

# MATERIALS RESEARCH SOCIETY-NATIONAL SCIENCE FOUNDATION PREM RESEARCH SCHOLARS SUMMIT POSTER SESSION

WEDNESDAY, APRIL 12
5:00 -7:00 PM
Moscone West, Level One, Exhibit Hall



# **POSTER GUIDE**

Poster ID	Presenter	Affiliation
PREM 01	Juan Bernal Romero	California State University Northridge
PREM 02	Swosti Choudhury	California State University Northridge
PREM 03	Alec Milbourne	California State University Los Ángeles
PREM 04	Jael Xitlali Fregoso	California State University Northridge
PREM 05	Bianca Brown	Spelman College
PREM 06	Jordan Brown	Spelman College
PREM 07	Christian Johnson	Spelman College
PREM 08	Jayda Shine	Spelman College
PREM 09	Elmon Anthony Merriman	Clark Atlanta University
PREM 10	Kathleen Bailey	Texas State University
PREM 11	Arriana Bisram	University of Delaware
PREM 12	Poster Retracted by Author	
PREM 13	Mason Brady	Fort Lewis College
PREM 14	Hannah Carlson	Fort Lewis College
PREM 15	Ajeya Dixon	Norfolk State University
PREM 16	Sahra Genc	Fort Lewis College
PREM 17	Liam Harrigan	Norfolk State University
PREM 18	Poster Retracted by Author	
PREM 19	Tekiyah Robinson	Norfolk State University
PREM 20	Dakota Rodriguez	Fort Lewis College
PREM 21	Poster Retracted by Author	
PREM 22	Ian VanHorn	Fort Lewis College
PREM 23	Jazz Geter	Hampton University
PREM 24	Alexa Livingstone	Hampton University
PREM 25	Breon McCray	Hampton University
PREM 26	Victoria Vinson	Howard University
PREM 27	Jaiden Moore	Jackson State University
PREM 28	Yifang Qi	Jackson State University
PREM 29	Zoe Schott	Jackson State University
PREM 30	Moses Ashie	North Carolina A & T State
PREM 31	Sheilah Cherono	North Carolina A & T State
PREM 32	Tyffani Royal	North Carolina A & T State
PREM 33	Broke Smith	North Carolina A & T State
PREM 34	Makeiyla Begay	Navajo Technical University
PREM 35	Jonathan Chinana	Navajo Technical University

PREM 36	Layla Marie James	Navajo Technical University
PREM 37	Keanu Simpson	Navajo Technical University
PREM 38	Katelyn Wilson	Navajo Technical University
PREM 39	Netanya Faith Dennis	North Carolina Central University
PREM 40	Shaila Jackson	North Carolina Central University
PREM 41	Patrick Jacobs	North Carolina Central University
PREM 42	Dionne Mitchell	North Carolina Central University
PREM 43	Poster Retracted by Author	
PREM 44	Poster Retracted by Author	
PREM 45	Sofia Sanchez Lemus	North Carolina Central University
PREM 46	Amyra Black	Tennessee State University
PREM 47	Grady Clopton	Tennessee State University
PREM 48	Karla Robles	Tennessee State University
PREM 49	Christopher Buford II	Tennessee State University
PREM 50	Ethiopine Choping	Tennessee State University
PREM 51	Geordan Dorsey	Fisk University
PREM 52	Antonio Moore	Fisk University
PREM 53	Rigo Mayorga Luna	Texas State University
PREM 54	Mackenzie Otakpor	Texas State University
PREM 55	Kushal Thapa	Texas State University
PREM 56	Edgar Torres	Texas State University
PREM 57	Adelyne Towne	Texas State University
PREM 58	Nolan Herbort	University of Texas at El Paso
PREM 59	Kausik Kolluri	University of Texas at El Paso
PREM 60	Paul G. Nalam	University of Texas at El Paso
PREM 61	Francelia Sanchez	University of Texas at El Paso
PREM 62	Richard Harry	Tuskegee University
PREM 63	Lyndon Smith Jr.	Tuskegee University
PREM 64	Faruk Soso	Tuskegee University
PREM 65	Shaskya Castaño	University of Puerto Rico, Mayaguez
PREM 66	Alberto Tous	University of Puerto Rico, Mayaguez
PREM 67	Wilnelia M. Barea	Universidad Ana G. Méndez-Cupey
PREM 68	Angélica del Valle	Universidad Ana G. Méndez-Turabo
PREM 69	Yannelly A. Serrano-Rosario	University of Puerto Rico, Río Piedras
PREM 70	Alexis Agosto	University of Central Florida
PREM 71	Dylan Jeff	University of Central Florida
PREM 72	Troie Journigan	University of Central Florida
PREM 73	Luis Tomar	University of Central Florida
PREM 74	Cecilia Abella	University of Hawaii at Manoa
PREM 75	Shelby Mitchell	University of Hawaii at Manoa
PREM 76	Tracee Nguyen	University of Hawaii at Manoa
PREM 77	Jade Paranhos Lopes	University of Hawaii at Manoa
PREM 78	Joshua E. Chaparro-Mata	University of Puerto Rico, Mayaguez
PREM 79	Gabriela A. Marrero-Hernández	University of Puerto Rico, Cayey
PREM 80	Emmanuel Rosa-Delgado	University of Puerto Rico, Humacao

PREM 81	Grace M. Sánchez-Santiago	University of Puerto Rico, Humacao
PREM 82	Anthony Martinez	University of Texas, Arlington
PREM 83	Manuel Rodriguez	University of Texas, Arlington
PREM 84	Hannah Umoeka	University of Texas, Arlington
PREM 85	Narcedalia Anaya-Barbosa	University of Texas Rio Grande Valley
PREM 86	Allan Cedillo	University of Texas Rio Grande Valley
PREM 87	Adriana Chapa	University of Texas Rio Grande Valley
PREM 88	Carlos Delgado	University of Texas Rio Grande Valley
PREM 89	Fabián Rodríguez	University of Texas Rio Grande Valley
PREM 90	Shadman Sakib	University of Texas Rio Grande Valley
PREM 91	Islam Uddin Shipu	University of Texas Rio Grande Valley
PREM 92	Fernando Viesca	University of Texas Rio Grande Valley
PREM 93	Jazzniah Compton	Xavier University of Louisiana
PREM 94	Ayssia Crockem	Xavier University of Louisiana
PREM 95	Kirsten Grant	Xavier University of Louisiana
PREM 96	Trinity Hixson-Wells	Xavier University of Louisiana
PREM 97	Kutemwa Masafwa	Xavier University of Louisiana



# PREM Affiliation: California State University - Princeton University

#### PREM01

Influence of Graphene Layer on the Adsorption and Dissociation of Water on Ru(0001) and Ir(111) Juan Jaime Bernal Romero, Jael Fregoso, Vanessa Carbajal & Li Gao

California State University, Northridge Contact author: li.gao@csun.edu

Generation of hydrogen from water dissociation is one promising strategy to meet the rapidly increasing demand for renewable energy and sustainable development. The adsorption and dissociation of water on the bare and graphene-covered Ru(0001) and Ir(111) surfaces has been studied by combining X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). The dissociation of water was observed for the bare Ru surface but not for the bare Ir surface. The influence of graphene layer on water adsorption and dissociation on these two metal surfaces has been investigated through temperature-dependent and dosage-dependent XPS measurements. The effect of water dosing on the morphology of graphene layer was also observed in STM measurements.

# PREM02

Competing Orders and d-wave Superconductivity in t-J Model on Square Lattice Swosti Choudhury & Donna Sheng California State University, Northridge Contact author: swosti.choudhury.472@my.csun.edu

We study the ground state properties of a t-J model with additional neighboring Coulomb interaction for four-leg ladder square lattice systems. We use the density-matrix renormalization group and verify the robustness of the superconducting pairing correlations and understand its competing orders.

# PREM Affiliation: California State University, Los Angeles - The Pennsylvania State University

# PREM03

Use of Sr(B,B')O<sup>3</sup> Perovskites for Transparent Semiconductors

<u>Alec Milbourne</u><sup>1</sup>, Francisco Marques Dos Santos Vieira<sup>2</sup> & Ismaila Dabo<sup>2</sup>

<sup>1</sup>California State University, Los Angeles, <sup>2</sup>The Pennsylvania State University

Contact author: amilbou2@calstatela.edu

Over the past several decades concerns about environmental degradation and climate change brought about through use of fossil fuels has led to increased interest in finding solutions to energy generation not reliant on petrochemicals. Photovoltaics have thus far offered a promising alternative. Photovoltaics require a transparent conductor (TC) for proper energy generation with the current state of the art material used for this purpose being indium tin oxide (ITO). Despite the promising uses and good efficiency of modern photovoltaics the requirement of ITO is presenting logistical and financial issues in sourcing indium that are hindering the mass scale adoption of renewable energy that is required to combat global emissions. The logistical and financial issues associated with indium have motivated the search for alternative transparent conductors. One such promising family of transparent conducting materials is cubic Strontium oxide perovskites. This family of materials has previously been shown to display good optical and electronic properties for potential use as a TC, however despite promising characteristics no single perovskite has shown to display these characteristics while also being stable. High entropy perovskites show better potential as stable TCs but their composition, processing, structure, property relations remain unidentified. In this study density functional was used to study single and double perovskites in order to elucidate these relationships. To accomplish this goal, the influence that magnetic ordering has on the structure of perovskites was taken into consideration by measuring the enthalpies of a variety of single perovskites under 4 different magnetic orderings, those being ferromagnetic (FM), and 3 anti-ferromagnetic (A, C, G). Based on this information, the mixing enthalpies of various double perovskites were computed. Results from this study were determined and found that under FM and G-anti-ferromagnetic orderings the 3d transition metals under study were on average more amenable to forming solid solutions and that engineering of these materials with these magnetic orderings is predicted to stabilize these high entropy perovskites.



# PREM Affiliation: California State University - Princeton University

#### PREM04

Influence of Graphene Layer on the Adsorption of Water on Ru(0001) and Ir(111) Investigated with Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy

Jael Fregoso, Li Gao & Juan Jaime Bernal Romero

California State University, Northridge Contact author: li.gao@csun.edu

Generation of hydrogen from water dissociation is one promising strategy to meet the rapidly increasing demand for renewable energy and sustainable development. A facility has been set up to investigate the dissociation of water on catalytic surfaces by combining scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). The adsorption of water on the Ru(0001) and Ir(111) surfaces has been studied by combining XPS and STM. The experiments were performed on bare metal surfaces, graphene covered metal surfaces, and doped-graphene covered metal surfaces. The dissociation of water was observed on the Ru samples but not on the Ir samples. The influence of (doped) graphene layer on water adsorption and dissociation has been investigated through temperature-dependent and dosage-dependent XPS measurements. The effect of water dosing on the morphology of graphene layer was observed in STM measurements. Therefore, this facility allows the investigation of the correlations between structural properties and chemical reactions. Our studies are valuable for assessing the performance of new catalytic materials that could be employed in practical-scale renewable energy applications.

# PREM Affiliation: Clark Atlanta University - Spelman College - Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials

# PREM05

Synthesis of Transition Metal Halides: Discovering Ferroelectric Materials

Bianca Brown<sup>1</sup>, Tyrel Mcqueen<sup>2</sup>

<sup>1</sup>Clark Atlanta University, <sup>2</sup>John Hopkins University Contact author: Bianca.brown1@students.cau.edu

Ferroelectricity, magnetism, has long been discovered and explained by different research groups. Since magnetics is such a promising field of study, we have decided to look into how to expand into inorganic and organic bonds. By looking into ferroelectric polymers, and aiming to have these polymers to self-assemble in new ways to further create new innovative technology. These polymers will self-assemble due to the dipolar interaction between the ferroelectric oxides. Here we have taken the geometrically forced polar bond of Nb3Cl7X(S, Se, Te) and are testing to see if we can create that bond as well as seeing if the bond has a magnetic field. The different variations we are trying are sulfur, selenium, and tellurium which we will be using chemical vapor transport to create. Our transport agent will be ammonium chloride, which will help the formation of crystals at the hot end of the temperature gradient. Running X-ray diffraction, XRD, and single crystal diffraction will let us know if we have created different variations. As well as taking a closer look and using Energy Dispersive X-Ray Spectrometry, EDS/EDX, map scans for further investigation on the stoichiometry of the different variations. Once those structures are created and tested we will then run a voltage test to ensure that said structure contains a magnetic source. The magnetic single-crystal structures are proven to be magnetic by using a capacitor and attaching a voltage by watching to see if the graph makes a field loop. Which will be tested using Physical Property Measurement System, PPMS, and checking its resistivity measurements.



#### PRFM06

Electronic and Vibrational Properties of Electron-Doped Transition-Metal Nitride Halides RNX (R = Zr and X = Br, I) from First Principles Jordan Brown<sup>1</sup> & Betül Pamuk<sup>2</sup>

<sup>1</sup>Clark Atlanta University, <sup>2</sup>Cornell University

Contact author: jordan.brown2@students.cau.edu

Using density functional theory (DFT), we study transition-metal nitride halides RNX (R = Zr; X = Br, I). The metal nitride halides RNX form two different polymorphs ( $\alpha$  and  $\beta$ ) in their layered crystallized structures. The parent compounds are band insulators, that when electron-doped, become superconductors. We used DFT calculations to obtain the energy as a function of electron density. We will discuss the electronic band structure of RNX materials and the effects of electron doping on these materials in β-form. Superconductivity is one of the most captivating quantum experiences that the natural world has created. It is the property of certain materials to conduct electricity or electron transport below what is known as the transition or critical temperature Tc with zero resistance. We are conducting this superconductivity on the metal nitride halides MNX (M= Zr; X= Br, I), which are indirect gap semiconductors with a layered structure, by electron doping. These compounds are considered band insulators, so we are using these two-dimensional host crystals to intercalate with the alkali metal lithium to assist in modifying the physical attributes without altering the fundamental crystal structures at high temperatures. Zirconium nitride layers are considered a promising superconductor, similar to CuO2 for the purpose of doping by intercalation which manipulates the aperture within the crystal structures, and a high level of doping is conceivable exclusive of hosting chaotic induced scattering sites onto electronically active sites (1). We looked at other superconducting materials such as ZrNCl to help give us insight into these newly developed series of superconductors based on layered structure nitrides. Research had shown for ZrNCl that at a low-doping regime the superconducting critical temperature increases. We performed first-principle calculations by using the Quantum-ESPRESSO software package. Throughout our process, we generated experimental cell parameters using previous research as well as convert the cell parameters for our electron-doped beta structures from hexagonal to rhombohedral cell. The different pseudopotentials were generated with a non-relativistic calculation and the Exchange-Correlation potential has been defined utilizing the PBE functional. Our interest was in the halides and knowing what would happen if we switched chloride in previous research (2-3) with bromide and iodide that are being used in our research. We found that the  $\alpha$ -form polymorph crystallizes in the orthorhombic space group Pmmn (#59).  $\beta$ -form polymorph crystallizes in the rhombohedral R3m(166). So, we studied both semiconducting structures and compared their electronic structures using DFT. β -ZrNCl in previous research also existed for  $\beta$ -ZrNBr. For future work, we would like to the vibrational properties better known as the phonons. We also would like to calculate the superconducting temperature.

# PREM07

Developing Computational Algorithms for Solid State Properties of Multiferroics Christian Johnson & Natarajan Ravi Spelman College

Contact author: christianjohnson@spelman.edu

The purpose of this study is to develop computational modeling by developing programs in the Python coding language for a variety of situations, ranging from optimization of spectral data to the computation of electric field gradient tensors. Google Colab, an online Integrated Development Environment (IDE) for python, in combination with library packages such as NumPy and SCIPY are effectively used for this purpose. The experimental data used for comparison purpose is generated by 57-Fe Mössbauer spectroscopy. Lorentzian line functions are used to obtain the least-squares fit of the experimental data. Additionally, using detailed crystal structures of selected ferrite materials, the electric field gradient tensor at the Fe-site is computed to be compared to experimentally determined quadrupole splitting. This work is supported by the NSF PREM – Emergent Interface Materials, Grant 2122147.

# PREM08

BaFe<sub>12</sub>O<sub>19</sub> as a Multiferroic Material Jayda Shine & Natarajan Ravi Spelman College

Contact author: jaydashine@spelman.com

A thin-film study using 57Fe Mössbauer spectroscopy is undertaken to enhance our understanding of ferroelectric/magnetic properties of some novel materials. One of the materials of current great interest, barium magnet (BaFe12O19), is grown on SGO substrate and is about 28 nm thick. This system is prepared by using Molecular Beam Epitaxial (MBE) method with 30% enriched 57Fe isotope in collaboration with our PREM partners at Cornell University. Conversion electron Mössbauer spectroscopy is being developed to study the depth profile and the nucleation process of the magnetic interactions in this material. Calibration of the detector system, data analysis including line shape function, writing python codes for field gradient calculations in Colab platform are currently underway. Details of the experimental technique, computational modeling, and optimization of the data will be presented. This work is supported by the NSF PREM - Emergent Interface Materials, Grant 2122147.

Oxide-Conducting Polymer Interfaces. Interactions between 4-Arm Hyperbranched PPI and LuFeO<sub>3</sub>

Elmon Merriman<sup>1</sup>, YiLin Li<sup>2</sup>, Xiao-Qian Wang<sup>1</sup>, Darrell Schlom<sup>2</sup>, Ishrat Khan<sup>1</sup>

<sup>1</sup>Clark Atlanta University, <sup>2</sup>Cornell University

Contact author: Elmon.Merriman@students.cau.edu

Interface membranes consisting of organic–inorganic composite (OIC) have received great attention over the past decades due to their enhanced performances in many applications. Conducting hyperbranched (perylene)-based polyimides (PPI), thermally stable to nearly 600 °C, (organic) [PPI]/ferroelectric LuFeO3 (inorganic) heterostructure are prepared to develop advanced materials with diverse optical and electronic properties. The novel PPI polymers have been synthesized with unique conducting properties made by templating the assembly of conducting PPI on ferroelectric crystals from the ordered polarization motifs provided by inorganic ferroelectric oxide. We performed first-principles calculations to clarify the interaction between LuFeO3 and polyimide (PPI) polymer. The 4-arm PPI repeating unit matches well with 8×8 LuFeO3 supercell, which shows the 4-arm PPI stays parallel to the LuFeO3. The computational study is validated by studying the interaction using spectroscopic (FT-IR, UV-Visible and NMR methods) and microscopic (SEM) techniques. The PPI and LuFeO3 composites are prepared by coating the ferroelectric crystals with a thin layer of the polymers.

#### PRFM10

Structure Analysis of Ruthenium-Titanium Oxide Oxygen Evolution Electrocatalysts using X-ray Photoelectron Spectroscopy Kathleen O. Bailey, Luis A. Albiter, Fernando Godinez Salomon & Christopher P. Rhodes Texas State University. Contact author: cprhodes@txstate.edu

Proton exchange membrane water electrolyzers (PEMWE's) allow electrochemical splitting of water into hydrogen and oxygen and can be powered by renewable energy sources (.e.g solar, wind), resulting in generation of "green hydrogen". The large-scale adoption of PEMWE's is hindered by the sluggish kinetics and cost of the oxygen evolution reaction (OER) catalyst at the anode. The current state-of-the-art OER catalysts are iridium-based; however, iridium is a rare element in the Earth's crust and is extremely expensive which results in high catalyst costs. Ruthenium oxide (RuO2) OER catalysts are of interest due to their higher activity and lower cost compared to iridium oxide; however, RuO2 is unstable and corrodes over time. By incorporating titanium into ruthenium oxide at various concentrations, Ru1-xTixO2 (x=0-50 at. %), the catalyst stability is improved. X-ray photoelectron spectroscopy (XPS) was used to characterize the surface of this catalyst. XPS analysis showed that the surface of the synthesized catalyst was more enriched with titanium compared to the bulk material. XPS also showed that the addition of titanium into the ruthenium oxide shifted the O2s region to a higher binding energy. This shift could explain the improved stability due to the strength of bonds increasing. Analyzing the surface structure of the synthesized catalyst allows for further development of high activity, lower cost, and high stability ruthenium-based catalysts that can improve the efficiency and lower the cost of PEMWEs.

# PREM Affiliation: Delaware State University - Claflin University - University of Delaware

# PREM11

Recombinant Synthesis and Characterization of Thermoresponsive Biopolymers for Designing Molecular Actuators Arriana M. Bisram, Sai S. Patkar, Cristobal Garcia Garcia & Kristi L. Kiick

University of Delaware

Contact author: Abisram@udel.edu

Resilin is an elastomeric protein derived from insects that demonstrates stimuli responsiveness and elasticity. This resilin can be conjugated with a coiled-coiled peptide center, which allows the unit to be responsive to stimuli such as pH, temperature, and chemical environment. The resilin unit in the polypeptide also gives mechanical advantages like low stiffness and extensibility. In addition to a resilin unit being attached to the peptide center, chemical handles can be utilized to perform orthogonal chemistries through implementation of amino acid residues. This work aims to express and characterize sequences with Lysine (K), Tyrosine (Y), Methionine (M), and Phenylalanine (F) chemical handles, which have amino acids incorporated for amine and oxidative reactive chemistries. As well as sequences with Cysteine (C) chemical handles, which have thiol-reactive chemistries. The goal is to investigate and compare the yield, purity, composition, and phase transition temperature of those polypeptides. To yield the desired protein sequence, recombinant synthesis in E. coli bacteria was utilized and followed by denaturing purification. The protein was then analyzed using SDS-PAGE and MALDI-TOF MS in order to characterize the molecular weight of the produced protein and the presence of impurities within the yield. This allowed for the verification of the polypeptide presence after expression and purification. Afterward, UV-vis was used in order to analyze the phase behavior of the polypeptide in response to temperature. The optical density at 350 nanometers was observed with regard to the temperature range, allowing us to find the point of phase transition. Results showed that all sequences demonstrated a phase transition during cooling, indicating that the sequences are responsive to temperature. The stimuli-response to temperature shows that temperature resulted in a change of chain dimensions for these sequences, and they therefore can be utilized as molecular actuators.

# PREM Affiliation: Fort Lewis College - Norfolk State University - University of Colorado, Boulder, STROBE

#### PREM13

Open ddPCR
Mason Brady, Ian Van Horn & Yiyan Li
Fort Lewis College
Contact author: mrbrady1@fortlewis.edu

Droplet Digital PCR (ddPCR) is a method of rapid bacterial quantification in a liquid culture or solution. The development of an open source ddPCR system will allow this technology to become more fiscally available. The development of this open source system utilized reused optical components, including a Photomultiplier Tube (PMT) from a flow cytometer, aligned using optical fittings. The signals received from the PMT were passed through a circuit containing bandpass resistor-capacitor filters and various amplifiers. FITC fluorescent microspheres were used to test the potential limits of the system's ability to quantify different concentrations of positive bacterial droplets in a sample. Error in the creation of FITC suspension samples has prevented a concrete test of accuracy of the system. To reduce this error, particles were manually counted under a microscope before passing the sample through the ddPCR system. This method of sample creation allowed for a 90% accuracy in quantification of particles, however this method is not feasible to test the system on a larger scale due to the impracticality of manually counting large amounts of fluorescent microspheres. The system has yet to be tested on plasmid transformed bacteria.

#### PREM14

Thrust Measurement System for Characterization of a 2D Monolithic Chip Utilizing Oxidized Porous Silicon Propellant

Hannah Carlson<sup>1</sup>, Wilder Jensen<sup>1</sup>, Dakota Rodriguez<sup>1</sup>, Julie Nelson<sup>1</sup>, Lyrik Lee<sup>1</sup>, Brian Tsosie<sup>1</sup>, Yiyan Li<sup>1</sup>, Prashanth Bangalore<sup>2</sup>, Billy Nollet<sup>1,2</sup>

& Jeff Jessing<sup>1</sup>

<sup>1</sup>Fort Lewis College, <sup>2</sup>AGILE Space Industries

An oxidized porous silicon (PSi) micro-thruster has the potential to replace liquid propellants in satellite micro-thruster positioning systems. Satellites typically use liquid propellants in their micro-thrusters because the liquid is more easily controlled than solid propellants. However, liquid propellants are much more expensive and heavier than solid propellants. The focus of this study is to characterize the energy, thrust and impulse of a porous silicon based micro-thruster. Porous silicon is an ideal candidate because, when ignited after being chemically oxidized, it produces a highly energetic micro-explosion that can be adjusted by varying the anodization time which varies the pore depth in the cell. The larger the pores volume equates to a higher energy output. The oxidizer used in this experiment was sodium perchlorate that was mixed into a solution with methanol and deposited onto the cell using a micropipette. In order to determine if PSi could be utilized as a potential micro-thruster, the detonation energy and associated thrust must be determined. Using previously developed microfabrication techniques, the oxidized PSi was formed with a monolithic structure for on-chip detonation. In this study, the reaction (i.e., explosion) time of the PSi was determined to be in the millisecond range through high-speed imaging. The energy of the denotated oxidized PSi was found using a Parr 6200 Calorimeter. Benzoic acid tablets have typically been used to calibrate calorimeters; however, gunpowder was used to calibrate due to the short reaction time of oxidized PSi. To measure the thrust and impulse of the microthruster, a thrust measurement stand was specially designed due to the small scale of the system. The test stand uses a load cell connected to an amplifier for high-speed data acquisition. The signal from the load cell is then read by a National Instruments data acquisition (DAQ) card linked to a LabVIEW program to record and compile the load cell data at high speed. Final analysis occurs in MATLAB to convert the signal from an analog input into a force. The test stand was calibrated based on known masses placed upon the top plate. From this research the thrust, impulse, and energy characteristics of porous silicon have been quantified. Future work will focus on the optimization of the nozzle fabrication, porous silicon formation, and the oxidizer application to maximize thrust and reproducibility.

# PREM15

Crystal Growth and Magnetic Properties of MgCr<sub>2</sub>O<sub>4</sub> Ajeya Dixon, Doyle Temple & Leroy Salary Norfolk State University Contact author: a.dixon101395@spartans.nsu.edu

Spinels containing transition metals or rare earth elements have been extensively studied as prime candidates to exhibit geometric magnetic frustration. Chromium-rich spinels, such as ZnCr2O4 and MgCr<sub>2</sub>O<sub>4</sub>, have attracted particular attention due to antiferromagnetic ordering transitions at low temperatures that are coupled to lattice distortions. Recently, we have produced MgCr2O4 rods using grinding and sintering methods. This is to prepare to produce single crystal using floating zone crystal growth technique in order to perform structural and magnetic characterizations in the near future. Testing of the rod materials using X-ray powder diffraction refinement indicates that the crystal structure is cubic having Fd-3m symmetry.



Morphological and Mechanical Characterization of a Novel Porous Silicon Membrane used in a Lung-on-a-Chip System Sahra Genc<sup>1</sup>, Dakota Rodriguez<sup>1</sup>, Alex Motler<sup>1</sup>, Sally Thompson<sup>1</sup>, Owen Hill<sup>1</sup>, Farjana Showme<sup>1</sup>, Leif Gislason<sup>1</sup>, Aaron Simien<sup>1</sup>, Sarah Schreiner<sup>2</sup>, Adrian Gestos<sup>2</sup>, Virginia L. Ferguson<sup>2</sup> & Jeff Jessing<sup>1</sup>

<sup>1</sup>Fort Lewis College, <sup>2</sup>University of Colorado, Boulder

Contact author: sggenc@fortlewis.edu

In the last decade, organ-on-a-chip technology has been heavily researched as an alternative to animal models and the traditional cell culture in the biomedical field. This technology could ultimately be used to develop accessible personalized medicine. In our research we focused on a Lung-on-a-Chip incorporating a novel fabricated porous silicon biomembrane. This porous silicon biomembrane mimics the functionality of the interstitial space (approximately 1  $\mu$ m in thickness) that separates the epithelial and endothelial cells seen in vivo. Previously we have reported the fabrication process used to create this novel membrane. A primary goal of the fabrication process is to produce a thin, through-etched porous silicon membrane that has a high degree of uniformity in thickness, porosity and predictable Young's Modulus. Preliminary characterization results reported both the membrane structure and the biocompatibility with cultured lung cells. In this current study, modifications to the fabrication process to yield more reproducible results were made, and we focused on the mechanical and morphological characterization of the membrane using scanning electron microscopy and nano-indentation. A small parametric study was performed with nano-indentation with the goal to characterize the Young's Modulus of the porous silicon membrane and to compare with in vivo interstitial space values and with other engineered membranes as reported in literature.

### **PREM 17**

Crystal growth and magnetic properties of Ba-doped CaFe<sub>2</sub>O<sub>4</sub> Liam B. Harrigan, Sunil K. Karna & Doyle Temple Norfolk State University

Contact author: <u>L.b.harrigan@spartans.NSU.edu</u>

The oxide compounds containing iron are widely studied because of many interesting phenomena including charge disproportionation, spin polarization, and the magentoresistive effect. CaFe2O4 crystallizes in the orthorombic Pbnm structure which consists of distorted FeO6 distorted octahedra through edge- and corner-sharing with intercalated Ca atoms. We have recently grown a large single crystal of Ba-doped CaFe2O4 by the optical floating-zone method and performed structural and magnetic characterization. we have doped the CaFe2O4 structure with Ba in up to 2.5% of the Ca-sites. Through x-ray diffraction and Rietveld refinement of the structure, we observed a contraction in the lattice parameters with increasing Ba. We also observe a change in the original CaFe2O4 antiferromagnetic ordering temperature in our magnetic susceptibility measurements after doping with Ba.

# PREM19

Single Crystal Growth of Non-Symmorphic Material CuBi $_2O_4$  Tekiyah Robinson, Doyle Temple, Leroy Salary, Ajeya Dixon Norfolk State University

Contact author: t.a.robinson101160@spartans.nsu.edu

Topological materials having eight-fold electronic degeneracy protection by nonsymmorphic symmetries of a crystal exhibit double Dirac fermions which have been predicted in CuBi2O4. In addition, more recent and accurate density functional theory calculations demonstrate that it should be an antiferromagnetic Mott insulator. Here, we have grown CuBi2O4 single crystal using floating zone crystal growth technique. First, polycrystalline CuBi2O4 was synthesized by the direct solid-state reaction of Bi2O3 and CuO in a 1:1 molar ratio, mixed thoroughly using a mortar and pestle. X-ray diffraction was employed to check phase purity of the polycrystalline samples and confirmed that CuBi2O4 crystallizes in the space group P4/ncc which consists of planar [CuO4]6– units with Bi3+ ions occupying the spaces between units. The resistivity and magnetoresistance measurements are planned to do in near future on CuBi2O4 single crystal.



Development of a 2D Monolithic Micro-Thruster Capable of On-Chip Detonation Utilizing Oxidized Porous Silicon Propellant Dakota Rodriguez, Julie Napora, Lyrik Lee, Hannah Carlson, Wilder Jensen, Brian Tsosie, William Nollet & Jeff Jessing Fort Lewis College

Contact author: derodriguez@fortlewis.edu

Many satellites in space utilize micro-thrusters to perform small adjustments to their position. The most common type of micro-thruster uses hydrazine combined with an oxidizer as a liquid propellant. The use of a liquid propellant increases the complexity of the design by needing fluid systems that are difficult to integrate and have large mass. This has led to interest in using micro-thrusters with solid propellant, specifically using microfabrication techniques to integrate the solid propellant into the micro-thruster. Here, we developed a monolithic structure that utilizes a spark gap for on-chip detonation of oxidized porous silicon (PSi). Porous silicon is used because of the high specific surface area and the dangling bonds that form in the pores so when oxidized, the PSi becomes highly reactive. With a twoinch p-type silicon wafer as the substrate, we refined a method to construct the micro-thruster using common microfabrication techniques and electrochemical anodization to form the PSi. Thermally grown oxide is used to create a spark gap and act as an insulator between the bulk silicon and the deposited metal layer. The deposited metal will be chromium due to its compatibility with hydrofluoric acid (HF) used in later processing. The metal layer will have enough voltage applied to it so that the electric breakdown strength of air is exceeded to cause spark generation, which detonates the PSi. To pattern the rocket cells on the micro-thruster, photolithography is employed to create an etch mask. The etch mask is used to protect certain areas of the thin film stack from the etchants that are used to remove the chromium and thermal oxide to expose the bulk silicon. Etching the thin film stack forms the geometry of the rocket cells. Formation of PSi is achieved through electrochemical anodization using HF. The depth and size of the pores will affect the thrust output of the micro-thruster, so a specific current density is targeted to maintain constant thrust output. To make the PSi reactive, a sodium perchlorate solution is deposited and then dried which chemically oxidizes the PSi creating a solid propellant on the micro-thruster. The amount of oxidizer used will also affect thrust output, so a micropipette is used to deposit constant volumes of sodium perchlorate solution. Wires are bonded to the chromium surface where a voltage can be applied to cause ignition. A test stand is being constructed to measure the thrust output of the micro-thruster. In application, many of these micro-thrusters would cover a satellite that could be precisely detonated to perform the small maneuvers necessary for re-adjustment. Using a solid propellent based micro-thruster with on-chip detonation gives an advantage by reducing the design complexity, mass, and environmental impact of the satellite.

# PREM22

*Open ddPCR*Mason Brady, <u>Ian Van Horn</u> & Yiyan Li
Fort Lewis College

\*Co-Presenter of PREM13

# **PREM Affiliation: Hampton University - Brandeis University**

# PREM23

Lanthanide Metallogels Constructed Using Visible-Light-Switchable Amino Acid Functionalized Aryalazopyrazole Ligands Jazz Geter & Kesete Ghebreyessus

**Hampton University** 

Contact author: Jazz.geter@my.hamptonu.edu

An emerging strategy for the fabrication of supramolecular materials is the use of metal-ligand interactions to trigger and modulate self-assembly, and tune the properties of the resulting soft materials. Herein, we report the design and synthesis of new amino acid functionalized arylazopyrazole (AA-azo) based photoresponsive low-molecular-weight ligands. The new photoswitchable ligands thus obtained exhibited lanthanide ions-induced self-assembly (Ln(III) = Eu(III), Tb(III)) to form supramolecular gels in methanol/water through the metal-ligand interaction under alkaline conditions. The metallogels were characterized by different spectroscopic and microscopic techniques. Scanning electron microscopy (SEM) imaging studies revealed that the morphology of the xerogels is highly influenced by the type of metal ions and amino acid ligands used. The metallogels display partial gel-to-sol transition due to the photo-induced reversible trans-to-cis isomerization of the azo moiety upon alternating blue and green light irradiation.



Near-Infrared Emission Studies of Er3+ Doped Halide Perovskites (CsPbCl3, CsCdCl3) for Applications in the ~1500-1700 nm Spectral Region Alexa Livingstone<sup>1</sup>, Uwe Hommerich<sup>1</sup>, Al Amin Kabir<sup>1</sup> & S. B. Trivedi<sup>2</sup>

<sup>1</sup>Hampton University, <sup>2</sup>Brimrose Technology Corporation of America, Sparks Glencoe

Contact author: alexa.livingstone@my.hamptonu.edu

The near-infrared region (1500-1700nm) is an important part of the electromagnetic spectrum due to its applications for eye-safe lasers and optical communications. In this research, we prepared Er doped halide perovskites (Er:CsPbCl3 and Er:CsCdCl3) and evaluated their near-IR emission properties. The investigated materials were prepared by solid-state melting synthesis employing high purity starting materials of CsCl, PbCl2, CdCl2 and ErCl3. The melting points of CsPbCl3 and CsCdCl3 are 553°C and 600°C, respectively. Following optical pumping using a laser diode at 800 nm, Er: CPC exhibited a broad near-IR emission peaking at ~1545.3 nm. Under similar experimental conditions, Er: CCC showed two near-IR emission bands centered at ~1545.6 nm and ~1678.6 nm. Based on the Er3+ energy level diagram ("Dieke-diagram") the ~1545 nm emission was assigned to the 4l13/2 -> 4l15/2 transition of Er3+ ions. In addition, the ~1678 nm band observed from Er: CCC was assigned to the 4l9/2 -> 4l13/2 transition. Spectral resolution studies allowed to determine the bandwidth (FWHM) of the 4l13/2 -> 4l15/2 peak emission line to be ~9.3 nm for Er: CPC and ~10.9 nm for Er: CCC, respectively. The 4l9/2 -> 4l13/2 peak emission line at ~1678 nm from Er: CCC had a bandwidth of ~14.2nm. More details of the near-IR spectroscopic of Er3+ doped CsPbCl3 and CsCdCl3 and its relevance for photonic applications will be presented at the conference.

# PREM25

Simulation Design and Spectral Analysis of Arylazopyrazole Polydimethylsiloxane(AAP-PDMS) Waveguide

<u>Breon McCray III¹</u>, Golsa Mirbagheri¹, Kesete Ghebreyessus¹, Uwe Hömmerich¹, Demetris Geddis¹ & Seth Fraden², ¹Hampton University, ²Brandeis University

Contact author: Breonmccray@gmail.com

In this work, Arylazopyrazole Polydimethylsiloxane(AAP-PDMS), as a new photo switch, flexible polymer composite is synthesized and spectral characterized with X-Ray Diffraction(XRD), Scanning Electron Microscope(SEM), and finite element method (HFSS). The organic AAP-PDMS thin film shows reactive index change in trans-to-sic states on exposure to ultraviolet(UV) and green lights. In addition, the tunable AAP-based waveguide is designed with the finite element method, representing different modes during photoisomerization. AAPs molecules observed conformational change upon alternating irradiation of UV/Visible lights. The observations made apparent the potential of AAP-PDMS's usage for optoelectronic devices.

# **PREM Affiliation: Howard University - Columbia University**

# PREM26

Surface Functionalization & Solution Exfoliation of Graphullerite Victoria Vinson<sup>1</sup>, Elena Meirzadeh<sup>2</sup>, Xavier Roy<sup>2</sup> & Colin Nuckolls<sup>2</sup> <sup>1</sup>Howard University, <sup>2</sup>Columbia University

Contact author: vinsovic004@gmail.com

The Roy and Nuckolls groups have recently devised a synthetic route to yield large, two-dimensional (2D), polymerized C60 crystals. C60 fullerene is reacted with magnesium (Mg) metal, in order to synthesize highly reduced C60 sheets, containing Mg counter-ions. Once the Mg is de-intercalated, we are left with a neutral, purely carbon-based material. Because it's analogous with the layered, hexagonal graphite, this new carbon allotrope is named graphullerene and its 3D van der Waals solid, graphullerite. Our three main goals over the course of the project have been to synthesize larger crystals (tens of microns), functionalize the sheets, and to exfoliate graphullerite via solution exfoliation. By doing so, we can utilize the sheets in solution chemistry, in order to tune their electrical, magnetic, chemical, or optical properties. We've used various molecules for the functionalization, with the purpose of making graphullerite soluble in organic solvents such as dimethylformamide (DMF) and tetrahydrofuran (THF). Using solution exfoliation techniques, we've been able to obtain large tri-layer, bi-layer, and monolayer de-intercalated graphullerene sheets.



# PREM Affiliation: Jackson State University - University of California, Santa Barbara

#### PREM27

Perovskite Solar Cells Prepared in Ambient Environment Jaiden Moore, Yifang Qi, Paresh Chandra Ray, Qilin Dai Jackson State University
Contact author: jaidenmoore16@icloud.com

Perovskite solar cells (PSCs) have attracted a lot of attention in recent years due to their high efficiency. However, the recorded performance (25.7%) is still lower than the theoretical Shockley-Queasier limit because the traps and defects still remain at the interface of perovskite and other layers. And one promising method is to modify the perovskite surface by polymers and other organic materials owing to the controllable properties of the organic functional groups in the materials. Herein, polylactic acid (PLA) with CH3 and C=O functional groups is introduced to passivate the interface between the perovskite and hole-transport layer. The perovskite solar cells are fabricated by one-step method in ambient environment. The SnO2 layer is spin coated by 7000 rpm for 30s as electron transport layer and P3HT is applied as hole transport layer. And the gold is deposited as electrode in the perovskite solar cells. The UV-vis absorption spectra of perovskite films with and without PLA passivation shows the perovskite peaks at ~800 nm, which means the perovskite can absorb the sunlight before 800 nm. Steady-state photoluminescence (PL) and time-resolved PL (TRPL) measurements of perovskite films on FTO are carried out to study the influence of PLA passivation on charge extraction and lifetime. The PL spectrum of the perovskite film with PLA passivation exhibits a higher intensity, which indicates the PLA passivation suppresses the carrier non-radiative recombination of perovskite films. Besides, the TRPL spectra can be fitted by the biexponential decay equation. And the fitted lifetime of perovskite without and with PLA passivation are 190 ns and 330ns. Thus, the PLA passivation enhances the lifetime of perovskite films and further improves the performance of devices. Furthermore, the PCE of the PSCs increases from 9.3% to 12.6 %, and the Voc enhances from 0.67 V to 0.80 V as the device is treated by PLA passivation.

#### PREM28

Passivation Influence of PEDOT:PSS on the Inverted Perovskite Solar Cells <u>Yifang Qi</u>, Jaiden Moore, Zoe Scott, Paresh Chandra Ray & Qilin Dai Jackson State University Contact author: qilin.dai@isums.edu

Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is a popular hole transport material in perovskite solar cells (PSCs). However, the devices with PEDOT:PSS exhibit large open-circuit voltage (Voc) loss and low efficiency, which is attributed to mismatched energy level alignment and the poor interface of PEDOT:PSS and perovskite. Here, we design three polymer analogues to polyaniline (PANI), PANI-Carbazole (P1), PANI-Phenoxazine (P2) and PANI-Phenothiazine (P3) with different energy levels to modify the interface between PEDOT:PSS and the perovskite layer and improve the device performance. The effects of the polymers on the device performance are demonstrated by evaluating the work function adjustment, perovskite growth control, and interface modification in MAPbI3-based PSCs. Low bandgap Sn-Pb-based PSCs are also fabricated to confirm the effects of the polymers. Three effects are evaluated through the comparison study of PEDOT:PSS-based organic solar cells (OSCs) and MAPbI3 PSCs based on the PEDOT:PSS modified by P1, P2 and P3. The order of contribution for the three effects is work function adjustment>surface modification>perovskite growth control. MAPbI3 PSCs modified with P2 exhibit a high open-circuit voltage (Voc) of 1.13V and a high-power conversion efficiency (PCE) of 21.06%. This work provides the fundamental understanding of the interface passivation effects for PEDOT:PSS-based optoelectronic devices.



Fabrication of High-Efficiency Perovskite Solar Cells Zoe Schott, Yifang Qi, Paresh Chandra Ray & Qilin Dai Jackson State University

Contact author: Zoejanelle39@gmail.com

Perovskite solar cells have emerged as a promising candidate for next-generation photovoltaic devices due to their high efficiency, lowcost fabrication, and tunable bandgap. The preparation of perovskite solar cells involves several critical steps, including the synthesis of high-quality perovskite materials, the optimization of the device architecture, and the development of efficient charge transport layers. The most commonly used perovskite material is methylammonium lead iodide (MAPbI3), herein the MAPbI3 perovskite solar cells were fabricated. The perovskite precursor solution contains 922 mg of lead iodide (PbI2), 318 mg methylammonium iodide (MAI), 1400 uL dimethylformamide (DMF) and 152 uL dimethyl sulfoxide (DMSO). For the perovskite solar cells fabrication, the FTO glass is cut into pieces for a certain size 1.4cm x 1.4 cm and then the glass is etched by zinc powder and HCl solution for 5 minutes. Then the etched FTO glass substrates are cleaned by sequential sonication in acetone, distilled water, and methyl alcohol for ten minutes each. The FTO glass substrates are dried by N2 and then treated with ultraviolet ozone for 30 min. After that, tin oxide (SnO2) solution is spin coated with 7000 rpm for 30 s and heated at 150 °C for 30 min and then, substrates are transferred to the air glovebox. The perovskite precursor solution is spin coated on the SnO2 layer with 4000 rpm for 30 s and the 50 uL ethyl acetate (EA) is dropped on the surface at 9 s. Then the wet films were annealed at 100 °C for 30 min. After the FTO substrates cool down to room temperature, the perovskite films were passivated by phenethylammonium iodide (PEAI) to optimize the device performance by the in situ passivation method developed by our group. The device efficiency increases by 25% as PEAI is used to passivate the perovskite films. The mechanism of the improved device performance is systematically studied by time-resolved photoluminescence (TRPL) and electrochemical impedance spectroscopy. Improved charge transport is attributed to improved device performance. Therefore, we develop a facile method to fabricate high-performance solar cells.

# PREM Affiliation: North Carolina A&T State University - Cornell University

#### PREM30

Hydrothermal Synthesis of Porous Iron Oxide Nanoparticles for Wastewater Treatment Moses Ashie<sup>1</sup>, Bishnu P. Bastakoti<sup>1</sup>, Mohan K. Bhattarai<sup>2</sup>, Ram S. Katiyar<sup>2</sup>, Gerardo Morell<sup>2</sup> & Kiran Subedi<sup>1</sup> North Carolina A&T State University, <sup>2</sup>University of Puerto Rico

Contact author: bpbastakoti@ncat.edu

To remediate water pollution due to the release of organic waste substances, highly porous iron oxide nanomaterials were synthesized via a block copolymer-assisted hydrothermal method. Characterization of synthesized materials using X-ray diffraction, electron microscopy, and Raman spectroscopy revealed the formation of crystalline nanoparticles with porous nanostructure. X-ray diffractometer spectra obtained shows the hexagonal phase symmetry of  $\alpha$ -Fe2O3. A particle diameter of  $^{\sim}$  50 nm as well as its magnetic properties was observed. The effectiveness of our synthesized nanoparticles was investigated on the treatment of a sample wastewater of Congo red (CR) as an organic pollutant. The interference of the CR molecules with our Fe2O3 nanoparticles shows effective adsorption. In comparison study, degradation of the CR was experimented and confirmed by the use of H2O2 as an oxidizer in the presence of visible light. The ease of excitation and reduction of Fe3+ ions to Fe2+ through the Fenton mechanism significantly results in the generation of electrons and holes which aids in the degradation process. This adsorption technique is much more efficient, and cost-effective. The recoverability and reuse of the nanoparticles due to their magnetic behavior make the technique highly useful.



Characterization of Pulsed Laser Deposited Titanium Nitride and Oxynitride Thin Films for Alternative Energy Applications

Sheilah Cherono<sup>1</sup>, Manosi Roy<sup>1</sup>, Kaushik Sarkar<sup>1</sup>, Jacob Som<sup>1</sup>, Abiodun Odusanya<sup>1</sup>, Mark Pfeifer<sup>2</sup>, Darrah Dare<sup>2</sup>, Valentin Craciun<sup>3</sup> & Dhananjay Kumar<sup>1</sup>,

<sup>1</sup>North Carolina A & T State University, <sup>2</sup>Cornell University, <sup>3</sup>National Institution for Laser, Plasma and Radiation Physics. Contact author: scherono@aggies.ncat.edu

Single crystalline titanium nitride (TiN) and partially oxidized titanium nitride (TiNOx) thin films have been grown in a rock-salt structure on sapphire substrates using high vacuum conditions. Pulsed laser deposition (PLD) technique was used to prepare the TiN and TiNOx thin films with different number of pulses ranging from 150-5000 on sapphire substrate. X-ray Diffraction and Reflection (XRD, XRR) were used for structural property analysis, and UV-vis and X-ray Photoelectron Spectroscopy (XPS) were used for optical and chemical properties.

The film thickness was varied in the length scale from a few unit cells to several unit cells. X-ray photoelectron spectroscopy (XPS) analysis has shown that oxygen content of the TiNOx films increases with film thickness (or deposition time), which in turn, affects the exposure time of the ablated materials to the residual oxygen in the deposition chamber (the source of TiN oxidation). The lattice constant of the TiNOx films, measured using XRD, is found to increase with the oxygen content in the film that is validated by the density functional theory (DFT) calculations. The lattice constant increase is explained using enhanced electrostatic repulsion between O2- orbitals in the absence of vacant Ti3+ sites; in order to maintain charge neutrality within the lattice, one Ti3+ cation vacancy is created for every three substitutions of N3- ions by O2- ions. We have observed an asymmetric 'V' shape variation in the optical bandgap as a function of film thickness. The bandgap values decreased from 3.89 eV to 3.30 eV as the film thickness increased from 1.5 nm to 4 nm and then increased from the minimum of 3.30 eV to 3.87 eV as the film thickness increased from 4 nm to 30 nm. The bandgap variation following the left arm of the V-curve is attributed to the quantum confinement effect, while the variation of the bandgap following the right arm of the V-curve is believed to be associated with the increased defects density of the Ti3+ cations that is caused by the charge imbalance in the TiNOx lattice due to partial substitution of N3- by O2- ions. Bandgap and chemical states of TiN/TiNOx thin films can be modulated by varying number of pulses (thickness) and then can used in the next generation of optoelectronic devices.

# PREM32

Effects of Temperature on Ruthenium Oxide Thin Films Using Pulsed Laser Deposition Tyffani Royal, Brooke Smith, Jacob Som & Dhanjay Kumar North Carolina A&T State University Contact author: dkumar@ncat.edu

Within this report, experiments were conducted to determine what effects temperature has on thin film composition, crystalline orientation, and roughness. Ruthenium Oxide (RuO2) thin films were grown using pulsed laser deposition with different substrate temperatures (100, 300, 500). The properties of the thin films were observed using X-Ray diffraction, scanning electron microscopy, and atomic force microscopy measurements. It has been observed that the increase in temperature causes an increase in density, and roughness. The RuO2 thin films made at 500°C are able to form on a substrate with strong crystalline orientation. This information can become vital in how thin films are made for their intended purpose.

# PREM33

Pulsed Laser Deposition and Characterization of Titanium Nitride and Oxynitride Thin Films for Alternative Energy Applications Brooke Smith, Dhananjay Kumar & Jacob Som

North Carolina A&T

 $Contact\ author:\ bksmith 2@aggies.ncat.edu$ 

TiNxOy (TiNO) thin films have been grown using a pulsed laser deposition process with a wide range of x and y realized by varying the oxygen pressure. X-ray diffraction, scanning electron microscopy, and atomic force microscopy measurements have been carried out to evaluate the phase purity and microstructures of TiNO films. The electrocatalytic activities of these films were performed in KOH solution for oxygen evolution reaction. It has been observed that the electrocatalytic activities of these films depend on the growth conditions. Films grown under low oxygen partial pressure (5 mTorr) showed an overpotential of 340 mV to achieve a current density of 10 mA/cm 2, whereas the TiNO film grown under high oxygen partial pressure of 25mTorr displayed the lowest overpotential of 290 mV at the same current density. This range of overpotential observed in this study is among the lowest values reported for any oxynitride systems.



# PREM Affiliation: Navajo Technical University - Harvard University

#### PREM34

Low-Cost Paper-Based Electrodes to Detect Ascorbic Acid, Dopamine and Uric Acid

<u>Makeyla Begay</u><sup>1</sup>, Katelyn Wilson<sup>1</sup>, Justin Platero<sup>1</sup>, Joshua Platero<sup>1</sup>, Jasmine Charley<sup>1</sup>, Michael Nelwood<sup>2</sup>, Khaled Abdelazim<sup>2</sup> & Thiagarajan Soundappan<sup>1</sup>

<sup>1</sup>Navajo Technical University, <sup>2</sup>Harvard University

Contact author: makeiyla.begay@student.navajotech.edu

The Navajo Nation has high rates of cancer, heart disease, and diabetes. Ascorbic Acid (AA), Dopamine (DA), and Uric Acid (UA) are essential biomolecules that we at Navajo Technical University (NTU) have started research on to detect and analyze. This study aimed to identify critical concerns and present our research to the people to assess knowledge of the research conducted here at NTU and gauge interest in research topics. We are also optimizing a suitable paper-based electrode to detect these essential biomolecules. These biomolecules each serve an important role in the human body. AA is a nutrient that forms muscle, cartilage, and collagen in bones and blood vessels. Side effects from AA can cause kidney stones and severe diarrhea. DA is a neurotransmitter that is involved in the central nervous system. When DA is low, it can make one feel unmotivated and tired, and many other symptoms linked to depression and Parkinson's disease. UA is found in blood, passes through the kidneys, and exits the body in urine. We utilize a potentiostat to detect these essential biomolecules with our three-electrode setup. The Linear Sweep Voltammetry helps us view the oxidation peaks detected for all three biomolecules, and the Cyclic Voltammetry technique allows us to view the reduction peaks in DA. Low detection limits of these biomolecules may possible by using the proper nano-materials.

#### PREM35

Simplifying the Design of a Tendon Actuated Soft Gripper into an Easy-To-Follow, Low-Cost Toolkit for K-12 Students <u>Jonathan Chinana</u><sup>1</sup> & Abigail Lockhart Calpito<sup>2</sup>

<sup>1</sup>Navajo Technical University, <sup>2</sup>Harvard University

Contact author: jonathan.chinana@student.navajotech.edu

The Soft Robotics Toolkit is an open-source platform that was created at the Harvard Biodesign Lab to educate students, teachers, and hobbyists on the fundamentals of electronics, soft robotics, and engineering. The main goal of this toolkit was to take the combination of gathered research out of the lab and into a classroom setting. After a successful pilot of a new tendon-actuated soft gripper (TASG) kit across various high schools in India, several improvements to the design of this educational toolkit were identified, such as lowering the production cost and simplifying the use of complex electronics. The soft gripper toolkit currently has a plug and play aspect which does make it easy to assemble, but also hinders students overall learning objectives and doesn't fully immerse them in the engineering design process. The aim of this research is to update the current design of the TASG toolkit by using accessible materials to reduce production cost and by simplifying the electronic circuit design by moving from custom built printed circuit boards (PCB) to off-the-shelf reconfigurable electronics. To do this, we switched out the custom PCBs from the previous soft gripper design and inserted a breadboard with an Arduino microcontroller: this change will allow students the ability to program, manipulate, and test off-the-shelf electronic components on a circuit of their own. We expect that these design changes will give students more creative control of how they want to structure their soft grippers and electronics, while giving educators the confidence to understand and implement the toolkit in their engineering focused curriculum.

# PREM36

*Ultra-Fast and Highly-Sensitive ddPCR for Infectious Disease Diagnostics*<u>Layla Marie James</u><sup>1</sup>, Katelyn Wilson<sup>1</sup>, Jean Serrano<sup>2</sup>, Yang Wang<sup>2</sup>, David A. Weitz<sup>2</sup>, Irene Ane-Anyangwe<sup>1</sup> & Abraham Meles<sup>1</sup>
<sup>1</sup>Navajo Technical University, <sup>2</sup>Harvard University
Contact author: layla.james@student.navajotech.edu

Digital droplet polymerase chain reaction (ddPCR), a method in which DNA is amplified and contained in a water-oil-based droplet, has become an attractive assay for clinical diagnostics as it provides high sensitivity to detect pathogenic genetic material. However, in order to expedite ddPCR for rapid diagnosis, we are integrating nanoplasmonic-based heating for ultrafast PCR thermo-cycling. To achieve this, we incorporate gold nano-rods in the ddPCR solution while avoiding their direct contact with PCR reagents inside the droplets; this avoids inefficiencies in PCR amplification due to interactions of the gold nano-rods with the proteins/enzymes. Our approach was to generate stable double emulsions that will contain the PCR solution protected by an ultra-thin oil shell, as the nano-rods are diluted into the outer aqueous phase. This study used glass-capillary micro-fluidic devices to create double emulsions. We learned that a highly viscous oil solution provided better control of the oil shell thickness with varying flow rates. Additionally, the double emulsions exhibited mechanical stability as they remained intact after manual pipetting. Overall, this system provides the basis for successfully integrating ultrafast PCR amplification via nanoplasmonic heating with highly-sensitive ddPCR detection.



How S.T.E.M. is Embedded in Navajo Weaving Keanu Simpson<sup>1</sup>, Melissa Saltwater<sup>2</sup> & Franklin Sage<sup>1</sup> <sup>1</sup>Navajo Technical University, <sup>2</sup>Harvard University Contact author: keanu20simpson@gmail.com

Weaving has been a life staple for the Native American, Navajo people. In this research, we are showing that Science, Technology, Engineering, and Mathematics (S.T.E.M.) is embedded in Navajo weaving, and that Navajo people are S.T.E.M. people within their own right. With the help of a Navajo elder, we were able to translate Navajo weaving knowledge into S.T.E.M., while also keeping it all traditional. The findings in this research helped in proving that S.T.E.M. is embedded in Navajo weaving, and that Navajo people are S.T.E.M. people within their own rights, through their own culture.

#### PREM38

Design and Fabrication of Flexible Paper-based, Electrochemical Sensors to Detect the Presence of Heavy Metals in Ground Water <a href="Matelyn Wilson">Katelyn Wilson</a>, Justin Platero</a>, Michael D. Nelwood</a>, Khaled Abdelazim</a>, Jasmine Charley</a>, Makeiyla Begay</a>, Samantha Francis</a> & Thiagarajan Soundappan</a>

 $^{1}$ Navajo Technical University at Crownpoint, NM,  $^{2}$ Harvard University at Cambridge, MA

Contact author: katelynwilson0214@gmail.com

The history of mining and mineral extraction across the Navajo Nation has resulted in considerable contamination of the land and the groundwater resources, which is a significant environmental concern. Through a partnership between Navajo Technical University and Harvard University, we have designed and fabricated flexible, paper-based sensors in tandem with electrochemical techniques such as cyclic voltammetry, differential pulse voltammetry, and anodic stripping voltammetry to determine heavy metal concentrations in test samples. We have selected to fabricate paper-based electrochemical sensors because; they are low-cost, easy to make, environmentally friendly, and can be deployed for field testing across the Navajo Nation. Furthermore, the linear electrochemical response and sensitivity of these electrodes, for detecting heavy metals, makes them well suited for real-time sensors in field-testing applications.

# PREM Affiliation: North Carolina Central University - The Pennsylvania State University

# PREM39

<u>Netanya Faith Dennis</u> North Carolina Central University

# PREM40

Modification of PANI with Carbon Nanodots for Enhanced Optoelectronic Properties Shaila Jackson, Ufana Raiz & Darlene Taylor North Carolina Central University Contact author: uriaz@nccu.edu

The present work reports synthesis of polyaniline (PANI) using different oxidants such as ammonium dichromate, ferric chloride and ferrous sulphate to study the morphologies and the variations of the electronic transitions upon doping with sulphuric and hydrochloric acids. The PANI was characterized using FTIR, UV-visible and scanning electron microscopy (SEM). Carbon nanodots (CND) were loaded in different amounts to investigate the change in the fluorescence properties of these polymers upon addition of carbon nano-dots. The nanohybrids hold potential application in designing smart packaging materials.

# PREM41

Investigation of Light Interaction with Silver Dots
Patrick Jacobs & Yongan Tang
North Carolina Central University
Contact author: pjacobs7@eagles.nccu.edu

Plasmonic nanostructures can strongly enhance light-matter interactions by confining light to the nanoscale in the form of surface plasmon polaritons. Surface plasmons can miniaturize optical devices to the nanoscale, and also generate extremely high electromagnetic intensities that create strong light-matter interactions. We investigated the light interacting with silver nanodots. This study is carried out with wavelengths of visible and near-infrared light using Finite Difference Time Domain (FDTD) method. Our simulations show that the dimensions of the silver dots and their size significantly affect the optical reflectance of the light. The optical reflectance in the spectrum of certain wavelengths is observed. These research results have possible applications in developing optical detectors and biosensing.

Fabrication of Stretchable Laser-Induced Graphene Strain Sensors for the Detection of Human Hand Motion Dionne Mitchell<sup>1</sup>, Monther Al Siyabi<sup>2</sup>, Vinay Kammarchedu<sup>2</sup> & Aida Ebrahimi<sup>2</sup>

<sup>1</sup>North Carolina Central University, <sup>2</sup>PENNState University

Contact author: dmitch80@eagles.nccu.edu

Flexible strain sensors have gained attention in various fields ranging from human motion detection in healthcare to soft robotics. Traditional metallic strain sensors lack flexibility and require elaborate fabrication techniques. Laser-induced graphene (LIG) are three-dimensional carbon-based nanomaterials that exhibit high thermal and electrical conductivity. LIG is a promising alternative to traditional strain sensors due to the efficient one-step fabrication process, excellent conductivity, and ability to modify the product for the desired use. We herein describe the preparation and testing of flexible LIG strain sensors for the detection of human hand motion. During fabrication, we examined the fiber height, color, and resistance to produce the most sensitive and resilient device. The completed graphene product was transferred to various stretchable materials to analyze the efficacy of the device in detecting high and low strain. To analyze the device the change in resistance during shear and tensile strain were recorded along with detecting a change in resistance of 9 different hand motions. After analysis, it is concluded that the flexible LIG strain sensors were successful in responding sensitively to each motion performed and provide promising results for flexible strain sensing.

#### PREM45

2-D Intercalated Structures Based on Hybrids of Vanadium Pentoxide with P-Phenylene Sofía Sánchez Lemus, Ufana Riaz & Darlene Taylor North Carolina Central University Contact author: uriaz@nccu.edu

The present work reports solid-state intercalation of p-phenylenes in the interlayer space of vanadium pentoxide with a view to study the effect of space confinement on the optoelectronic properties of the conjugated oligomers as well as vanadium pentoxide. The organic-inorganic nanohybrids were characterized using, FTIR, UV-visible, X-ray diffraction (XRD) and scanning electron microscopy (SEM), atomic force microscopy (AFM). Bandgaps were determined using the UV-visible data and were found to show variation with the side chain functional groups of p-phenylenes. The study could be helpful in designing next generation solar cells with controlled properties.

# PREM Affiliation: Tennessee State University - Fisk University - Illinois Materials Research Science and Engineering Center

# PREM46

Surface Modification of WSe<sup>2</sup> via Oxygen Plasma and DI Water Rinse Amyra Black<sup>1</sup>, Arend van der Zande<sup>2</sup>, Kelly Hiyuan<sup>2</sup> & Siyuan Huang<sup>2</sup> <sup>1</sup>Tennessee State University, <sup>2</sup>University of Illinois Urbana-Champaign Contact author: amyrablack404@gmail.com

Ninety—eight percent of the human genome has been sequenced, figuring out the 2% percent is important because we can begin creating individualized medicines. Sequencing DNA can help understand the protein which can then be used to create treatment for diseases a majority of which are related to protein deficiency. Nanopore is a promising next generation sequencing method, creating a nanopore-based on 2D materials is a promising solution. Improving on 2D nanopore requires a better spatial resolution and shorter nanopore channel. However, when the negatively charged DNA is sequenced it creates a dominating interlayer resistance. The resistance of the WSe<sub>2</sub> tends to dominate the resistance within the nanopore. A method of controlling the resistance of the WSe<sub>2</sub> is an oxygen plasma p-doping method. During the oxygen plasma treatment, the top layer of the WSe<sub>2</sub> turns to MoS<sub>2</sub> but is degraded after a DI rinse. This study will be using Atomic Force Microscopy to observe the surface modification of the WSe<sub>2</sub>.



First-Principles Study on Polarization Dependent Optical Properties of Transition Metal Doped β-Ga<sub>2</sub>O<sub>3</sub>
<u>Grady Patrick Clopton</u><sup>1</sup>, Channyung Lee<sup>2</sup>, Joel Varley<sup>2</sup>, Michael Scarpulla<sup>2</sup>, Andre Schleife<sup>2</sup> & Elif Ertekin<sup>2</sup>
<sup>1</sup>Tennesse State University, <sup>2</sup>University of Illinois at Urbana Champaign
Contact author: gclopton@tnstate.edu

β-Ga2O3 has attracted interest for use as a material for power-switching devices due to its ultra-wide bandgap, high breakdown field, and availability of affordable large-diameter single-crystal wafers. Before we can utilize Ga2O3 in such devices, it is critical to understand fundamental aspects of defects and doping, including how defects incorporate into the lattice, how they affect carrier concentrations, and how they affect mobilities. One challenge in achieving control over defects in Ga2O3 is that it is often difficult to characterize and identify defects that are intentionally or unintentionally present in synthesized material. In this work, we use first principles modeling and simulation based on density functional theory to explore the possibility of pleochromism in transition metal doped Ga2O3. Pleochromism is an optical phenomenon where a material shows different colors when observed from different directions, particularly under polarized light. We explore the optical response of Ga2O3 with transition metal impurities Cr, Ir, and Fe. Specifically, we compute the electronic band structure and optical absorption spectrum of supercells containing substitutional defects for Cr, Ir, and Fe in various charge states. Due to the anisotropy of the crystal structure, we find that each defect exhibits a pleochroic signature: a direction and polarization dependent optical absorption spectrum that is unique to the transition metal impurity.

# PREM48

Electrohydrodynamic Fabrication of Core-Shell Microparticles for Controlled-Release Immunotherapy of Ovarian Cancer Karla Robles<sup>1</sup>, Todd Giorgio<sup>2</sup> & Richard Mu<sup>1</sup>

¹Tennessee State University, ²Vanderbilt University

Contact author: karlanatalyrobles@gmail.com

The low success rates of immune checkpoint-inhibitors (CPIs) in the treatment of ovarian cancer may be attributed to low bioavailability following administration. Local administration of CPIs, i.e. intraperitoneal, rather than intravenous, in mouse models can improve therapy by increasing proximity of the treatment to the cancer target. However, injections need to be administered every other day to achieve the desired therapeutic effects. Microencapsulation techniques, such as the electrohydrodynamic atomization (EHDA) or electrospray method, can prove useful in developing controlled-release biomaterials for prolonged bioavailability. We propose a single-administration treatment using microparticles with an immune checkpoint inhibitor core encapsulated within a biodegradable PLGA shell. In the electrospray technique, syringe pumps dispense core and shell material solutions through a coaxial steel needle which receives a high voltage. When the electric charge build-up overcomes the solutions' surface tension, monodisperse particles are deposited onto a grounded collector. Here, we develop and categorize controlled-release microparticles for immunotherapy using EHDA. The preliminary results show scanning electron micrographs of microcapsules with a PEG core and PLGA shell of 1-3 µm.

# PREM49

<u>Christopher Buford II</u> Tennessee State University

# PREM50

First-Principles Study of Photoelastic Effect in Zinc Blende Gallium Phosphide

Ethiopine Choping<sup>1</sup>, Junehu Park<sup>1</sup>, Cindy Wong<sup>1</sup>, Yifan Yao<sup>1</sup>, Yi-Ting Lee<sup>1</sup>, André Schleife<sup>1</sup> & Elif Ertekin<sup>2</sup>

<sup>1</sup>University of Illinois Urbana-Champaign, <sup>2</sup>Tennessee State University.

Contact author: ethiebernard@gmail.com

Zinc Blende Gallium Phosphide (GaP) is a wide bandgap semiconductor. It is a III-V semiconductor that is widely used for its electroluminescent properties in electronic devices. The zinc-blende structure of this GaP compound creates a cubic shape where each gallium (Ga) atom is at the center of the cubic structure and the phosphides (P) at the four corners (1). The GaP structure was simulated using the density functional theory (DFT) to investigate the changes in the elastic moduli under photoexcitation. The electronic structure was simulated under hot-electron Fermi distributions with temperatures between 0.1 eV to 1.0 eV, as a first approximation of a thermalized photoexcited state. The simulation was used to demonstrate how the elastic moduli would change at varying electron temperatures. The simulation determined that at high energies the electrons in the GaP structure has a higher probability of moving from the valence band to the conduction band between 4 eV to 6 eV.



The Growth of Gallium Oxide Nanowires
<u>Geordan Dorsey</u><sup>1</sup>, Antonio Moore<sup>1</sup>, Warren Collins<sup>1</sup>, Richard Mu<sup>2</sup> & Akira Ueda<sup>1</sup>
<sup>1</sup>Fisk University, <sup>2</sup>Tennessee State University
Contact author: geordand26@yahoo.com

The growth of  $\beta$ -gallium oxide (Ga2O3) nanowires has been achieved by the solid-liquid method. In Argon atmosphere, pure gallium was heated to produce gallium vapor and oxidized by introducing oxygen gas with a certain flow rate at high temperatures (~1000°C) with a vertical tube furnace. Since  $\beta$ -Ga2O3 is the most thermodynamically stable phase of Ga2O3 at standard temperature and pressure, and has the monoclinic crystal structure,  $\beta$ - Ga2O3 nanowires are grown in a specific direction. For the growth of  $\beta$ - Ga2O3, two kinds of substrates were prepared: The first kind is the quartz substrates coated with Ga2O3 thin film of 100 nm by using an electron beam evaporator, and the second kind is quartz substrates deposited with gold nanoparticles with a DC sputtering coater. The correlation between the gold nanoparticle diameter and the thickness of Ga2O3 nanowire was studied. The growth orientation was also investigated for these two kinds of substrates. Acknowledgements: The authors acknowledge the support of the NSF through the Partnership for Research and Education in Materials (PREM) program DMR-2122169, the University of Illinois at Urbana-Champaign Materials Research Science and Engineering Center DMR-1720633 and HRD-1924241 under HBCU-RISE Program at Tennessee State University, and NIH U54 pilot research program.

#### PREM52

The Growth of Nano-Phase Gallium Oxide under Vacuum

Antonio Moore<sup>1</sup>, Geordan Dorsey<sup>1</sup>, Lei Qian<sup>1</sup>, Warren Collins<sup>1</sup>, Richard Mu<sup>2</sup> & Akira Ueda<sup>1</sup>

<sup>1</sup>Fisk University, <sup>2</sup>Tennessee State University

Contact author: AXMoore27@my.fisk.edu

The growth of  $\beta$ -gallium oxide (Ga2O3) has been carried out by using an electron beam evaporator. Under the vacuum of around 10-5 Torr, pure gallium was heated to produce gallium vapor by electron beam and oxidized by introducing oxygen gas with a specific flow rate with a leak valve. Since  $\beta$ -Ga2O3 is the most thermodynamically stable phase of Ga2O3 at standard temperature and pressure and has a monoclinic crystal structure, the resulting  $\beta$ - Ga2O3 nanowires grew in a specific direction based on material conditions during nucleation. For the growth of  $\beta$ - Ga2O3, two kinds of substrates were prepared: quartz substrates coated with Ga2O3 thin film (100 nm) by using an electron beam evaporator, and quartz substrates deposited with gold nanoparticles of varying thickness using a sputtering machine. The correlation between the gold nanoparticle diameter and the thickness of Ga2O3 nanowires was studied. The crystal growth orientation was also investigated as a function of coating material for both types of substrates with a Scanning Electron Microscope and X-ray diffraction.

# PREM Affiliation: Texas State University - University of Texas at Austin - Center for Dynamics and Control of Materials

# PREM53

Charge Transfer through Individual DNA Molecules Measured by Mechanically Detected Electric Charge Sensing
<a href="mailto:RigoLuna">RigoLuna</a>, Noah Austin-Bingamon, Binod D.C, Mitchell Ford, Damilola Runsewe, Tania Betancourt & Yoichi Miyahara, Texas State University.

Contact author: rml74@txstate.edu

# \*Also presented at EL12.03.02, Apr 11, 2023, 4:00PM, Moscone West, Level 1, Exhibit Hall.

DNA is a programmable and quickly synthesized material that has gained significant interest in the development of nano-scale devices, including as a charge-transfer medium for molecular nano-electronics. However, a thorough understanding of the electrical properties of charge transfer within the DNA molecule is necessary to make these devices practical. Previous attempts to characterize the electrical properties of individual DNA molecules have produced conflicting results due to differing experimental setups. In our research, we aim to characterize individual hybridized DNA molecules attached to gold via thiol-linkers using a non-contact mechanical method via AFM. Our method should provide a more accurate measurement of charge transfer in individual DNA molecules and also minimize deformation to the molecule. With this method, we hope to gain a better understanding of the electrical properties of charge transfer within DNA molecules, which could lead to the development of more efficient and reliable molecular nano-electronic devices.



The Investigation of the Injectability and Cytocompatibility of Dynamic Poly(ethylene glycol) Hydrogels

Mackenzie U. Otakpor¹, Andi Crowell², Kushal Thapa¹, Thomas FitzSimons², McKenzie Siller¹, Adrianne Rosales² & Tania Betancourt¹

¹Texas State University, ²The University of Texas at Austin.

Contact author: mackotak@gmail.com

Hydrogels are composed of hydrophilic polymers that are crosslinked to form a network. Hydrogels are often used to mimic the extracellular matrix (ECM), which contains macromolecules and minerals that aid in the physical and chemical support of cells. Hydrogels have found applications in biomedicine as tissue engineering scaffolds, wound healing materials, and drug delivery devices. Dynamic hydrogels, specifically, contain crosslinks that can be modulated by a range of internal and external stimuli, making them uniquely suitable to changing tissue microenvironments or to the need for on-demand drug release.

A 4-arm poly(ethylene glycol) macromer with benzal-cyanoacetamide end groups (PEG-RBCA) and 4-arm poly(ethylene glycol) macromer with thiol end groups (PEG-thiol) was used in this work to create dynamic hydrogels. The hydrogels were further loaded with poly(ethylenedioxythiophene) (PEDOT) nanoparticles which act as photothermal agents, enabling laser-induced modulation of hydrogel crosslinking by affecting the equilibrium of the dynamic bonds. The injectability and cytocompatibility of the hydrogels were investigated. To better understand the injectability and the mechanical compatibility of the hydrogels with the host tissue, we studied the rheological properties of the hydrogels and examined the injection force required for the administration of the hydrogels. To investigate the cytocompatibility of the hydrogels, two cell viability assays were used: Live/Dead assay and 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium (MTS) assay. Studies were conducted with fibroblast cells and human MDA-MB-231 breast cancer cells.

The goal of these studies was to examine the potential of these dynamic hydrogels for biomedical applications. Rheological studies demonstrated that the hydrogels possessed viscoelastic properties similar to those of tissues and that these properties could be tailored by utilizing varying precursor molecular weight and functionality. The injectability studies demonstrated that the hydrogels are injectable with a clinically relevant force. Finally, preliminary cell viability studies demonstrated that the hydrogels are cytocompatible.

# PREM55

Hydrogels Crosslinked with Dynamic Thia-Conjugate Bond and Incorporated with Poly(ethylenedioxythiophene) Nanoparticles as Photothermally Responsive Controlled Release System

<u>Kushal Thapa</u><sup>1</sup>, Joanna Zepeda<sup>1</sup>, McKenzie Siller<sup>1</sup>, Edgar Torres<sup>1</sup>, MacKenzie Otakpor<sup>1</sup>, Thomas FitzSimons<sup>2</sup>, Anne Crowell<sup>2</sup>, Adrianne Rosales<sup>2</sup> & Tania Betancourt<sup>1</sup>

<sup>1</sup>Texas State University, <sup>2</sup>The University of Texas at Austin.

Contact author: k\_t260@txstate.edu

# \*Also presented at SB07.02.06, Apr 11, 2023, 2:15PM, Moscone West, Level 2, Room 2018.

Hydrogels are a class of soft materials formed by crosslinking of hydrophilic polymers. The nature of crosslinks in the molecular level determines the properties of the hydrogels in the macroscopic level. In our research, we utilized thia-conjugate bond as means of crosslinks in our polyethylene glycol (PEG) based hydrogel. This dynamic covalent bond provides self-healing ability to the hydrogel [1]. Additionally, the equilibrium of the crosslinking reaction can be shifted with thermal, mechanical, or pH stimulus [2]. For the bulk hydrogel, this translates to a controllable transition between gel and sol state by modulating these stimuli. We investigated the thermal response of the hydrogel with the aim of developing an on-demand, pulsatile drug delivery system. Further, we incorporated poly(ethylenedioxythiophene) or PEDOT nanoparticles within the hydrogel to facilitate photothermal modulation of the drug release through administration of clinically relevant near-infrared (NIR) light.

We used Michael addition of thiol-ene pairs from four-arm PEG thiol (PEG-SH) and four-arm PEG benzylcyanoacetamide (PEG-BCA) to form dynamically crosslinked hydrogels. PEDOT nanoparticles were synthesized using an emulsion polymerization process and were entrapped within the hydrogel. Additionally, BSA-FITC, a fluorescently labeled protein, was loaded into the hydrogel-PEDOT complex and its release behavior into buffer upon direct thermal stimulation and photothermal stimulation with 808-nm laser was investigated. The injectability of the hydrogels was studied using hypodermic needles. The biocompatibility of the hydrogel-PEDOT complex was characterized on MDA-MB-231 cell line using the MTS and live-dead assay.

PEDOT nanoparticles had an average size of 56.3 nm and absorbance peak at 780 nm. The photothermal stimulation of these nanoparticles with an 808 nm laser showed a fast increase in temperature plateauing within the first five minutes. The nanoparticles also showed photothermal stability on repeated pulsatile laser stimulation. As for the hydrogel-PEDOT complex, drug release studies showed time-dependent release profile for thermal stimulation while photothermal stimulation showed time-independent release profile. The hydrogel-PEDOT complex was also shown to be injectable through a 28-guage hypodermic needle. The biocompatibility of the hydrogel-PEDOT complex was characterized on MDA-MB-231 cell line using the MTT assay and the results showed that this complex is not cytotoxic.

Our dynamically crosslinked hydrogel loaded with PEDOT nanoparticles showed photothermally stimulated drug release in a clinically relevant environment. [1] FitzSimons, Macromolecules, 2020, 53, 3738-3746; [2] FitzSimons, ACS Polym Au, 2022, 2, 129-136.

Photothermally Responsive Dynamic Hydrogels Incorporating Reversible Thiol/Ene and Irreversible Maleimide/Thiol Crosslinking for Pulsatile Drug Delivery

Edgar Torres<sup>1</sup>, Kushal Thapa<sup>1</sup>, Thomas FitzSimons<sup>2</sup>, Mckenzie Siller<sup>1</sup>, Joanna Zepeda<sup>1</sup>, Adrianne M. Rosales<sup>2</sup> & Tania Betancourt<sup>1</sup>

¹Texas State University, ²The University of Texas at Austin.

Contact author: e\_t217@txstate.edu

Hydrogels are three-dimensional hydrophilic polymer networks with tissue-like properties that have been used in biomedical applications for several decades. In our laboratory, a pulsatile drug delivery system based on dynamic poly(ethyleneglycol) (PEG) hydrogels crosslinked via thiol/ene Michael addition was previously explored. These hydrogels were designed to be photothermally activated upon irradiation of embedded poly(ethylenedioxythiophene) (PEDOT) nanoparticles. While showing great promise, the dynamic nature of the crosslinks of these hydrogels led to the uncontrolled hydrogel dissolution and consequent release of entrapped agents when no stimulation was applied when in an unconstrained aqueous environment. In this work, 4-arm-PEG-Maleimide (PEG-Mal) is investigated as a potential solution providing a secondary crosslink to contain the unwanted release. To synthesize the hydrogel, a Michael addition of thiol-ene functional four-arm PEG-benzylcyanoacetamide, PEG-thiol, and PEG-Mal was conducted. Various molar ratios of the three precursors were explored. The hydrogel was loaded with PEDOT nanoparticles to provide it with photothermal properties, and BSA-FITC, a fluorescently labeled protein, acted as a therapeutic mimic. The release of BSA-FITC upon application of heat or laser irradiation of the hydrogels was confirmed visually and spectroscopically. Results showed that no undesired release of BSA-FITC occurred from hydrogels that included PEG-Mal, in contrast to those lacking these stable crosslinks. Further studies will be carried out to verify the addition of PEG-Mal as a viable option for the preparation of hydrogels for the pulsatile release of therapeutic agents.

# PREM57

**Electroactive Polymer Nanofibers** 

<u>Adelyne Towne</u><sup>1</sup>, Madeleine Pastore<sup>1</sup>, Nicolas Lontkowski<sup>1</sup>, Marvin Santiago<sup>1</sup>, Zachary Brotherton<sup>2</sup>, Nathaniel Lynd<sup>2</sup> & Jennifer Irvin<sup>1</sup> <sup>1</sup>Texas State University, <sup>2</sup>University of Texas at Austin.

Contact author: act109@txstate.edu

As electroactive polymers (EAPs) switch between two stable oxidation states, changes in conductivity, color and volume are exhibited. These characteristic changes have given rise for EAP use in a myriad of applications such as energy conversion and storage, electrochromics, water purification, and biomaterials as biosensors. Nanofibrous EAPs may provide a high surface area, modifiability in the presence of nanoparticles for various applications and tunability of properties applicable. Polymer nanofibers can be produced via the process of electrospinning, but EAPs lack effective polymer chain entanglement necessary to form solutions of adequate viscosity for nanofiber formation. Instead, EAPs can be incorporated as coatings on the surface of electrospun polymers. This poster will present effective methods to coat commodity polymers (polyacrylonitrile and polycaprolactone) with EAPs polypyrrole and poly(3,4-ethylenedioxythiophene), as well as approaches of pretreatment of nanofibers for optimal coating uniformity. Synthesis and characterization of a propargyl ether-modified poly(ethylene oxide) (PPGE) will be discussed, as well as attempts to graft electroactive monomers to PPGE using click chemistry and attempts to electrospin via blending with PEO as a carrier polymer.

# PREM Affiliation: The University of Texas at El Paso - University of California at Santa Barbara

# PREM58

Characterization and Synthesis of Pulsed-Laser Deposited Ba(Fe0.7Ta0.3)O3 $-\delta$  Thin Films Nolan T. Herbort, Ramana C.V.

University of Texas at El Paso

Contact author: rvchintalapalle@utep.edu

Research and development activities in the topical area of semiconducting metal oxides (SMO) for application in a wide variety of sensors for utilization in domestic and industrial sectors is continually rising. The strong, continued interest in SMOs is p rimarily driven by the increased market size of sensors for consumer and industrial applications. Optimization of industrial processes require rapid sensor responses, and along with these optimizations they reduce the amount of hazardous chemicals being released into the environment from these processes. Recently, Ba(Fe0.7Ta0.3)O3 $-\delta$  (BFTO) has been evolved as an efficient oxygen sensor material with a functionality over a broad temperature and oxygen partial pressure range. However, efforts directed to understand the fundamental scientific aspects of crystal chemistry and phase stabilization, especially as a function of variable thermochemical synthetic conditions, in BFTO materials is meager. In this context, in the present work, we focused our efforts on the synthesis and characterization of bulk and thin film Ba(Fe0.7Ta0.3)O3 $-\delta$  (BFTO30) materials. The BFTO compounds were synthesized using the conventional high-temperature solid-state chemical reaction method. The structure and phase stability of the BFTO bulk materials studied in order to optimize the bulk target, which was used to fabricate thin films by pulsed-laser deposition (PLD). The BFTO films were made by PLD by varying the deposition temperature and oxygen pressure. The effect of these thermodynamic parameters on the structure, composition, and optical properties is established.

Two-Photon Excitation of InGaN Nanowires

Kausik Kolluri<sup>1</sup>, Emma M. Sundin<sup>2</sup>, Debabrata Das<sup>2</sup>, Chintalapalle V. Ramana<sup>2</sup> & Chunqiang Li<sup>2</sup>

<sup>1</sup>University of California Santa Barbara, <sup>2</sup>University of Texas at El Paso

Contact author: kkolluri@ucsb.edu

The unique properties of semiconductor nanowires offer a gateway to improvements in light emitting devices, energy harvesting and conversion. However, in order to better understand the optical properties of these materials, we conducted two-photon excitation photoluminescence (PL) spectroscopy experiments on indium gallium nitride (InGaN) nanowires, which have important applications in light emission diodes (LEDs), and photovoltaics. These nanowires were grown on silicon substrates by molecular beam epitaxy (MBE). We used a house-built two-photon microscope with a tunable femtosecond laser to excite these InGaN nanowires over the infrared excitation spectrum. The PL spectrum peaks at 500 nm. Results show absorption peaks above the band gap that are dependent on the excitation wavelength. At these peaks, the PL emission intensity is additionally dependent on the linear polarization angle of the illumination laser. These results indicate two-photon excitation of discrete quantum energy levels in these nanowires, revealing previously unreported energy states in these materials. This discovery will lead to new understanding of electronic and optical properties of InGaN nanowires.

# PREM60

 $\textit{Fabrication and Characterization of High Quality Rutile-Phase } \textit{GeO}_{2} \textit{Films on MgO} (100) \textit{ for Application in Optoelectronics}$ 

Paul Nalam, Debabrata Das & C. V. Ramana

The University of Texas at El Paso Contact author: pgnalam@miners.utep.edu

Ultra-wide bandgap materials (UWBG) with energy bandgaps  $^{\sim}4\text{eV}$  or larger are currently of immense interest for the development of devices for high-power electronics, deep-ultraviolet (DUV) optoelectronics, energy harvesting, electrocatalysis and quantum information processing. In this context, the functional metal oxide GeO2 is important for its large bandgap (4.5-6.0 eV), ambipolar dopability and large thermal conductivity. GeO2 exists primarily in two crystalline polymorphs: the rutile / tetragonal (r) phase and the  $\alpha$ -quartz / hexagonal (h) phase. Both polymorphs exhibit interesting and useful optical and opto-electronic properties. However, since it exists in multiple metastable phases with similar formation energies, isolated synthesis of multiple polymorphs with high crystal quality is challenging and has hindered its adoption into advanced optoelectronic applications. Here, we employed radio-frequency magnetron sputtering, which is a relative cost effect method, to deposit r-GeO2 thin films on MgO (100) substrates in a controlled oxidation environment. The lower degree of interfacial lattice mismatch between r-GeO2 and MgO enabled to tune the degree of epitaxy of the thin film based on the oxidation environment. The surface morphology, growth mechanism, optoelectronic properties, crystallography, and chemical stoichiometry of these thin films are studied in detail using atomic force microscopy, UV-Vis, Photoluminescence spectroscopy, Ellipsometry, X-ray diffraction, Transmission electron microscopy and X-ray photoelectron spectroscopy.

# PREM 61

Pulsed Laser Deposition of  $\theta$ -Ga $_2$ O $_3$  Tungsten Alloy for Self-Biased Solar-Blind Ultraviolet Photodetectors Francelia Sanchez Escobar, Debabrata Das & C. V. Ramana

University of Texas at El Paso

Contact author: fsanchezes@miners.utep.edu

The energy consumption has increased over the last decades due to the technological advancements which require high energy-efficient multifunctional devices. Self-assembled vertically aligned  $\beta$ -Ga2-xWxO3 nanocomposite (GWO-VAN) architecture were grown on silicon platform by pulsed laser deposition for the application in low-cost self-biased solar-blind UV photodetector. The W-enriched vertical  $\beta$  Ga2-xWxO3 nanocolumns inside the W-deficient  $\beta$ -Ga2-xWxO3 matrix were fabricated by controlling the growth parameters. The presence of  $\beta$ -Ga2-xWxO3 was confirmed from structural and morphological characterization using x-ray diffraction, x-ray spectroscopy, HAADF-STEM and atom probe tomography. Furthermore, photoluminescence spectroscopy assisted to understand the dynamics of photo-absorption and the recombination between energy states. Cost-effective MSM-type UV PD was fabricated using  $\beta$ -Ga2-xWxO3 VAN as the active material with a silver top metal contact. The device was characterized to test its responsivity, detectivity, among other measurements.



# PREM Affiliation: Tuskegee University - University of Nebraska-Lincoln

#### PREM62

Enhanced Magneto-Electric Coupling Effect of KLTO Reinforced Polyvinylidene Trifluoroethylene Nanocomposites for E-Textile Smart Surfaces

Richard Harry<sup>1</sup>, Shaik Zainuddin<sup>1</sup>, Robyn Mabra<sup>1</sup>, Navadeep Shrivastava<sup>2</sup> & Ziping Luo<sup>2</sup>

<sup>1</sup>Tuskegee University, <sup>2</sup>Fayetteville State University.

Contact author: rharry3999@tuskegee.edu

The utilization of polymers within the microelectronics sector has become more prevalent in advanced applications due to their easy processibility, versatility, and tailorable properties. In recent years, polymers have been used in sensors, spintronics, separator membranes for Li-ion batteries, dye-sensitized solar cells, supercapacitors, fuel cells, etc. Co-polymer polyvinylidene-co-tri fluoroethylene (PVDF-TrFE) has been assessed broadly across sensor technology applications and proved capable as a coupled ferroic component in magneto-electric systems. To ascertain the unique functionality of the polymeric material, nanomaterials with targeted functionality are used as nanofillers. Layer perovskites have been reported, such as the Ruddlesden-Popper phase, Dion-Jacobson phase, and Aurivillius phase, in which K2La2Ti3O10 nanoparticles are a formulation of interest. This study investigated the magneto-electric properties of PVDF-TrFE nanocomposites loaded with K2La2Ti3O10 (KLTO) nanoparticles. At first, The KLTO was synthesized using the modified Pechini method. Next, these compounds were added to PVDF-TrFE at varying weight percentages of 1, 5, and 10 wt. % and then formed into flexible nanocomposite thin films via solvent casting. Nanocomposites were annealed at 150oC for 2 hrs to enhance β-phase crystallinity. Films were fabricated and processed at dimensions of 8-20µm thickness, 35 mm length, and 35 mm width. The morphology of the nanocomposites was observed using SEM at a magnification of 2000x in the 10µm range, which showed a robust distribution of KLTO nanoparticles within the PVDF-TrFE matrix, with few aggregated sites within the observed region. Differential scanning calorimetry (DSC) was performed to observe the phase transition properties of KLTO@PVDF-TrFE nanocomposites, which determined the average Curie temperature and melting temperatures 119oC and 147oC, respectfully, increasing the nominal temperatures by up to 2.3% via the addition of 10wt% KLTO@PVDF-TrFE. The XRD patterns of bulk and exfoliated KLTO nanoparticles exhibited high crystallinity, with a high distribution of elements within the structure. Ferroelectric hysteresis loops were given from the Radiant Multiferroic Analyzer, which increased peak polarization at a breakdown field of 2000kV/cm with the addition of 5wt%KLTO@PVDF-TrFE. Magnetic tests were done using Vibrating Sample Magnometer (VSM), which yielded the magnetic polarization concerning changes in field magnitude. The highest magnetic moment occurred with the addition of 10wt% KLTO@PVDF-TrFE with a saturated magnetization value of 3.66 emu/g. Magnetoelectric coefficients were calculated based on the polarization and saturated magnetization values, which indicated the magnitude of the coupling effect to be highest within the 5wt%KLTO@PVDF-TrFE nanocomposites. Results from this study determined that KLTO@PVDF-TrFE is suitable for etextile sensor systems in various industries, including consumer electronics, transportation, and aerospace sectors.

# PREM63

Synthesis and Characterization of BiFeO₃ Particles Doped with Zn and Ti Lyndon Smith¹, Vijaya Rangari¹, Kayleigh McElveen² & Rebecca Lai²¹Tuskegee University, ²University of Nebraska-Lincoln. Contact author: lsmith7435@tuskegee.edu

Bismuth ferrite particles doped with Zn and Ti with a nominal composition of BiFe0.96(Zn, Ti)0.02O3 were synthesized using a nano-agitator milling method for electrical applications. The particles were milled for 4 hours, then calcined in air at 650°C, 700°C, 750°C, 800°C, and 850°C for 2 hours. The particles were then characterized using SEM/EDAX, XRD/JADE, and SQUID. Polarization curves were also measured along with leakage current for the sample calcined at 750°C. Compared to neat BiFeO³ synthesized using a similar method, the leakage current density was reduced by a factor of about 50. Rietveld refinement was performed on the XRD patterns to determine the relative weight fractions of phases and approximate crystallite sizes. From 700°C to 800°C, the hexagonal phase (BiFeO3) was predominant. At the highest temperatures, 800°C and 850°C, a Bi- and O-deficient sillenite phase formed (Bi22Fe2O36) along with an orthorhombic phase (Bi2Fe4O9). At lower temperatures, Bi25FeO40 was the primary sillenite phase. Crystallite sizes ranged from ~50.6 nm – 65.8 nm for the hexagonal phase, ~73.2 nm – 86.8 nm for the sillenite phase. The orthorhombic phase only formed in significant amounts at 850°C and had a crystallite size of ~82.5 nm. The remnant magnetization at 300 K was 0.0507 emu/g for the sample calcined at 750°C.



Fabrication and Investigation of the Coupling Effect of Flexible PVDF-TrFE/Zinc Nickel Ferrite Nanocomposite Films Faruk Soso & Vjaya Rangari

Tuskegee University Alabama

Contact author: vrangari@tuskegee.edu

Thin flexible polyvinylidene fluoride – trifluoro ethylene (PVDF – TrFE) copolymer films were incorporated with ferromagnetic zinc nickel ferrite at different weight ratio of (1%, 3%, %5, and 10%) via magnetic staring and ultrasonication to ensure adequate dispersal of the nanoparticles in the matrix. The spin coating technique was used to produce quality void free films and the ZNF nanoparticles were prepared by the bead milling approach, using metal oxides and acetates as the precursors. The prepared nanoparticle powder was gradually calcined to 1000°C holding it for five hours at the rate of 10°C per minute. The structure, morphology, electrical, magnetic, thermal, and mechanical properties of the samples were characterized by XRD, SEM, LCR, VSM, TGA, and mechanical testing analyzer. The X-ray diffraction confirmed the incorporation of the crystallized nanoparticle and the ferroelectric polar Beta phase of PVDF-TrFE. Thermal analysis showed improved thermal properties as the increased nanoparticles were tailored on the films. The elastic modulus and dielectric properties of the film were studied showing significant improvement upon increased loading of the nanoparticles in the films. The magnetic properties of the synthesized ZNF films were studied showing magnetic saturation at room temperature. These interesting properties of ZNF/PVDF-TrFE lead to some switching actuation which signifies the films could be used in microelectronics.

# PREM Affiliation: University of Puerto Rico-Mayagüez - University of Wisconsin-Madison

#### PREM65

Study of the Effect of Surfactants on the Stability and Structure of Liquid Crystal Emulsions Stabilized with Nanoparticles under Static and Dynamic Conditions

Shaskya Y. Castaño-Castellar & Aldo Acevedo

University of Puerto Rico at Mayagüez Contact author: Shaskya.castano@upr.edu

Liquid crystal (LC) droplets show great promise as platforms for sensing applications of chemical or biological analytes and in controlled release delivery systems. Nevertheless, stabilization of the emulsions to retain the ordered arrangements and physical properties of LC is still a challenge. In this work, we evaluate the inclusion of ZnO nanoparticles to the stabilizing layer of LC emulsions and its interactions with three commercial surfactants: sodium dodecylsulfate (SDS), Triton-X, and dodecyltrimethylammonium bromide (DTAB). Emulsions were prepared by mixing from 5 to 20 v/v% of 5CB with previously prepared nanoparticle-surfactant complexes, glycerin and water. The stability of the complexes and emulsions under static and dynamic conditions was monitored by measuring interfacial tension using the pendant drop method, drop size distribution from optical micrographs, zeta-potential by dynamic light scattering, and steady-state shear viscosity with a rotational rheometer. Inclusion of the nanoparticles decreased the interfacial tension. While ZnO-DTAB combination was unable to stabilize the emulsions, those prepared with the SDS and Triton-X complexes showed a synergistic improvement of their stability at the lower LC content. Steady droplet size distribution and zeta-potential were observed for at least 30 days. In addition, the emulsions were able to sustain shear rates of up to 100 s-1 without showing signs of coalescence or thixotropic behavior.

# PREM66

Bimetallic Be/Cu Pillared-Layered Porous Coordination Polymer for Selective CO<sub>2</sub> Removal via Adsorption Alberto M. Tous-Granados¹, Juan C. Muñoz-Senmache¹, Rodinson R. Arrieta-Perez² & Arturo J. Hernández-Maldonado¹¹University of Puerto Rico at Mayagüez Campus, ²Universidad de La Sabana, Bogotá Colombia Contact author: arturoj.hernandez@upr.edu

The rational exploration of new chemical configurations within the structural confinements of porous coordination polymers (PCPs) continues to play a major role in developing novel functional adsorbents. In this respect, a bimetallic beryllium/copper [Cu2(pzdc)2(Be(pyac)2)]n [pzdc: pyrazine-2,3-dicarboxylate; Be(pyac)2: Bis[3-(4-pyridyl)pentane-2,4-dionato]beryllium(II)] pillared-layered PCP was synthesized for the first time. N2 (-196 °C) and CO2 (-78 °C) equilibrium adsorption data confirmed a microporous complex with a surface area of about 284 m2 g-1. A thermal gravimetric analysis showed that the PCP is thermally stable to about 250 °C. Moreover, in situ high-temperature powder X-ray diffraction showed that the metal—organic structure reversibly contracts or expands upon the presence of a guest species (i.e., water) or temperature. The bimetallic Be/Cu complex also displayed strong CO2-adsorbent interactions, evidenced by a larger heat of adsorption (41 kJ mol-1) compared to similar but monometallic PCPs. Furthermore, the Be/Cu PCP exhibited an ideal adsorbed solution theory (IAST) selectivity >60 for separating CO2/N2 (15:85) mixtures at 25 °C and 1 atm, which is higher than the values obtained for monometallic PCPs.



# PREM Affiliation: Universidad Ana. G. Mendez - University of Puerto Rico-Rio Piedras - Cornell High Energy Synchrotron Source

#### PREM67

Biotemplation of Titanium Dioxide Nanoparticles Using Oregano Ghost Leaf Wilnelia Barea Carrión & Lymari Fuentes Claudio
Ana G Méndez University, Cupey Campus
Contact author: wbarea1@email.uagm.edu

Dye Sensitized Solar Cells (DSSC) are an alternative for the energy crisis that we are confronting these days. Like many other options it has advantages such as being flexible and giving the opportunity of less expensive production. However, one of it disadvantages is the aggregation of the most common semiconductor used for the photoanode, titanium dioxide (TiO2). This project seeks alternatives to reduce the aggregation of TiO2 particles to improve dye adsorption and solar light harvesting on these devices. For this, the leaves of Plectranthus amboinicus (oregano) are used as soft biotemplates to control the synthesis of TiO2. This leaf provides a complex structure and different chemical components that could affect the physical-chemical properties of the nanoparticles. In order to understand the contribution of the components of the leaf on the resulting particles, the properties of TiO2 biotemplated with the whole leaf are compared with those of TiO2 particles biotemplate with a ghost leaf. The ghost leaf acts as a vessel for the synthesis of the particle without the presence of all the components of the whole leaf. The contribution of the components of the whole leaf are evaluated by comparing particle size, energy band gap, X-ray diffraction and surface morphology for both biotemplated samples.

#### PREM68

Angelica del Valle Universidad Ana G. Mendez-Turabo

#### PREM69

<u>Yannelly A. Serrano-Rosario</u> University of Puerto Rico, Rio Piedras

# PREM Affiliation: University of Central Florida - University of Washington

# PREM70

Observation of Flat Bands in Niobium Halide Semiconductor

<u>Alexis Jadiel Agosto</u><sup>1</sup>, Sabin Regmi<sup>1</sup>, Tharindu Warnakulasooriya Fernando<sup>2</sup>, Yuzhou Zhao<sup>2</sup> & Anup Pradhan<sup>1</sup>

<sup>1</sup>University of Central Florida, <sup>2</sup>University of Washington

Contact author: Alexi.Agosto@knights.ucf.edu

Kagome materials are potential systems for Dirac fermions and flat bands, which make them suitable grounds for the study of topology and electronic correlations in geometrically frustrated quantum materials. This study investigates the electronic structure of one such material, a niobium halide semiconductor, with a breathing kagome lattice of niobium atoms. We reveal the presence of multiple flat and weak dispersing bands, that are well captured in theoretical band calculations as well. Being a layered van der Waals material with a magnetic monolayer, this system will open up avenues toward the study of electronic correlations, magnetic order, and their interplay in two dimensions as well as toward its potential applications.

# PREM71

An Extensive Raman Study on Quantum Material Nb3Cl8: From Bulk to Thin Layers

<u>Dylan Jeff</u><sup>1</sup>, Favian Gonzalez<sup>1</sup>, Kamal Harrison<sup>1</sup>, Andres Pereira Bonilla<sup>1</sup>, Alex Agosto<sup>1</sup>, Yuzhou Zhao<sup>3</sup>, Tharindu Fernando<sup>3</sup>, Humberto R Gutierrez<sup>2</sup>, Madhab Neupane<sup>1</sup>, Jihui Yang<sup>3</sup>, Xiaodong Xu<sup>3</sup>, Ting Cao<sup>3</sup> & Saiful Khondaker<sup>1</sup>

<sup>1</sup>University of Central Florida, <sup>2</sup>University of South Florida, <sup>3</sup>University of Washington.

Contact author: djeff09@knights.ucf.edu

The Niobium halide (Nb3X8,X = CI, I,Br) family of quantum materials crystallize in a breathing Kagome lattice, a structure which allows for exotic electronical and magnetic properties to arise in the 2d limit. Amongst these properties, Nb3Cl8 features topologically flat bands in its electronic structure and has shown ferromagnetic orderings. Studies on the photon-phonon interactions in the material are lacking, therefore an extensive Raman experiment was performed to probe the material's vibrational modes as it is mechanically exfoliated from bulk crystal to thin layers. Bulk Nb3Cl8 crystals were grown via chemical vapor transport and characterized via x-ray diffraction and Raman spectroscopy. Polarized Raman experiment at different temperatures were carried out to study the material's vibrational modes and assign them to their respective symmetrical representations. Results from the layer-dependent study show phonon confinement effects in the Raman spectra of Nb3Cl8 evident from peak broadening and slight downshifting. Finally, excitation-dependent studies were performed to find excitation sources that are in resonance with the material. Through this, a thorough understanding of Nb3Cl8's phonons in the 2d limit was developed, laying the groundwork for future work involving the material and bringing forth new pathways for further research.



High Harmonic Generation from Epitaxial Zinc Oxide Films

<u>Troie Journigan</u>, Yangyang Liu, Christian Cabello, Tran Chau Truong, Dipendra Khatri, S Novia Berriel, Parag Banerjee & Michael Chini University of Central Florida

Contact author: michael.chini@ucf.edu

High harmonic generation (HHG) is a non-perturbative nonlinear optical process in which the interaction of an intense, low-frequency laser field with an atomic, molecular, plasma, or solid target results in the emission of ultrashort bursts of high-frequency photons. HHG from solid materials is linked to laser-driven electron trajectories in the lattice potential, and, as a result, the harmonic emission yields information on crystal properties such as electronic band structure, crystal symmetry, and polarization states [1-3]. Among solid targets, thin-film samples are especially attractive for HHG experiments, for both practical and scientific reasons. HHG in bulk materials has been shown to distort spectral features due to nonlinear propagation of the intense driving laser through the medium [4]. On the other hand, epitaxial growth of thin films on certain substrates can lead to crystal structural orientations and electronic states which are not accessible in bulk material [5]. In the two-dimensional limit, HHG in monolayer materials have revealed enhanced light-matter interactions and unique behavior associated with Berry curvature and valley polarization [6]. Hence, HHG in thin films is a promising platform for examining of new optical and electronic properties as well as improved understanding of the microscopic physics of HHG. In this study, we use intense, femtosecond, mid-infrared laser pulses to drive HHG in thin Zinc Oxide (ZnO) films grown epitaxially on R-plane sapphire substrates through plasma-assisted atomic layer deposition. In particular, we analyze the dependence of the film thickness and preparation on the harmonic spectrum. Most interestingly, we find that the as-grown ZnO films yield both even and odd harmonics, while annealed samples produce only odd harmonics. The generation of even harmonics can be attributed to broken inversion symmetry in the as-grown crystal, which yields an asymmetric response in the time-dependent polarization, while the generation of only odd harmonics indicates the loss of this asymmetry during the annealing process. Hence, our results indicate the presence of a polar phase in the as-grown samples, which is absent in the annealed films. We further study the dependence of the harmonic spectrum on the crystal orientation with respect to the laser polarization direction. We find that the annealed samples show an isotropic orientation dependence, with no preferred orientation with respect to the laser polarization, while as-grown samples exhibit periodic dependence on the polarization direction of the laser. The periodicity of both the even and odd harmonics is consistent with that of orientation-dependent measurements of HHG from bulk ZnO samples, thereby indicating that the as-grown samples have a similar structural symmetry to the bulk [1]. However, the isotropic response of the annealed samples suggest a structural transformation into a centrosymmetric form. To characterize the structural morphology of the films, we perform transmission electron microscopy (TEM) imaging of both the as-grown and annealed films. The TEM images of the as-grown samples indicate monocrystalline epitaxial growth of R-plane ZnO, while the annealed samples are consistent with a polycrystalline ZnAl2O4 spinel structure. Our combined HHG and TEM studies indicate that harmonic generation provides an all-optical technique to observe signatures of polarity as well as a method for distinguishing between monocrystalline and polycrystalline phases.

# PREM73

**Luis Tomar** 

University of Central Florida

# PREM Affiliation: University of Hawaii at Manoa - University of Washington

# PREM74

Modification of MgB $_2$  and CaB $_6$  through Ultrasonication for Gas Sorption Cecilia Abella, Isabella Kotsol & Godwin Severa University of Hawaii at Manoa

Contact author: cmabella@hawaii.edu

The harmful impacts of fossil fuels on the environment, including air and water pollution and greenhouse gas emissions, underscores the importance of transitioning to cleaner energy sources. Hydrogen is an ideal clean energy solution due to its high energy density, which is nearly three times that of diesel and gasoline. Hydrogen can be stored as compressed gas, cryogenic liquid or in solid state materials. The focus of this project is on developing solid state hydrogen carrier/storage materials, specifically metal borides of calcium and magnesium for hydrogenation to metal borohydrides. Due to their high gravimetric and volumetric density, calcium borohydride (Ca(BH<sub>4</sub>)<sub>2</sub>) and magnesium borohydride (Mg(BH<sub>4</sub>)<sub>2</sub>) serve as promising candidates for hydrogen storage applications. However, the hydrogen cycling of the metal boride/borohydride system is challenged by poor thermodynamics and kinetics at relevant conditions. Consequently, there is a need to broaden knowledge on syntheses of modified metal borides for hydrogenation to metal borohydrides at moderate conditions.

Ultrasonication technique is a viable method for creating modified nanostructured metal borides for hydrogenation to borohydride. Ultrasonication utilizes the principle of cavitation to disrupt the metal and boron bonding interactions within metal borides. In this work, modified MgB<sub>2</sub> and CaB<sub>6</sub> were prepared by direct tip sonication at 40% amplitude using a 22 KHz sonicator. Additives, such as morpholine and quinoline were utilized to assist in formation of the nanostructured, defected metal borides from the bulk borides. The best sonicated samples had the metal borides homogeneously suspended in the solvent, suggesting nanostructuring of the metal borides. Following sonication the products were dried in a vacuum oven and hydrogenated for 72 hours at 250°C and 120 bar. Results of the characterizations, using FTIR, TGA-DSC, and XRD, before and after hydrogenation will be presented.



Pressures Influence on Volume and Spin Crossover for Fe<sub>4</sub>(OAc)<sub>10</sub>[EMIM]<sub>2</sub> Ionic Liquid

Shelby Mitchell<sup>1,2,3</sup>, Ryan Beck<sup>5,6</sup>, Tian<sup>5,6</sup>, Edward Bruffey<sup>1,4</sup>, Phuong Nguyen<sup>1,3</sup>, Colleen Kelley<sup>1,4</sup>, Stella Chariton<sup>7,8,9,10</sup>, Xiaosong Li<sup>4,5</sup>, Godwin Sereva<sup>1,2,3</sup> & Przemyslaw Dera<sup>1,2,3</sup>

<sup>1</sup>University of Hawaii at Manoa, <sup>2</sup>MRE-C PREM, <sup>3</sup>Hawaii Institute of Geophysics and Planetology, <sup>4</sup>Hawaii National Energy Institute, <sup>5</sup>University of Washington, <sup>6</sup>MEM-C, <sup>7</sup>Argonne National Laboratory, <sup>8</sup>GeoSoilEnviro, <sup>9</sup>CARS, <sup>10</sup>University of Chicago.

Contact author: smitch22@hawaii.edu

We synthesized a novel iron(II) 1-Ethyl-3-methylimidazolium acetate ionic liquid compound, Fe4(OAc)10[EMIM]2. The Fe compounds contain Fe2+ octahedral chains that are coordinated by the acetate groups. The EMIM do not directly interact with the Fe2+, but instead contribute to the structural framework of the compound through van der Waals forces. The octahedral coordination arrangement is important, because it is most conducive to spin crossover (SCO). SCO occurs in octahedral transition-metal complexes with the electron configuration of 3d4 to 3d7. In Iron(II) complexes, SCO between the paramagnetic high-spin state and the diamagnetic low-spin state can be induced by temperature, pressure, light, and other stimuli. We investigated using pressure to induce a SCO.

We conducted a variable pressure single crystal synchrotron X-ray diffraction experiment with Fe4(OAc)10[EMIM]2 in Ne pressure transmitting medium. The experiment revealed a discontinuity in pressure-dependence of volume at 6.5 GPa, which indicates a volume expansion and is most likely associated with incorporation of Ne atoms into structural voids. Up to the 7.5 GPa, the highest pressure reached in the experiment, we did not observe a clear evidence of SCO. The experiment was complemented with a series of first principles Density Functional Theory calculations. Calculations were performed using the Vienna ab initio simulation program (VASP). The projector augmented wave method and Perdew-Burk-Erzerhof exchange correlation functional was used. The calculations confirm that the ambient state of the sample corresponds to a high-spin configuration of the iron ions. The DFT calculations were performed twice for a high spin and low spin electron configuration and indicate occurrence of SCO at 47 GPa, much above the range of pressure covered in the in situ XRD experiment. The unit cell volumes calculated using the high spin configuration agree well with the experimental data up to the volume expansion point.

#### PREM76

Low Temperature Solvothermal Synthesis of Calcium Hexaboride and Zirconium Diboride <u>Tracee Nguyen</u><sup>1</sup>, Ricardo Rivera<sup>2</sup>, Isabella Kotsol<sup>1</sup>, Brandi Cossairt<sup>2</sup> & Godwin Severa<sup>1</sup>

<sup>1</sup>Hawai'i Natural Energy Institute, <sup>2</sup>University of Hawai'i, Honolulu

Contact author: severa@hawaii.edu

Traditional synthesis approaches for metal borides, such as annealing and solid-state methods, require high temperatures to meet the high melting point of boron, making these processes energy inefficient and challenging to scale up. More recently, solution-based approaches have been introduced for the synthesis of transition metal borides, such as the synthesis of nickel boride using a modified polyol synthesis proposed by Schaefer et al. This work presents alternative solvothermal synthesis methods for calcium hexaboride (CaB6) and zirconium diboride (ZrB2). Under controlled temperature conditions, a metal precursor, such as calcium hydride or zirconium (IV) chloride was reacted with a borohydride salt, in attempts to form a metal boride, at temperatures below 350°C. The products of the solvothermal reactions are currently being characterized by a variety of techniques including x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and nuclear magnetic resonance spectroscopy (NMR). XRD shows only the presence of the anticipated chloride metal salts, suggesting that the metal boride phase is amorphous. The results of these characterizations and syntheses will be presented.

# PREM77

Synthesizing Printed CuInSe₂ for Thin-Film Technology Jade Paranhos Lopes & Nicolas Gaillard University of Hawaii at Manoa Contact author: jade.yards@gmail.com

Thin film solar cells is an emerging technology providing a cheaper alternative to commonly used monocrystalline silicon solar cells, and is consistently improving in efficiency. CuInSe2 ink (CISe) is used because of its high optical absorption, low toxicity, and optimum band gap of 1.0 eV for solar energy conversion. In order to reduce manufacturing costs, solution-based processing techniques are investigated in this communication.

In order to fabricate the solar cells, molybdenum (Mo) is first deposited onto a 1"x1" soda lime glass (SLG) substrate using RF magnetron sputtering. The CISe ink is then fabricated using thiourea, indium (III) chloride, and copper (I) chloride dissolved in HPLC grade methanol. This solution is spin coated 10 times onto the Mo-SLG substrates, and placed on a hot plate where methanol evaporates. Lastly, in order to crystalize the spin coated CISe precursor, samples are loaded into a vacuum furnace where they undergo selenization at high temperatures.

In order to further investigate the optimal ink properties of CISe, the Cu/In compositional ratio was altered. The typical 0.8 ratio used did not produce the expected photoluminescence data when investigated, in order to optimize the molecular ink 4 CISe samples were synthesized with ink ratios at 0.5, 0.6, 0.7, and 0.8. The results from this research will continue to improve the study for higher efficiency low-cost thin film solar cells.

# PREM Affiliation: University of Puerto Rico, Humacao & Cayey - University of Pennsylvania

#### PREM78

Topography and SERS Study of MagnetronSsputtering PVD of Ag Nanoparticles for Ultrasensitive, Large Area PlasmonicSsensor Joshua E. Chaparro Mata<sup>1</sup>, Edgard O. Díaz<sup>2</sup>, Gabriel García<sup>2</sup>, Camila Negrón<sup>1</sup>, Adrian Camacho<sup>2</sup>, Adam Alfieri<sup>3</sup>, Lorena C. Reyes<sup>2</sup>, Surrenda B. Anantharaman<sup>3</sup>, Deep Jariwala<sup>3</sup>, Erich Stach<sup>3</sup> & Francisco Bezares<sup>1</sup>

<sup>1</sup>University of Puerto Rico at Mayaguez, <sup>2</sup>University of Puerto Rico at Cayey, <sup>3</sup>University of Pennsylvania. Contact author: joshua.chaparro1@upr.edu

Ag nanoparticles have unique physical and chemical properties, which make them suitable for a wide range of applications in various fields, such as electronics, catalysis, biomedicine, and environmental protection. To grow these nanoparticles, magnetron sputtering physical vapor deposition (MSPVD) was used due to its relatively low costs, reliability, precision, as well as its flexibility. In particular, our experiments focus on the fabrication of large-area (wafer scale), ultra-sensitive, and highly reproducible Surface-enhanced Raman spectroscopy (SERS) sensors. 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. We leveraged this relationship to optimize SERS signal enhancements and performed TEM and SEM measurements to study the physical mechanisms underlying the deposition of the Ag nanoparticles. In particular, TEM images clearly demonstrate that more than one nanoparticle size distribution can result, depending on deposition time and/or substrate temperature. Furthermore, a comparative analysis was performed to determine which growth parameters give the highest SERS peak intensities. It was determined that the growth parameters can be easily tuned to produce large-area, ultra-sensitive sensors (106 enhancement factors), and a relationship to the physical and plasmonic properties was established. These results provide great insight into the physics governing the growth dynamics of MSPVD-fabricated nanoparticles and its relationship to their plasmonic and optical properties.

#### PREM79

DFT Calculations of Thin-Film SrFeO<sub>2.5</sub> and SrCoO<sub>2.5</sub>

<u>Gabriela Marrero Sánchez</u>, Yalexander Sanchez-Navarro & Juan A. Santana University of Puerto Rico at Cayey. Contact author: gabriela.marrero6@upr.edu

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 and thin-film SrFeO2.5 and SrCoO2.5 to study their OVCs ordering. The results from PBE+U show that OVCs in SrFeO2.5 will have perpendicular orientation under compressive strain and parallel under tensile. In the case of SrCoO2.5, OVCs will be parallel to the substrate under compressive and tensile strain.



Detection of Wells in Images of Paper Based 96-wells Plates

Emmanuel Rosa Delgado<sup>1</sup>, Gabriela B. Gómez Dopazo<sup>2</sup>, Renis J. Agosto Nieves<sup>2</sup>, Vibha Bansal<sup>2</sup>, José O. Sotero Esteva<sup>1</sup>
University of Puerto Rico at Humacao, <sup>2</sup>University of Puerto Rico at Cayey
Contact author: emmanuel.rosa2@upr.edu

During the last decade there has been a fast development of paper-based devices for chemical assays that, in combination with widely available image acquisition devices and data science techniques, replace other materials and sophisticated equipment thus increasing accessibility, and lowering costs and their impact to the environment. An example of such devices is the standard 96-wells plates. Devices reported in literature consist of well patterns made by transferring impermeabilizing waxes and/or polymers onto commercially available 2D paper. Recently our group reported new methods for producing 3D microwell paper-based plates. They are prepared using a cellulose acetate solution poured into a 3D printed template followed by a sequence of post treatment that includes impermeabilization of the whole plate. The wells may have conical and round bottomed shapes. A prototype of a computer dashboard also has been developed which is able to work in an efficient way towards the analysis of colorimetric assays using these paper-plates. The aim is to replace expensive analysis equipment and allow measurements in the field using computers as well as smartphones and tablets. The dashboard allows the user to load the image of a plate either by uploading a previously taken photo of the plate or by directly accessing the device's camera. In this work we present the successful implementation of methods for automatically detecting the paper-plate wells. It overcomes particular challenges posed by the use of hand-held cameras and paper-plates such as keystone and illumination effects as well as the curved shape that 3D paper plates often possess. It also eliminates the user intervention required for this task, or at least significantly reduces it, when compared to existing applications. The implemented process is as follows. First image segmentation is performed to extract the plate from the picture. The Sobel filter edge detection method is applied to a copy of plate image after preprocessing using a Multidimensional Gaussian Filter. Straight borders are inferred by applying minmax and least squares interpolation to coordinates. Then two strategies are used to detect wells. A reverse of the keystone correction of the plate is applied to the CAD design of the plate template and registered onto the plate image thus obtaining the coordinates of the borders of the wells. This strategy works best with relatively flat plates. A second strategy consists of finding circular shaped objects by applying a Hough transform after adjusting the contrast of a grayscale copy of the plate's image producing the coordinates of the center and radius of most of the wells. Missing wells are inferred by interpolation. This method works better for bent and/or irregular plates. Software used includes the Streamlit Python library for the dashboard and the SciPy, scikit-image, and OpenCV libraries for image processing. A custom function was programmed for the keystone correction.

# PREM81

Linking Pillararene and Hemicryptophane to Cellulose Purification Filters for Removal of Ions from Potable Water <u>Grace Sánchez</u><sup>1</sup>, Fabián González<sup>1</sup>, Aria Fodness<sup>2</sup>, Ivan Dmochowski<sup>2</sup> & Ezio Fasoli<sup>1</sup>

<sup>1</sup>University of Puerto Rico at Humacao, <sup>2</sup>University of Pennsylvania
Contact author: grace.sanchez3@upr.edu

Pillararenes (PA) and hemicryptophane are a new class of macrocycles that have drawn attention because of their host guest properties with a variety of inorganic and organic molecules. PA have been studied for their ability to encapsulate heavy metals and organic molecules within their aromatic rings. Hemicryptophanes have been found to host anions such as fluoride. The objective of this work is to functionalize a cheap, environment-friendly soft material (cellulose) with newly discovered macrocyclic compounds, 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. Hemicryptophane is currently under synthesis by linking cyclotriveratrylene (CTV) cap and tris(2-aminoethyl)amine (TREN) as the anion binding site. Cellulose matrix were functionalized with propargyl bromide and epichlorohydrin to create a linker for attachment of the macrocycles. The chemically modified membranes were characterized by FT-IR spectroscopy SEM microscopy. As an alternative approach PA were mixed at different w/w ratio with cellulose nanofibrils and immobilized on membranes. The different purification devices were tested for their ability to trap cations as well as organic pollutants.



# PREM Affiliation: University of Texas, Arlington - Northwestern University

#### PRFM82

Sub-Thermal Electron Transport in Silicon System at Room Temperature

Anthony Martinez<sup>1</sup>, Pushkar K. Gothe<sup>1</sup>, Ojas T. Bhayde<sup>1</sup>, J. Tyler Gish<sup>2</sup>, Vinod Kumar Sangwan<sup>2</sup>, M. R. Tiscareno<sup>1</sup>, Thevnin Rumende<sup>1</sup>, Michael P. Rabel<sup>1</sup>, Gumaro Garcia Gonzalez<sup>1</sup>, Adrian Gomez<sup>1</sup>, Jiechao Jiang<sup>1</sup>, Yi-De Liou<sup>1</sup>, Ye Cao<sup>1</sup>, Efstathios Meletis<sup>1</sup>, Mark C. Hersam<sup>1</sup>, Seong Jin Koh<sup>1</sup>

<sup>1</sup>The University of Texas at Arlington, <sup>2</sup>Northwestern University, Evanston

Contact author: anthony.martinez5@mavs.uta.edu

In solids at room temperature, electrons are thermally distributed over available states following the Fermi-Dirac statistics. This electron thermal smearing, however, is typically undesirable as it nullifies or degrades many novel electronic and spintronic phenomena. For example, the Coulomb blockade in single-electron transistors can be wiped out at room temperature unless the single-electron charging energy is made much larger than the room-temperature thermal energy. The electron thermal smearing is also the root cause of the excessive heat generation (or power consumption) of the currently most advanced transistors. Here we present CMOS-compatible device architecture that enables sub-thermal electron transport in a silicon-based system at room temperature. The device is composed of a stack of thin film layers on top of a silicon substrate, with layers of 50 nm Cr (source), tunneling barrier 1 (0.5-2 nm Al2O3 or 4 nm Cr2O3), 5 nm SnO2, tunneling barrier 2 (2 nm SiO2), and Si (drain). Electrons tunnel from Cr to SnO2 layer, then tunnel to Si. Current-voltage (I-V) measurements of the fabricated devices show abrupt current jumps, demonstrating sub-thermal electron injection to Si. The corresponding differential conductance (dI/dV) plots show extremely narrow widths in the differential conductance peaks. The full width at half maximum (FWHM) of the dI/dV peaks is as small as 0.025 mV, corresponding to an effective electron temperature of 0.08 Kelvin at room temperature. The I-V and dl/dV measurements were also carried out at low temperatures, down to 77 Kelvin. No changes in their I-Vs and dl/dVs were observed compared to the room-temperature measurements, indicating that the electron transport in the fabricated devices is not a thermally activated process. From transmission electron microcopy (TEM) analysis, we find that the microstructure of the SnO2 layer and the interface between Cr and SnO2 layers play a critical role in the observed sub-thermal electron transport. The ability to enable subthermal electron transport in a silicon system at room temperature may find many applications, such as transistors that can operate with extremely low energy consumption. This work was supported by the National Science Foundation (DMR-2122128, DMR-1720139, and ECCS-2031770).

# PREM83

Manuel Rodriguez

University of Texas, Arlington

# PREM84

Fast, Portable, and Sensitive Detection of Covid-19 Oligonucleotides Through Formation of Core-Satellite Plasmonic Nanostructures Hannah Umoeka<sup>1</sup>, Vineet Kumar Jayakrishnan<sup>1</sup>, Luis Dibert<sup>1</sup>, Anthony Martinez<sup>1</sup>, Chinmay Nitin Afzulpurkar<sup>1</sup>, Mileend Pankajbhai Sharma<sup>1</sup>, Vinod Kumar Sangwan<sup>2</sup>, Mark C. Hersam<sup>2</sup> & Seong Jin Koh<sup>1</sup>

<sup>1</sup>The University of Texas at Arlington, <sup>2</sup>Northwestern University, Evanston.

Contact author: hannah.umoeka@mavs.uta.edu

A method that enables a fast, portable, and sensitive detection of specific pathogens, such as Covid-19, would play an important role in ensuring public health and responding to public health emergencies. Currently, the polymerase chain reaction (PCR) or reverse transcription PCR (RT-PCR) provide very sensitive detection of specific sequences of DNA/RNA of pathogens. These methods, however, require a substantial amount of time (> 1 hour), trained personnel, and lab space, which are not desirable features in many circumstances. Here we present an approach in which specific sequences of oligonucleotides can be detected within 5 minutes on a small (6 mm by 9 mm) silicon or glass substrate. This is demonstrated using 67-mer oligonucleotides having Covid-19 sequence as a model system, with detection sensitivity reaching 500 fM. In our approach, target Covid-19 oligonucleotides are sandwiched between a 50 nm capture Au nanoparticle (C-AuNP) and 30 nm probe Au nanoparticles (P-AuNPs), producing a core-satellite nanostructure on a Si or glass substrate. The formation of core-satellite nanostructures is detected by the red shift of plasmonic resonance peak in reference to the plasmonic resonance peak of the control (no Covid-19 oligonucleotides). Our method realizes a fast detection of the Covid-19 oligonucleotides with a total hybridization time only 3 minutes. In addition, the relative absorbance of the red-shifted plasmon resonance peak is correlated with the concentration of the target oligonucleotides, enabling a quantitative detection of target oligonucleotides. The small footprint of the detection unit (6 mm by 9 mm) also allows pathogen detection in the field or large-scale detection of numerous samples at the same time. The ability of our method to provide fast (<5 min), sensitive (currently 500 fM), and quantitative detection of specific sequences of oligonucleotides, along with the small footprint (6 mm by 9 mm) of the detection unit, has the potential to be used to initially screen various pathogens in the field and could serve as an important tool to quickly respond to public health emergencies. This work was supported by the National Science Foundation (DMR-2122128, ECCS-2031770, and DMR-1720139).



# PREM Affiliation: University of Texas, Rio Grande Valley - University of Minnesota

#### PREM85

*Understanding Polymer Shear Profiles When Processed by Micro-Compounders*Narcedalia Anaya Barbosa<sup>1</sup>, Joshua Goetz<sup>2</sup>, Christopher J. Ellison<sup>2</sup> & Frank S. Bates<sup>2</sup>
<sup>1</sup>University of Texas Rio Grande Valley, <sup>2</sup>University of Minnesota
Contact author: narcedalia.anayabarbosa01@utrgv.edu

# \*Also presented at SB07.03.06, Apr 11, 2023, 5:00PM, Moscone West, Level 1, Exhibit Hall.

This research provides a better understanding of the rheological behavior of polyethylene at different processing conditions using the DSM Xplore 5 and 15 cc micro-compounders. Polymers used were high density polyethylene (HDPE) with a linear architecture, low density polyethylene (LDPE) showcasing a long chain branched structure, and linear low density polyethylene (LLDPE) exhibiting a short chain branched architecture. Measurements obtained in the micro-compounders were compared to those obtained with an ARES-G2 rheometer for a range of shear rates (50, 100, 150, 200 and 250 RPM), temperatures (150oC, 200oC), fill volumes (80%, 90%, 100%) and polymers. The measurements were used to evaluate the accuracy of the micro-compounders and scalability between the systems. Comparing the rheometer data and micro-compounder predictions can aid in identifying differences related to the polymer architecture and help to understand the impact of simple and extensional shear on the polymer when it is processed.

#### **PREM 86**

Production of Piezoelectric Structural Health Monitoring Sensor for Composite Structural Panels on Spacecrafts <u>Allan Cedillo</u> &Karen Lozano

The University of Texas Rio Grande Valley Contact author: allan.cedillo01@utrgv.edu

Companies such as Boeing and Airbus have transitioned from alloys to reinforced composites for structural panels on their aircrafts. Significant improvements have resulted from this transition such as weight reduction and improved mechanical/thermal resistive properties. As the positive outcomes of composites are notable, it is of interest to widen the use use of these materials in the aerospace industry. A challenge to overcome relies on the ability to implement Structural Health Monitoring sensors (SHMs) that can withstand harsh environments. The purpose of this project is to develop an SHM sensor to be mounted unto a composite panel and capable of converting it into a smart panel. The SHMs will be used as a form of a Nondestructive Testing technique to provide data on the condition of the component's structure while in service. The SHM sensor will be composed of polyvinylidene fluoride (PVDF) nanofibers blended with polydiacetylene (PDA). The fiber based membranes will be developed using the Forcespinning® technique. PVDF nanofibers have been reported to possess promising mechanical/thermal properties combined with attractive piezoelectric response, adding the PDA will result in enhancing the sensing ability by promoting a colorimetric response to applied temperature. This project is ongoing, currently the focus is on optimizing nanofiber production parameters. Multiple parameters are being tested and fibers analyzed using scanning electron microscopy. A compromise among fiber yield, fiber diameter and homogeneity of the system (lack of beads) is being considered during the optimization process. Once the ideal system is developed, thermal, electrical, and mechanical characterization will be conducted on the developed samples and under certain stimuli to evaluate sensing response. As adequate material property data is gathered the integration between the nanofiber system and composite structure will be designed.

# PREM87

Improving the Dispersion of Silicon/Silicon Dioxide Quantum Dots Adriana Chapa<sup>1</sup>, Kristine Q. Loh<sup>2</sup> & Vivian Ferry<sup>2</sup>

¹The University of Texas Rio Grande Valley, ²University of Minnesota Contact author: adriana.chapa03@utrgv.edu

# \*Also presented at EL07.05.02, Apr 12, 2023, 5:00PM, Moscone West, Level 1, Exhibit Hall.

Luminescent Solar Concentrators (LSCs) are devices that can generate renewable electricity and are composed of a transparent waveguide that is coated with a luminescent solution. Silicon Quantum Dots (Si QDs) are semiconductor nanocrystals that broadly absorb UV light and photoluminesce near-infrared light. Si QDs can suit LSC applications as they are nontoxic, are made from an abundant element, and have succeeded in renewable energy technology. We use nonthermal plasma to synthesize Si QDs, but as-synthesized, Si QDs have a high defect density. A silicon dioxide (SiO2) shell can protect the Si QD core and reduce the defect density. Unfortunately, Si/SiO2 nanoparticles still agglomerate due to the nonpolar silicon hydride and polar silanol surface groups that prevent dispersion in either polar or nonpolar solvents. This work focuses on developing a method for the Si/SiO2 QDs to stay in a stable, homogeneous mixture. This study varied different aspects of the dispersion by experimenting with different ligands, pH levels, and solvents. We characterized the solutions by using FTIR, UV-Vis, and PL spectroscopies. We concluded that using PEG-Silane as a ligand in an acidic environment with a polar solvent led to a stable, homogeneous mixture with a high photoluminescence intensity.

Improved Nanofiber Morphology Control & Higher Production Yield through Electro-Centrifugal Spinning Carlos A. Delgado, Arturo Fuentes & Horacio Vasquez

University of Texas Rio Grande Valley

Contact author: cdelgadoreyna98@gmail.com

An experimental setup for Electro-Centrifugal Spinning (ECS), relatively novel method of creating nanofibers, was created to take advantages of the benefits of both Electrospinning (ES) and Centrifugal Spinning (CS). The project seeks to maintain the high CS nanofiber production yields, while additionally incorporating ES benefits such as high alignment, fine diameter and low variability of overall diameters. Initial tests using an Electro-Centrifugal Spinning (ECS) machine were conducted using PEO and DI H2O. SEM characterization of the produced fibers with different processing parameters (e.g., rotational speed and electric field voltage) are presented. Initial ECS experimental results show great potential for improved nanofiber morphology control and higher production yields.

#### PREM89

Role of Solvent Composition During Processing of Stimuli-Responsive PNIPAM/Silyl Methacrylate Copolymers Fabian A. Rodríguez<sup>1</sup>, Jason D. Linn<sup>2</sup>, Diana Y. Zhang<sup>2</sup>, Michelle A. Calabrese<sup>2</sup>

<sup>1</sup>UTRGV, <sup>2</sup>University of Minnesota

Contact author: fabian.rodriguez05@utrgv.edu

# \*Also presented at EL03.04.01, Apr 11, 2023, 5:00PM, Moscone West, Level 1, Exhibit Hall.

Electromagnetic radiation from the sun can produce changes in the internal temperatures of infrastructures. Offsetting this increase in temperature requires greater energy consumption. Therefore, the use of smart glass windows has increased as these windows restrict the passage of solar radiation that enters through exterior windows. Despite these favorable qualities, implementation of smart windows is limited due to high production and installation costs. Typically, smart windows are pretreated and requires standard windows to be replaced. Cost, therefore, becomes a barrier for businesses, schools, or individuals who are seeking to implement a green, energy efficient, alternative. To circumvent these costs while still meeting demands for greater energy efficiency, thermosensitive polymer coatings have been proposed as an alternative to traditional smart windows such as thermal glazes or hydrogel laminates.

In this study, poly(N-isopropylacrylamide-co-3(trimethoxysilyl)propyl methacrylate copolymer (PNIPAM -co-TMA) has been studied as thermal-responsive glass coatings due to optical properties stemming from thermally reversible phase changes. These phase changes result from the abrupt coil-to-globule transition where aqueous solutions shift from clear to opaque with increasing temperature. The thermoresponsive behavior of PNIPAM is favorable for sprayable smart window coatings for their ability to filter out light and heat from solar radiation. However, the presence of TMA, which allows PNIPAM coatings to bind to glass substrates, can lead to irrecoverable opacity due to crosslinking within the copolymer chain. Cloud point testing was utilized to characterize the optical response of PNIPAM-co-TMA over several thermal cycles as irrecoverable transmittances can be observed when the TMA crosslinks within the copolymer chain. However, systems composed of 95% mol of water and 5% mol of DMSO were able to recover their original clarity across various concentrations of TMA. These results are significant because co-nonsolvency allowed access to the collapsed, opaque, state using solvent mixtures instead of temperature. This may be advantageous for coating processes. Various co-nonsolvent systems were processed into coatings through either spin or drop coating. Finally, contact angles at 23C and 60C were collected for a coated slide. At room temperature, below the cloud point temperature, the coated slide had a contact angle of approximately 21 degrees. When the coated slide was heated to 60C a contact angle of 52 degrees was measured. These results verify that the PNIPAM-co-TMA solution maintains the characteristic hydrophobic phase change after the coating grafts onto the glass and subsequently permits this research to impact the use of polymer responsive coatings to improve energy efficiency.



Cellulose/Chitosan Composite Aerogel Based Triboelectric Nano-generator for Harvesting Mechanical Energy Shadman Sakib, André Ramos, M. Jasim Uddin University of Texas Rio Grande Valley

 $Contact\ author: shadman.sakib 01@utrgv.edu$ 

# \*Also presented at SB09.09.12, Apr 13, 2023, 5:00PM, Moscone West, Level 1, Exhibit Hall.

In our triboelectric layers high charge density is desired. This can be achieved with a combination of high surface area (provided by porous nano fiber mats) and dopants with high electropositive and high electronegative charge affinities. The high electronegative charge is desired for the alginic acid to promote the formation of the gel-like film and could be strengthened with calcium ions to allow the cross linking between the ions and the alginic acid. We envision the sliding contact to be the main method for charge generation in this context. The high structural strength and flexibility will be provided by a porous, flexible aerogel/xerogel complex matrix structure. Medical applications for these TENGs are the goal of this research, the fruits of this research will go into producing TENGs for small medical devices which would otherwise have to be charged or be powered by external batteries which currently makes them expensive and impractical. Expecting mothers with high-risk pregnancies have a big concern with their fetuses, and every minute counts, especially when it comes to them. For these exceptional cases, a way to constantly monitor vital signs for their fetuses is crucial especially if something happens and there is a need for corrective action or a physician intervention. Our device would be flexible, safe, and accurate to be embedded in everyday garments and used as a self-powered tool to monitor their fetus's health in real time and be able to alert the mother when things are starting to get serious and there is an urgent need for medical attention.

# PREM91

Manufacturing of Advanced Piezoelectric Nanogenerator by Functionalizing PVDF with LiTaO<sup>3</sup> and Multiwalled Carbon Nanotubes (MWCNTs) for Energy Harvesting and Sensing Applications

Islam Uddin Shipu, Adrian Portales, Rigobert Ybarra, Mohammed Uddin & Karen Lozano

University of Texas Rio Grande Valley

Contact author: <u>islamuddin.shipu01@utrgv.edu</u>

# \* Also presented at EL08.08.05, Apr 12, 2023, 5:00PM, Moscone West, Level 1, Exhibit Hall.

One of the freely available green energy sources that might be used to satisfy the small-scale energy need is mechanical energy. In order to capture mechanical energy, power the next generation of electronic gadgets, and health monitoring flexible piezoelectric nanogenerators made of light weight polymers and carbon nanotubes have drawn a lot of attention. Lithium tantalate (LiTaO³) nanoparticles were prepared and utilized to create a flexible piezoelectric nanogenerator (FPNG). A compact piezoelectric nanogenerator that successfully transfers mechanical energy into electricity was then created using lightweight polyvinylidene fluoride (PVDF), multiwalled carbon nanotubes (MWCNTs), and LiTaO³ nanoparticles. To create a piezoelectric composite film, LiTaO³ nanoparticles were first prepared and loaded into poly vinylidene difluoride (PVDF) and multi-walled carbon nanotubes (MWCNTs). This piezoelectric composite film was then placed between two copper electrodes to create an flexible piezoelectric nanogenerator (FPNG). It was thoroughly examined and adjusted how the concentration of LiTaO³ injected into PVDF and MWCNT affected the electrical performance of FPNG. 1.5%, 2.5%, 3%, and 5% LiTaO³ were used to manufacture the flexible piezoelectric films and then the films' XRD, XPS, SEM characteristics were analyzed as well as the voltage and current were measured. Open-circuit voltage and short-circuit current measurements for the 3 wt% FPNG were ~9V and ~60nA respectively. The nanogenerator was further put to the test by combining it with common electronic parts including capacitors, bridge rectifiers, and 10 LEDs. By transforming human walking force into energy, multiple piezoelectric films can light a room even without electricity. The FPNG was used to harness diverse biomechanical energy. This FPNG was also employed as a sensor for in vitro and in vivo biological applications such as blood flow, respiration, and muscle contraction.



Enhancement of PTFE-PVA Triboelectric Effect with Multiwall Carbon Nanotubes Coating Fernando Viesca, Diego de León, Jasim Uddin

University of Texas Rio Grande Valley

Contact author: fernando.viesca01@utrgv.edu

With the increased demand of energy brought by a developing society, an increased need for alternative energy solutions becomes important. Triboelectric nanogenerators (TENGs) have emerged as a promising solution for energy generation in small electronic devices. Improving the surface charge energy is essential to increase the electrical output performance of TENGs. In this study a TENG consisting of Forcespinning® (FS) Polytetrafluoroethylene nanofibers (PTFE-NFs) and Forcespinning® (FS) Polyvinyl alcohol nanofibers (PVA-NFs), as the negative and positive layers respectively, were fabricated. A modification to the PTFE-NFs were made by coating the surface of the PTFE-NFs with multiwall carbon nanotubes to generate higher electrical output. Multiwall carbon nanotubes (MWCNTs) were dispersed in a deionized water solution using three different surfactants: Sodium Dodecyl Sulfate (SDS), Sodium dodecylbenzenesulfonate (SDBS), and Triton X-100 (TX-100), then the dispersions were analyzed. PTFE-NFs were submerged into the dispersion for 24 hours to coat the surface of the NF mat and increase the electrical output, like voltage. A 25.4 x 25.4 mm2 PTFE-NFs/PVA NFs TENG device was created by using 3D Stereolithography (SLA) technology, where a simple spring contact separation system was selected. Thin copper foil was used as electrode for both nanofiber mats. PTFE-NFs were characterized using a Scanning Electron Microscope (SEM) and X-Ray Diffraction (XRD). The electrical performance was characterized using an oscilloscope with the addition of a potentiometer.

# PREM Affiliation: University of Texas, Rio Grande Valley - University of Minnesota

#### PREM93

Solid Polymer Electrolytes from Branched Phosphonium Ionenes with Elastomeric Properties Jazzniah Compton<sup>1</sup>, Hongyi Zhang<sup>2</sup>, Nicholas Boyton<sup>2</sup> Stuart Rowan<sup>2</sup> & Asem Abdulahad<sup>1</sup> <sup>1</sup>Xavier University of Louisiana, <sup>2</sup>University of Chicago Contact author: jcompton@xual.edu or aabdulah@xula.edu

Solid state lithium metal batteries are largely regarded as a safer alternative to traditional lithium-ion batteries that also have higher theoretical energy densities due to the solid lithium anode. However, realizing the full potential of lithium metal batteries requires a solid electrolyte that has ionic conductivity, high lithium cation transference, and sufficient mechanical properties. This research presents the synthesis and characterization of elastomeric hyperbranched phosphonium ionenes that incorporate organic ionic plastic crystals. Elastomeric hyperbranched phosphonium ionenes were polymerized by a modified Menshutkin reaction where the phosphino groups of 1,4-bis(diphenylphosphino)butane (f = 2 monomer) were reacted with 2,2-bis(((6-bromohexanoyl)oxy)methyl)propane-1,3-diyl bis(6bromohexanoate) (f = 4 branching monomer). Thermal analysis of these hyperbranched phosphonium ionenes showed that they have glass transition temperatures less than 0 °C and degradation temperatures of approximately 200 °C. Comparatively, hyperbranched phosphonium ionenes prepared by the A2 + B3 step-growth polymerization of 1,4-bis(diphenylphosphino)butane with 1,3,5tris(bromomethyl)bromide produced covalent networks with much higher glass transition temperature (>100 °C) and degradation temperatures (>300 °C). Despite their reduced temperature stability, the elastomeric branched phosphonium ionenes showed higher ionic conductivity. This is likely due to increased segmental motion suggested by their significantly reduced glass transition temperature as measured by differential scanning calorimetry. Ongoing work on these promising solid polymer electrolytes includes doping the elastomeric branched phosphonium ionenes with organic ionic plastic crystals (OIPCs) along with lithium-based salts. OIPCs are expected to further enhance the ionic conductivity. OIPC-doped phosphonium ionenes will be characterized for their ionic conductivity, lithium transference number, and charge/discharge properties in coin cell batteries.

# PREM94

<u>Ayssia Crockem</u> Xavier University of Louisiana



Optimizing the Formulation of a 3D-Printable Resin for Producing Ionic Liquid Based Gels Through Additive Manufacturing Kirsten Grant, Isaiah Washington, Meghan Mouton, Ai-Nhan Au-Duong & Asem Abdulahad Xavier University of Louisiana

Contact author: kgrant3@xula.edu

lonic liquids have been investigated for their utility as components in ion conductive electrolytes for lithium-ion batteries and for their ability to adsorb small molecule gases such carbon dioxide. Therefore, efficient and reproducible means of producing viable materials that are capable of incorporating large amounts of ionic liquid is of significant research interest. This project concerns the rapid preparation of ion gels using additive manufacturing by 3D-printing. Photo-curable resins that can be used as 3D-printable resins are appealing because of the reproducibility and rapid material synthesis that 3D-printing offers. 3D-printable resins comprised of butyl acrylate, 2-hydroxyethyl methacrylate, 1,6-hexanediol dimethacrylate crosslinker, and diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide (TPO) photo-initiator were used to prepare a 3D-printable resin. 1-Ethyl-3-methylimidazolium ethyl sulfate was incorporated to determine the structure property relationships of the 3D-printable resin as a function of ionic liquid incorporation. In addition, crosslinking density was varied by changing the percent incorporation of the 1,6-hexanediol dimethacrylate crosslinker. With 3D-printing times of less than 30 minutes, the formulated resins produce 3D-printed materials with elastomeric properties whose properties depend on crosslinking density. For example, thermal analysis using differential scanning calorimetry reveals that the glass transition temperature at 20 % crosslinker is 19.75 °C, and increasing the crosslinker to 40 % of the formulation by mass increases the glass transition temperature to 30.74 °C. Ongoing work includes expanding the 3D-printable monomers with larger pendant groups such as ethylhexyl methacrylate instead of butyl acrylate. It is anticipated that incorporating larger monomers will increase the free volume within the cured film to result in improved elastomeric properties.

# PREM96

Synthesis and Characterization of Solid Polymer Electrolytes From Partially Fluorinate poly(silyl ethers)

<u>Trinity Hixson-Wells</u>, Briya Kirksey<sup>1</sup>, Ai-Nhan Au-Duong<sup>1</sup>, Chibueze Amanchukwu<sup>2</sup> & Asem Abdulahad<sup>1</sup>

<u>Xavier University of Louisiana</u>, 2University of Chicago

Contact author: aabdulah@xula.edu

Current lithium-ion batteries rely on a flammable, liquid-based electrolyte that limits the lifetime of the battery and has the potential to explode when the battery casing is punctured. Towards improving safety and increasing their energy density, lithium metal batteries that employ a solid lithium anode and a solid polymer electrolyte (SPE) are of significant research interest. Current state-of-the-art SPEs have a limited voltage range of operation up to 4 V and many of the synthetic approaches to prepare polymers for SPEs lead to structures that include reducible double bonds. This study focuses on the synthesis and characterization of fluorinated poly(silyl ethers) with no double bonds. The synthesis of fluorinated poly(silyl ethers) in this study begins with the synthesis of fluorinated diallyl monomers 1,4-bis(allyloxy)-2,2,3,3-tetrafluorobutane, 1,6-bis(allyloxy)2,2,3,3,4,4,5,5-octafluorohexane. Diallyl monomers based on the ether repeat unit of poly(ethylene glycol) (PEG) which is known to solubilize and transport Li+ cations with high efficiency were also prepared. Specifically, 1,2bis(allyloxy)ethane, 3-(2-(2-allyloxy)ethoxy)prop-1-ene, and 4,7,10,13-tetraoxahexadeca-1,15-diene were prepared from the reaction of allyl bromide with ethylene glycol, diethylene glycol, and triethylene glycol, respectively. The successful synthesis of each monomer was confirmed by chemical characterization using 1H NMR and FTIR at product yields of >70 %. Subsequently, high molecular weight random copolymer poly(silyl ether)s were prepared by reacting the diallyl monomers with 1,1,3,3,5,5-hexamethyltrisiloxane in the presence of a platinum catalyst, where the polymer composition was varied by controlling the monomer feed ratio of the fluorinated diallyl monomers to the diallyl ether monomers. Currently, these unique Li+ conducting polymers are under investigation for their thermal properties. Also, electrochemical characterization reveals that the ionic conductivity and lithium transference number depend on the percent incorporation of the ether monomers.

# PREM97

<u>Kutemwa Masafwa</u> Xavier University of Louisiana

