience. The advantage with a low-code integrated tool development approach is to get more alternatives, such as obtaining information directly from One Drive to use it for the better functioning of the application and thus provide a better user experience. We used Power Apps for the application development, Power Automate to connect with other tools, One Drive to save and collect the images, and Power BI to create plots. The limitations could be, the necessity of a strong internet connection for development, requires payment to be able to use and prior knowledge or learning about all the components of the platform to be able to achieve successful results.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-15 "Deformed plate wells detection by means of image filters, keystone corrections and the Hough transform"

Emmanuel Rosa Delgado¹, Vibha Bansal², José O. Sotero Esteva¹

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²Department of Chemistry, University of Puerto Rico at Cayey, Cayey, PR 00737

Applications that use smartphone cameras for visual colorimetric analysis are often developed in combination with components that serve as sample holders, fluidic chambers, or active membranes. Using smartphones as handheld visual colorimetric analysis devices and sample managers with novel flexible materials raises challenges not present when using rigid materials and better-controlled settings. For instance, accurately finding where analytes are is crucial to a correct analysis.

This work has used deformed 96-wells plates as a model of devices that may be used in the field in combination with smartphone applications as colorimetric devices. An algorithm based on the application of the Hough transform followed by an interpolation is developed and tested with plate images under different illumination sources that have been deformed in a controlled fashion. The proposed method shows robustness in detecting the wells in all images of the test sets.

This work was funded by NSF under grant: DMR-PREM-2122102.

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O-7 "Autonomous deposition of polymeric and particle composites for structural control of soft materials"

Yvonne <u>Zagzag</u>, Minki Lee, Chinedum **Osuji** University of Pennsylvania, Philadelphia, PA, 19104

We use autonomous experimentation (AE) to control the structure of polymeric and particle composites and ultimately relate these structures to material parameters. Autonomous experimentation uses decision algorithms to plan and execute a series of material experiments iteratively. Specifically, an iterative research loop of planning, experiment, and analysis is carried out autonomously. Using the library of parameters that control particle and polymeric composite interactions and their morphologies in an AE process will allow us to direct the evolution of these materials to predictively manufacture network morphologies. These reproducible films will be useful for industrial purposes such as creating homogenous drying patterns for printing industries. By exploiting the mixing and subsequent deposition properties of polymers and particles dispersed in solvents and in liquid crystal monomers, we aim to artificially engineer an energy landscape that governs the resultant textures of chain-like and network-like structures that can be studied optically. Ultimately, we aim to enable AE to establish unique routes toward creating drop-cast samples associated with structural fingerprints. The development of this new research process, these iterative autonomous loops, is expected to increase the efficiency of soft matter science and shift the way our research is conducted.

O-8 "Directing Self-Assembly and Advancing Autonomous Experiments with Soft Materials"

Chinedum **Osuji**

Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA 19104

Controlling structure and thereby manipulating the properties of matter is a central concern for materials science. This talk approaches for directed self-assembly examines nanostructured systems such as block copolymers and liquid crystals to create useful materials, including single crystals and materials with bespoke textures. We describe the use of electrospray deposition as an approach to produce thin films of polymers and other materials at slow deposition rates that enable control of morphology. The platform developed for electrospray deposition enables automated and autonomous experiments to be performed. This talk will describe the design and features of the platform and cover ongoing experiments that use computer controlled liquid handling and optical irradiation to advance autonomous investigations.

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P-14 "Computational identification of the ferrimagnetic structure of $HSrCoO_{2.5}$ "

Andrea García, Juan Santana

Department of Chemistry, University of Puerto Rico at Cayey, Cayey, PR 00737

Multiferroics exhibit the rare and intriguing property of simultaneously possessing multiple ferroic orders, such as ferromagnetism, ferroelectricity, and ferroelasticity. The coexistence and coupling of these distinct ferroic states open up a realm of possibilities for the development of novel, multifunctional devices with applications ranging from energyefficient electronics to memory storage and sensing. Unfortunately, multiferroic materials demonstrating robust coupling between ferroelectric and ferromagnetic (or ferrimagnetic) states at room temperature have remained elusive. In this context, we suggest that introducing hydrogen into antiferromagnetic transition-metal oxides holds promise for achieving multiferroics with substantial magnetoelectric coupling. Using computational optimization of brownmillerite SrCoO_{2.5}, we demonstrate the position of the hydrogens can simultaneously manipulate the magnetization and stability of the structure. The structures with the tetrahedral cobalts in an antiferromagnetic state and the octahedral cobalts in a ferromagnetic state resulted in the lowest energies; and they had the hydrogens either facing downwards, upwards, and outwards. Overall, the structures with the hydrogens facing downwards had the lowest energies, resulting in the most stable ones.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-13 "Photoresponse properties of a broadband rGO-nSi photodetector"

José L. <u>Pérez Gordillo</u>¹, Anamaris Meléndez¹, Jorge J. **Santiago**², Nicholas J. **Pinto**¹, Idalia **Ramos**¹

¹Department of Physics and Electronics, University of Puerto Rico at Humacao, Humacao, PR 00791

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A photodetector constructed from reduced Graphene Oxide (rGO) shows respectable values for responsivity and fast response and recovery times at 0 voltage bias. rGO films made using a simple one-pot hydrothermal method have been characterized in previous work and show good electrical and optical properties. To fabricate our device, an rGO film is cleaved over the edge of an n-Si substrate. The electrical contacts between the rGO and n-Si allow efficient transfer of photogenerated charge carriers. The device shows a photoresponse at a broad spectral range of 250 to 631 nm, with a fast response and recovery times of a few milliseconds. The green and simple preparation of our rGO photodetector shows promising results for carbon-based electronics from renewable sources and compatible with silicon technology.

This work was funded by NSF under grant: DMR-PREM-2122102.

Panel "Best practices for recruiting, retaining, and supporting graduate students from MSIs"

This panel will explore topics around recruiting, retaining and supporting graduate students who earned their undergraduate degrees from minority serving institutions (MSIs). Panelists Andrea Marcano (PhD candidate at MIT), Deliris Ortiz, PhD (starting a postdoctoral fellowship at UM-Ann Arbor), and Idalia Ramos (PREM PI, Prof. of Physics & Electronics at UPR-Humacao) will share experiences and expertise to seed this discussion on broadening participation and student flourishing in STEM graduate programs. The panel will be moderated by Kristin Field, PhD (Education Director for the Penn NRT Soft AE Program).

P-12 "Analysis and sintering process characterization of carbon spheres prepared using hydrothermal method"

Emily <u>Morales</u>¹, Anamaris Meléndez¹, Idalia **Ramos**¹, César A. Nieves²

¹Department of Physics and Electronics, Humacao, PR 00791 ²Omya Technology Center Cincinnati, Blue Ash, OH 45242

We are studying the impact of precursor concentration and annealing temperature on the properties of reduced carbon spheres (rCS). Carbon spheres (CS) were synthesized by hydrothermal carbonization of sucrose, in concentrations of 0.1 M and 0.8 M, and then thermally reduced at 600°C in an inert atmosphere to eliminate functional groups and increase the carbon content. The thermal transformations occurring in the preparation of rCS are investigated through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) across a broad temperature range from 25 to 1000°C. The morphology, composition, structure, size distribution, and surface chemistry of the thermally reduced spheres are analyzed with SEM-EDS, FTIR, and XRD. No significant mass changes are measured for rCS up to 600°C. The results confirm the successful reduction of oxygen in CS as well as the thermal stability of the resultant rCS. The impact of sucrose concentration and reduction temperature on the properties of carbon spheres will be presented.

Carmen I. <u>Torres-Dávila</u>¹, Kamillie <u>Díaz-Dávila</u>², Nitza V. Falcón-Cruz¹, and Rolando **Oyola**¹

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Gold nanoparticles (AuNP) have the potential to be used in biomedical applications where interaction with many ligands can occur. Characterization of nanoparticle-ligand, i.e., binding constant and sites, can be measured using fluorescence quenching, a well-established approach. However, many reports identify potential experimental pitfalls of the technique when applied to ligand-AuNP interactions. Two significant pitfalls are 1) approximation of the free ligand concentration as the total ligand concentration and 2) corrections due to inner filter effects. Equilibrium binding isotherms are model-independent and reflect the relationship between the extent of ligand binding density and the free ligand concentration. This model-free approach allows for a quantitative description of the interactions independent of assumptions about the nature of the binding process. In this work, we applied a model-independent method of analysis to generate a true thermodynamic for the AuNP-Atto655 binding isotherm. Atto655 is a sensitive fluorescence probe that absorbs in the red region, minimizing inner filter effects. This model-free method will be compared to the noncooperative independent site model.

This work was funded by the NSF-DMR-2122102 program.

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Poster Presentations

- P-1 "Electrical characterization and ammonia gas response of a p-Si/n poly[benzimidazo- benzophenanthroline] thin film junction diode", Alejandro J. Cruz-Arzon¹, José Pérez¹, Idalia Ramos¹, Nicholas J. Pinto¹, Nitza Falcón², Rolando Oyola², Yue Jiang³, Nikita Gupta³ and A.T. Charlie Johnson³. ¹Dept. Physics and Electronics, UPRH; ²Dept. Chemistry, UPRH; ³Dept. Physics and Astronomy, PENN
- P-2 "Ionic liquid gate tunable diodes based on MoSe₂/doped Si hetero-junctions", Keiralys <u>Soto Ortiz</u>¹, Alexander <u>Real Quiñones</u>¹, Nicholas J. Pinto¹, C. Wen², Y. Suh and A.T. Charlie Johnson². ¹Dept. Physics and Electronics, UPRH; ²Dept. Physics and Astronomy, PENN
- P-3 "Silane Modified Fumed Silica for Liquid Marble Fabrication", Lyanivette <u>Alvarado López</u>¹, Luis A Delgado Rodríguez¹, Gustavo A Berríos Alvarado¹, Ezio Fasoli², Daeyeon Lee³, Vibha Bansal¹. ¹Dept. Chemistry, UPRC; ²Dept. Chemistry, UPRH; Dept. Chemical & Biomolecular Eng., PENN
- P-4 "Fabricating transparent microwell plates from cellulose acetate", Nathalia <u>Liu De Restrepo</u>1, Alexander Y. Ortiz Rivera1, Idalia Ramos2, Ivan J. Dmochowski3, Daeyeon Lee4, Vibha Bansal1. Dept. Chemistry, UPRC; Dept. Physics and Electronics, UPRH; Dept. Chemistry, PENN; Dept. Chemical & Biomolecular Eng., PENN
- P-5 "Glycerol as plasticizer agent in recycled cellulose acetate microwell plates", Gabriela A. Marrero Hernández¹, Idalia Ramos², Ivan Dmochowski³, Daeyeon Lee⁴, Vibha Bansal¹. ¹Dept. Chemistry, UPRC; ²Dept. Physics and Electronics, UPRH; ³Dept. Chemistry, PENN; ⁴Dept. Chemical and Biomolecular Eng., PENN
- **P-6** "Size and Interparticle Distance Control in Magnetron Sputtering Deposition of Noble Metals", Wanda <u>Rivera</u>¹, Camila <u>Negrón</u>², and Francisco **Bezares**². ¹UPRC; ²UPRM
- P-7 "Optical Properties of Random Arrays of Magnetron Sputtering Deposition of Ag Nanoparticles on Si Substrates", Joshua <u>Chaparro</u>, Jessiel <u>Vélez</u>, Germán <u>Vázquez</u>, Francisco **Bezares**. Dept. Physics, UPRM

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- "Development of a paper-based sensor for the detection of aromatic aldehydes and its implementation in the Experimenta con PREM workshop", Auriani Gómez, Yelisbeth Santa, Gabriela Villafañe, Ezio Fasoli. Dept. Chemistry, UPRH
- "Synthesis of Pillararenes and their attachment to cellulose membranes", Grace Sánchez¹, Yelisbeth Santa¹, Jubetzy Crespo², Ezio **Fasoli**¹, ¹Dept, Chemistry, ²Dept, Biology, UPRH
- P-10 "Fluorescence study of a fluorene-Shiff-base derivative for Ga³⁺ sensing", Nicole <u>De Jesús</u>, Nitza V. <u>Falcón Cruz</u>, Melvin De Jesús, Rolando Oyola. Dept. Chemistry, UPRH
- P-11 "Quantitative analysis using model-independent ligand binding density function applied to nanoparticle-ligand equilibrium", Carmen I. Torres Dávila¹, Kamillie Díaz Dávila², Nitza V. Falcón Cruz¹, Rolando **Oyola**¹. ¹Dept. Chemistry, UPRH; ²Escuela Superior Bellas Artes, Humacao
- P-12 "Analysis and sintering process characterization of carbon spheres prepared using hydrothermal method", Emily T. Morales Arroyo¹, Anamaris Meléndez¹, Idalia Ramos¹, César Nieves², ¹Dept. Physics and Electronics, UPRH; Omya Technology Center Cincinnati, Blue Ash, OH
- P-13 "Photoresponse properties of a broadband rGO-nSi photodetector", José L. Pérez Gordillo¹, Anamaris Meléndez¹, Nicholas J. Pinto¹, Jorge Santiago², Idalia Ramos¹. Dept. Physics and Electronics, UPRH; ²Dept. Electrical and Systems Eng., PENN
- P-14 "Computational identification of the ferrimagnetic structure of HSrCoO₂₅", Andrea García, Juan Santana. Dept. Chemistry, **UPRC**
- P-15 "Deformed plate wells detection by means of image filters, keystone corrections and the Hough transform", Emmanuel Rosa Delgado¹, Vibha **Bansal**², José O. **Sotero Esteva**¹. ¹Dept. Mathematics, UPRH: ²Dept, Chemistry, UPRC
- P-16 "Colorimetric assay analysis using Microsoft Power Platform", Frances J. Martínez Miranda, Emmanuel Rosa-Delgado, Génesis Pérez González, José O. Sotero-Esteva. Dept. Mathematics, UPRH

P-10 "Fluorescence study of a fluorene-Shiff-base derivative for Ga³⁺ sensing "

PREM

Nicole De Jesús, Nitza V. Falcón Cruz, Melvin De Jesús, and Rolando Ovola

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Quantitative metal analysis using fluorescence probes is becoming an alternative to atomic absorption or emission techniques. Gallium is commonly used in nuclear medicine and as an antimicrobial agent among metals. Gallium nanoparticles can potentially be used for drug delivery and in amyloidosis disease. However, determining the gallium content in nanoparticles is required for higher-quality control and quantitative work. This work presents the fluorescence properties of a fluorenyl-Shiff base derivative sensor at different pHs. Acidic conditions (pH <3) quench the probe's emission intensity, while alkaline (pH > 8) induces a high emission yield. The binding of Ga³⁺ ions to the probe was proven using gallium nitrate as a standard.

This work was funded by the NSF-DMR-2122102 program.

P-9 "Linking Pillararene to cellulose for the development of potable water purification filters"

Grace <u>Sánchez</u>¹, Yelisbeth <u>Santa</u>¹, Jubetzy <u>Crespo</u>², Ezio **Fasoli**¹

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Pillararenes (PA) are novel macrocyclic compounds made of repeating hydroquinone units that can establish host-guest properties with a variety of inorganic and organic molecules. This allows them to trap contaminants in potable water. The goal of the project is the immobilization of PA on chemically modified cellulose matrix with the aim of developing new purification devices for the removal of water pollutants (heavy metal and/or organic molecules).

Dimethoxy-pillararene (DMPA) was synthesized by reacting 1,4-dimethoxybenzene and paraformaldehyde in 1,2-dichloroethane in the presence of trifluoroacetic acid (TFA) as catalyst. The product was crystallized from acetonitrile and characterized by ¹H NMR and ¹³C NMR. DMPA was immobilized on cellulose nanofibrils. The resulting membrane was analysed through Scanning Electron Microscopy (SEM) and was tested for its ability to trap ions from a solution.

DMPA was also reacted with BBr_3 to selectively remove one methoxy group. The so formed product was purified by column chromatography and characterized by LC-MS and NMR.

Cellulose acetate filters commercially available from Steriltech were functionalized epichlorohydrin to create a linker for attachment of the PA. The chemically modified membranes were characterized by FT-IR spectroscopy SEM microscopy.

- P-17 "Optimized 3D-printed fluidic devices for separation of carbon spheres", Robert A. Rosario González¹, Kimberly M. Hernández Ferrer², Rolando Oyola³, Jorge J. Santiago Avilés⁴, José O. Sotero Esteva¹. ¹Dept. Mathematics, UPRH; ²Ramón Quiñones Medina High School, Yabucoa; ³Dept. Chemistry, UPRH; ⁴Dept. Electrical and Systems Eng., PENN
- P-18 "Overview of Neural Network architectures for the study of polymers", Michael J. <u>Rivera Lazú</u>¹, Sophia L. <u>Martínez Miranda</u>², Preston **Moore**³, José O. **Sotero Esteva**¹. ¹Dept. Mathematics, UPRH; ²Petra Mercado High School, Humacao; ³Dept. Chemistry and Biochemistry, Saint Joseph's University, Philadelphia
- P-19 "Effect of common smartphone image pre-processing techniques on colorimetry classification", Génesis N. <u>Pérez González</u>¹, Emmanuel <u>Rosa Delgado</u>¹, Ezio **Fasoli**², José O. **Sotero Esteva**¹. ¹Dept. Mathematics, UPRH; ²Dept. Chemistry, UPRH
- P-20 "All-solid-state thin-film batteries with solid electrolytes for medical applications", Carla Baez-Velázquez¹, Xavier Zayas-Rodriguez², Kyanelisse Flores Morales¹, R. S. Katiyar³, and D. Barrionuevo⁴. ¹Dept. Chemistry, UPRC; ²Dept. Natural Sciences, UPRC; ³Dept. Physics and Institute of Functional Nanomaterials, UPR-Río Piedras; ⁴Dept. Mathematics and Physics, UPRC
- **P-21** "Utilizing ferroelectric structures for energy storage applications", Edward Hickey-Figueroa¹, Patricia Gierbolini-Santos² and Danilo **Barrionuevo**³. Dept. Chemistry, UPRC; ²Dept. Biology, UPRC; ³Dept. Mathematics-Physics, UPRC
- **P-22** "Zinc oxide with silver nanoparticles for gas sensing applications", Yasmarie Colón-Sáez¹, Paola Garcia-Polanco², Wilfredo Otaño³, Danilo **Barrionuevo**³. ¹Dept. Chemistry, UPRC; ²Dept. Natural Sciences, UPRC; ³Dept. Mathematics and Physics, UPRC
- P-23 "Multiferroic characteristics of hafnium-doped material for neuromorphic computing applications", Eric Sánchez-Ayala¹, Cynthia Rodríguez-Cruz¹, Maria Rodríguez-Ortiz¹, and Danilo Barrionuevo², ¹Dept. Biology, UPRC; ²Dept. Mathematics-Physics, UPRC

P-8 "Development of a paper-based sensor for the detection of aromatic aldehydes and its implementation in the Experimenta con PREM workshop"

Auriani <u>Gómez</u>, Yelisbeth <u>Santa</u>, Gabriela <u>Villafañe</u>, Ezio **Fasoli** Department of Chemistry, University of Puerto Rico at Humacao, Humacao, PR 00791

Aromatic aldehydes are widely used as flavoring agents in food, perfume, and pharmaceutical industry. A chromogenic and fluorogenic cellulose sensor assay was developed for the qualitative and quantitative detection of aromatic aldehydes in a solid phase. The sensor is made of cellulose filter paper commercially available from Steriltech chemically modified with epichlorohydrin and para-amino benzamidine (pABA). The assay consist in the reaction of the sensor with glyoxal bisulfite and different aromatic aldehydes: benzaldehyde, furfural, vanillin, and cinnamaldehyde. The reaction leads to the formation of a fluorescent benzyl imidazolone, which is visible on the paper sensor. The assay weas tested for quantitative analysis, using a Fluorescence Spectrophotometer at 375 nm excitation and 500-600 emission. Results show a linear detection in the range of 25 to 1,000μM for benzaldehyde and 25 to 250μM for furfural.

This experiment was implemented as a workshop for Experimenta con PREM where high school students were exposed to the topic of sensors, fluorescence spectroscopy and were able to recognize and quantify the different aldehydes given to them.

P-7 "Optical Properties of Random Arrays of Magnetron Sputtering Deposition of Ag Nanoparticles on Si Substrates"

Joshua <u>Chaparro</u>, Jessiel <u>Vélez</u>, Germán <u>Vázquez</u>, Francisco **Bezares**

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Ag nanoparticles have unique optical and chemical properties, making them suitable for novel photonic applications. Although a great number of studies have established the fundamental physics underlying the photonic properties of these systems, many questions remained unanswered for the more specific aspects, such as those related to possible particle-particle interaction effects on periodic and random arrays of closelyspaced nanoparticles as well as the role of substrates in the plasmonic resonance under these conditions. In this work, we measure and compare the photoluminescence and extinction spectra of random arrays of Ag nanoparticles and characterized and monitored changes in their optical properties due to degradation over a period of approximately a year. The arrays of nanoparticles were fabricated utilizing the Magnetron Sputtering Physical Vapor Deposition (MSPVD) technique, with varying depositions parameters such as substrate temperature and deposition times and pressures. Interestingly, we show that the ratio of intensities of photoluminescence to extinction measurements at a given wavelength can be varied and it is possible to suppress one against the other by carefully designing the morphology as well as the size and interparticle distance of the nanoparticles in the arrays. Degradations effects on the optical properties will also be discussed.

This word was funded by NSF under grant: DMR-PREM-2122102.

ABSTRACTS Poster Presentations

P-1 "Electrical characterization and ammonia gas response of a p-Si/n-poly[benzimidazobenzophenanthroline] thin film junction diode"

Alejandro J. Cruz-Arzón¹, José Pérez¹, Idalia Ramos¹, Nicholas J. Pinto¹, Nitza Falcón², Rolando **Oyola**², Yue Jiang³, Nikita Gupta³, A.T. Charlie Johnson³

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We report on the electrical characterization and ammonia vapor (NH₃) response of a p-Si/n-poly[benzimidazobenzophenanthroline] (n-BBL) thin film junction diode. The presence of a depletion layer at the *n*-BBL/*p*-Si interface was verified *via* capacitance-voltage measurements, and the built-in potential was ~1.8V. Using the standard diode equation for data analysis, the turn-on voltage, rectification ratio, and ideality parameter of the diode were found to be 2, 16 and 6V respectively. The diode was also tested in the presence of NH₃ vapor where it retained its asymmetric J-V behavior with increased currents and an insignificant change in device parameters. NH3 is believed to interact with the adsorbed O_2^- species on the *n*-BBL surface liberating electrons that enhance the diode current. The response time, recovery time and sensitivity of the diode was 60s, 110s and 52% respectively. Removal of the gas restored the diode characteristics to their near original shape making it reusable. The diode was also electrically characterized as a function of temperature and found to retain its rectifying behavior down to 150K. The rectifying and gas sensing features make the diode multifunctional which expands the range of applications of this ladder-type conducting polymer.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-6 "Size and Interparticle Distance Control in Magnetron Sputtering Deposition of Noble Metals"

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Magnetron Sputtering Physical Vapor Deposition (MSPVD) of Ag nanoparticles on SiO₂ substrates has the potential for development of ultra-sensitive, large-area sensing and photocatalytic applications. Deposition parameters such as substrate temperature and deposition times and pressures are key factors for controlling the optical and morphological properties of these samples. However, many aspects remain unclear regarding the relationships between deposition parameters and physical properties. Here, we study Scanning Electron Microscopy (SEM) images of Ag nanoparticles on SiO₂ substrates fabricated by MSPVD through a complete range of temperatures (25-250 °C), times (3-15 s) and pressures (09.00 -19.00 mT). We show that it is possible to tune the nanoparticle sizes and interparticle distances, with a high degree of accuracy and consistency, to produce optimized Surface-enhanced Raman Scattering sensors, where these two variables are key. A simple, general model for Ag nanoparticle growth will also be discussed.

P-5 "Glycerol as plasticizer agent in recycled cellulose acetate microwell plate"

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Plastic is vastly used in research laboratories around the world and an average researcher produces 15 times more plastic waste than an individual. Most of this plastic waste comes from single use plasticware in the laboratory which includes microwell plates. There is, thus, a need to develop eco-friendly alternatives to these plastic laboratory consumables. In an effort to address this need, cellulose acetate (CA) microwell plates were developed in our laboratory. The plates were fabricated using a mixture of defined amounts of cellulose acetate, calcium carbonate, glycerol, and acetone. Following this, we have been studying the recyclability of these plates. The used CA plates were treated with different solutions to eliminate the reactants from the reactions performed in the plates, ground to fine powder, washed with different reagents, and finally used to fabricate new CA microwell plates. The plates obtained had crumbly texture. The fabrication was thus optimized with respect to glycerol content as the plasticizer. Adding higher amounts of glycerol improved the elasticity of the recycled plate.

This word was funded by NSF under grant: DMR-PREM-2122102.

P-2 "lonic liquid gate tunable diodes based on MoSe₂/doped Si hetero-junctions"

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We present our results on the fabrication and electrical characterization of CVD grown monolayer MoSe₂/doped Si heterojunction diodes at room temperature. Ionic liquid (IL) gating of monolayer MoSe₂ when connected in a field-effect transistor configuration shows that the charge transport is ambipolar. This motivated us to test the operation of MoSe₂/doped Si diodes fabricated separately using p- and ndoped Si substrates in the presence of an IL. By applying a gate voltage to the IL we were able to tune the diode parameters (i.e. rectification ratio, turn-on voltage and ideality parameter). Notable differences in the current-voltage (I-V) curves were observed depending on the type of doped Si that was used. Varying the gate voltage resulted in the diode exhibiting nonlinear rectifying characteristics in the first and third quadrant of the I-V plot for the $MoSe_2/p$ -Si diode, while the $MoSe_2/n$ -Si diode exhibited non-linear rectifying behavior only in the third quadrant of the I-V plot. Electrostatic current control at low voltages enhances the diode's functionality, making it useful in other applications besides rectification.

P-3 "Silane Modified Fumed Silica for Liquid Marble Fabrication"

Lyanivette <u>Alvarado López</u>¹, Luis A Delgado Rodríguez¹, Gustavo A. Berríos Alvarado¹, Ezio **Fasoli**², Daeyeon **Lee**³, Vibha **Bansa**l¹

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Liquid Marbles (LMs) are microspheres fabricated by rolling a microdroplet of a solution on a bed of hydrophobic nanoparticles. They offer a closed system wherein reactions can occur between entrapped reagents, or through injection of additional reagents. Robust and transparent LM were fabricated in our laboratory for colorimetric estimations. These LMs were fabricated using three types of coatings: 1) Fumed silica modified with hexamethyldisilazan (MFS); 2) Silica Gel modified with trichloro (1H,1H,2H,2H-perfluorooctyl) silane (T8 MSG); and 3) a mixture of both (MIX). LMs coated with T8 MSG and the MIX demonstrated higher resistance to coalescence and shearing forces. However, MFS and MSG consisted of different silanes, and this led to the question of what property confers stability upon the LMs: particle size or the degree of hydrophobicity of the silane. The study being reported in this poster addresses this question through modification of fumed silica with T8 and using this powder to fabricate LM and characterize it. Preliminary results for the coalescence study showed that the LMs coated with T8 MFS exhibit the same stability as those coated with MFS (Cab-O-Sil), indicating that it is the particle size, not hydrophobicity which confers the stability on LM in this case.

This work was funded by NSF under grant: DMR-PREM-2122102.

P-4 "Fabricating transparent microwell plates from cellulose acetate"

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In contemporary scientific laboratories, the proliferation of single-use plastics poses a severe environmental threat, prompting urgent efforts to adopt sustainable alternatives. This study addresses this concern by exploring cellulose acetatederived microwell plates as an eco-friendly alternative for traditional plastic plates. Derived from natural compounds, cellulose acetate (CA) offers a biodegradable alternative. However, transparent CA microwell plates formed in our laboratory displayed undesirable traits such as wrinkled texture and brittleness. Simple CA discs were used to optimize the fabrication process from hereon. Glycerol was introduced as a plasticizer and led to CA discs with improved elasticity. Optimal results were achieved at glycerol concentration of 0.5% (w/v). Glycerol, however led to loss of transparency which was resolved by incorporation of isopropanol in the CA dispersion. Further improvements in the disc quality were obtained through annealing and immersion of CA discs in NaOH bath. Plates exposed to 0.0025N NaOH exhibited outstanding transparency and flexibility. The study's future direction aims at the fabrication of a CA microwell plate using conditions optimized for CA discs, contributing to sustainable laboratory practices and reducing environmental impact.