13TH ANNUAL UNDERGRADUATE RESEARCH SYMPOSIUM

AUGUST 1, 2024 | 1:30 - 3:30 PM

ENGINEERING AND SCIENCE BUILDING LOBBY

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Welcome to the 2024 Undergraduate Research Symposium!

REU Students, Mentors, and Friends,

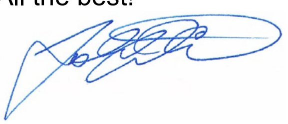
I am delighted and thrilled to extend my warmest welcome to the 13th Annual VINSE REU Poster Session and Concluding Banquet. This year has been nothing short of exceptional, thanks to the remarkable dedication and hard work of our talented REU students. Throughout the summer, we've enjoyed wonderful outings and social gatherings, fostering friendships that we hope will last a lifetime.

The VINSE REU program remains committed to equipping undergraduate students with the skills and creativity needed to excel as nanoscience and engineering researchers on a global scale.

Having run for 13 years, the VINSE REU program continues to thrive. I am honored to serve as Director for the next two years and look forward to collaborating with you in identifying the next cohort of outstanding students for this incredible opportunity.

Thank you once again for joining us, and we hope you thoroughly enjoy the celebrations ahead!

All the best!



Josh Caldwell

1. Brennah Kennedy *Bucknell University* VINSE NSF-REU
2. Aria Mingo *Cornell University* Chemical Biology NSF-REU
3. Claire Bougere *Louisiana State University* VUSE Summer Research Program
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8. Fiona Power *University of Miami* VUSE Summer Research Program
9. Grace Heilmann *University of North Carolina, Greensboro* Chemical Biology NSF-REU
10. Tianqi Sun *Georgia Institute of Technology* VUSE Summer Research Program
11. Jenna Jang *Vanderbilt University* VINSE Tech Crew
12. David Alejandro Flores Nasser *Pennsylvania State University* VINSE NSF-REU
13. Cait Bradley *Oglethorpe University* Chemical Biology NSF-REU
14. Kissamy Georges *University of Massachusetts, Dartmouth* VINSE NSF-REU
15. Thaissa Peixoto *Johns Hopkins University* VUSE Summer Research Program
16. Vivian Ma *Vanderbilt University* VINSE Tech Crew
17. Nicholas Gray *West Chester University* VINSE NSF-REU
18. Allison Portaro *University of Louisville* Chemical Biology NSF-REU

19. Kendall Kelly *University of Mississippi* VINSE NSF-REU
20. Carisa Lynch *Florida International University* VUSE Summer Research Program
21. Rafael Antonio Rodas Aguilar *Vanderbilt University* VINSE Tech Crew
22. Elvis Daniel Perez Galarza *Western Carolina University* Chemical Biology REU
23. Angelica Velasquez *University of Connecticut* Chemical Biology NSF-REU
24. Kaitlyn Kelly *University of Florida* VUSE Summer Research Program
25. Elliott Ballino *University of Scranton* Chemical Biology NSF-REU
26. Lisa Sebastian *Rose-Hulman Institute of Technology* VINSE NSF-REU
27. Tuong (Kathleen) Nguyen Dinh Cat *Franklin & Marshall College* VU Intern
28. Montana Price *Volunteer State Community College* Chemical Biology NSF-REU
29. Priya Soma Mathiy *Pennsylvania State* VUSRP
30. Erica Hengartner *University of Florida* Chemical Biology NSF-REU
31. Gladys Martinez Franco *California State Polytechnic, Pomona* VINSE NSF-REU
32. Ndi Winston Nfor Kanjo *Vanderbilt University* VINSE Tech Crew
33. Margaret Marte *Clemson University* VINSE NSF-REU
34. Noah Durlam *Valparaiso University* VINSE NSF-REU
35. Allison Wightman *Grinnell College* Chemical Biology NSF-REU
36. Dhemi Mislenkov *Saint Mary's College & University of Notre Dame* VUSE
37. Yukie Chang *Pomona College* VUSE Summer Research Program

1 | Brennah Kennedy | VINSE REU

Tunable Polaritonic Heat Conduction Through Modulating Metal Concentration in the Polariton Launcher

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Launching of phonon polaritons (PhPs) has been shown to improve the thermal conductivity of silicon carbide (SiC) nanowires by coating one or both ends of the wire with gold. However, this method, though effective, is challenging to replicate consistently. Using a standard electron beam-induced deposition (EBID) method, which allows for the local deposition of a platinum (Pt) and carbon (C) mixture, offers a more approachable way to launch PhPs as compared to the gold coating method. While the Pt/C mixture has been used in some studies for launching PhPs, its launch efficiency is yet to be explored. Here, we report on the effect of Pt concentration on the PhP launching efficiency of Pt/C mixtures and the resulting tunable thermal effects in SiC nanowires. First, by varying the EBID current, Pt weight percent concentrations between 28.24 and 67.14 were achieved, resulting in a limited range of Pt concentrations with a low saturation point. Therefore, to further improve the Pt concentration, a thermal annealing recipe was developed by adjusting the temperature and annealing time in an ambient ceramic oven. In this process, the carbon residue in the mixture gets vaporized and oxidized, which increases the Pt concentration to a maximum of 92 % (wt). In the end, thermal measurements of SiC nanowires with different configurations were carried out to estimate the thermal effects from EBID with different Pt concentrations. Results show a higher PhP thermal conductivity (kPhP) as the Pt concentration increases. The above findings contribute to developing a new PhP launching mechanism for heat conduction enhancement in polar solids.

Bio. Brennah Kennedy, a student in the 2026 class at Bucknell University, is majoring in Electrical and Computer Engineering with a concentration in Sustainable Energy and a minor in Environmental Studies and Sciences. She is particularly passionate about using her electrical engineering skills in conjunction with other disciplines to contribute to developing renewable energy resources. In the summer of 2023, Brennah completed research in curricular development and is currently involved in semester research focused on piezoelectric technology in pavement for energy harvesting applications in Palestine. She was accepted into VINSE REU's 2024 summer research program, where she is working in the Nanoscale Transport Phenomena Laboratory overseen by Dr. Deyu Li. Her research includes interdisciplinary aspects in mechanical engineering with a focus on thermal transport in nanowires via launching phonon-polaritons in microelectronics. Outside of research, she dedicates her time to starting and organizing clubs, like the Grand Challenge Scholars Program. This club helps enrich sustainability's presence on her campus while promoting professional and personal development in students. With her interests ranging from energy efficiency, renewable technology, and materials sciences to power electronics, she plans to pursue a Ph.D. and ultimately work at the National Renewable Energy Laboratory in Colorado.

Human Milk Oligosaccharides Ameliorate Nosocomial Infections as Protective Coatings

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Increasing rates of morbidity and mortality within hospitals are caused by pathogenic bacteria colonizing indwelling medical devices. This abiotic surface adherence is caused by the ability of bacteria to form biofilms. Bacterial biofilms are three-dimensional communities of microorganisms surrounded by a self-produced extracellular polymeric matrix. Bacterial biofilms confer increased resistance to antibiotics, resulting in invasive infections among immunocompromised patients. Human milk oligosaccharides (HMOs), the carbohydrate component of human breast milk, are known to promote growth of commensal bacteria while inhibiting the growth of pathogenic bacteria in the infant gut. Recent studies have shown that outside the neonate, HMOs have both antibacterial and biofilm-inhibiting properties. With this in mind, we employed HMOs as anti-adhesive coatings against various pathogens to assess abiotic bacterial adherence to various materials. HMOs were used to reduce bacterial adhesion on surfaces imitating those most commonly populated by nosocomial pathogens, including catheters, prostheses and pacemakers, among others. The ESKAPE pathogens (Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa and Enterobacter species) exhibit high antibiotic resistance and are responsible for 15.5% of hospital-acquired infections. Plastic surfaces (24-well plate base) and glass surfaces (glass coverslip) were exposed to HMOs for 12 hours. After the solution evaporated, bacterial cells were added to the surfaces and incubated. The next day, bacterial density (OD_{600}) and biofilm formation (OD_{560}) were spectrophotometrically determined. While HMO treatment did not elicit any changes in bacterial density, significant decreases in bacterial adherence were observed across strains assessed in this study. The results indicate that the addition of HMOs reduces the adherence of both gram-negative and gram-positive bacteria on both plastic and glass surfaces. This research highlights the potential for HMOs as protective coatings on indwelling medical devices to mitigate the spread of hospital-acquired infections.

Bio. Aria Mingo is a senior at Cornell University, majoring in Chemistry and minoring in Earth and Atmospheric Sciences. Under the mentorship of the Ober Group, she has conducted research focusing on polymeric additions to various transition metals and studying polymer-grafted nanoparticles (PGNs). In addition to her academic pursuits, Aria has worked as a Scribe at a medical center, gaining practical experience in healthcare documentation. She also served as a student intern at Argonne National Laboratory through Washington State University, where she contributed to the design of a copper precision target for laser analysis. Currently, Aria is interning at Vanderbilt University within the Townsend Lab, investigating the antimicrobial and antibiofilm properties of human milk oligosaccharides (HMOs).

Preparation of 3D-printed cell-laden hydrogels for analysis with imaging mass spectrometry

Claire Bougere[1], Margarita Orlova[4], Leon Bellan[2,4], Eric Spivey[2,3]
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[2]*Department of Biomedical Engineering, Vanderbilt University*
[3]*Vanderbilt Institute of Integrative Biosystems Research and Education*
[4]*Department of Mechanical Engineering, Vanderbilt University*

This project aims to identify and characterize different cell types when embedded in 3D-printed hydrogel structures using imaging mass spectrometry (IMS). For this research, HEK-293 cells expressing a histone H2B protein tagged with mCherry and Caco-2 cells modified to constitutively express green fluorescent protein (GFP) were the chosen cell types. Gelatin methacrylate (GelMA) was used to suspend the cells and formulate the hydrogel structures through 3D bioprinting with a CELLINK BIO X6 printer and temperature-controlled printheads. A confocal microscope was used to image the hydrogel structures and determine if the cell types were distinguishable by fluorescence after 3D printing. To prepare for IMS, the hydrogel structures were embedded in a mixture of fish gelatin and carboxymethylcellulose, cryogenically frozen, sliced, placed on indium tin oxide-coated glass slides, and coated with a chemical matrix. IMS was then used to identify and distinguish between the two cell types in the prepared sample. After optimizing the procedure and bioprinting the cell-laden structures, confocal microscopy confirmed the presence of the two cell types in specific locations within the GelMA structures. Matrix-assisted laser desorption/ionization (MALDI) IMS will further characterize the 3D-printed structures by providing a profile of small molecules, such as lipids and metabolites, for each examined cell in the sliced samples. The results of this research may have promising implications for improving analytical methods for studying cells embedded in 3D-printed structures. The results of this research will also support future research on fabricating and analyzing a microphysiological system that provides a functional model of simple, defined neural circuits.

Bio. Claire Bougere is a rising senior pursuing a Bachelor’s degree in Biological Engineering at Louisiana State University (LSU). She works in an on-campus biomedical engineering laboratory, where she primarily practices cell culture and protein analysis. She is a member of the LSU Ogden Honors College and has received the LSU Communicator Certificate. Claire is doing research at Vanderbilt University for Summer 2024 as a participant in the Vanderbilt University School of Engineering Summer Research Program.

4 | PARKER FRIEDLI | VINSE Tech Crew

Determining the Impact of Angled vs. Flat Sample Mounting in High-Density Feature Patterning

Parker Friedli[1], *Christina McGahan[2]*
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From hair-thin electrodes to optical metasurfaces for manipulating light, nanoscale devices often incorporate specifically patterned thin film coatings of various materials to enable specific functionalities. These patterned devices are fabricated through a sequence of lithography, thin-film deposition, and liftoff processes to pattern the desired film on a substrate. In the deposition chamber, angled sample mounting fixtures (angle plates) can benefit the liftoff process by enabling better pattern definition due to an improved line-of-sight compared to a flat plate. However, the increased complexity and time required for sample setup and deposition using an angle plate must be considered against potential improvements in final device performance. This work investigates the impact of angled vs. flat sample mounting on the quality of high-density feature patterning for nanoscale devices. After patterning silicon chips, film stacks of variable thicknesses (30-100 nm) and materials (Al, Ti-Au) were deposited using both flat and angled sample configurations. A general liftoff procedure was completed following deposition, and the resulting patterns were analyzed using image analysis software for successful liftoff of unwanted material. Preliminary results indicate samples where the flat plate was used are more likely to erase desired features during liftoff for films less than 100 nm thick. However, aside from the mentioned trend of erasure, there was no statistically significant advantage to using the angled plate compared to the flat plate with the features and densities tested. Thus, further testing should be completed with different patterns/feature densities and photoresist film thicknesses. The findings from this work will guide users in selecting the optimal deposition approach, considering the tradeoffs between setup complexity and the improved performance enabled by angled mounting.

Bio. Parker Friedli is a third-year at Vanderbilt University majoring in Mechanical Engineering. She joined the Tech Crew of Vanderbilt Institute of Nanoscale Science and Engineering (VINSE) in the Fall of 2023 to learn more about emerging nanotechnology fields, with a particular interest in nanofabrication, and the creation of nano electro-mechanical devices. Her cleanroom specialty lies in deposition and photolithography processes. She enjoys learning about others' research and helping out in the cleanroom whenever needed.

Computational Screening of Perovskite Oxides for Reversible Cl/Cl- Redox Reactions in Batteries

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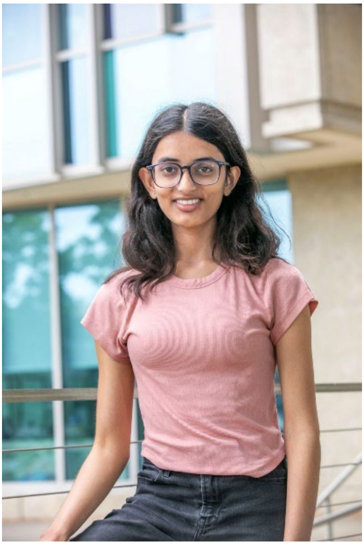
[2]Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, USA;
[3]Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, USA;

Currently, lithium-ion batteries are the gold standard in energy storage, and can commonly be found in devices from cell phones to electric vehicles. However, there is a research interest in alternatives such as Cl/Cl- anion redox batteries that could offer higher capacity. In order to solve a problem with current chloride-ion batteries, in which gaseous chlorine escapes, this project investigates the adsorption of chlorine onto perovskite oxide materials to find electrodes that can prevent chlorine evolution. VASP (Vienna Ab initio Simulation Package) was used to perform DFT (density functional theory) calculations on a variety of perovskites of the form $SrBO_3$, with B representing first-row transition metals. First, bulk and surface optimizations were performed on each perovskite. A geometric optimization was also performed on Cl_2. Additionally, the DFT+U correction was employed in order to account for the strongly correlated d electrons present in these perovskite oxides. Adsorption was investigated at the top, bridge, and hollow sites of the transition metals. Strength of adsorption between chlorine and the transition metal have been examined. However, the interaction between the chlorine atom and the transition metal has not been clearly examined. Thus, future work exploring the electronic structures is necessary to understand the main descriptors for the chlorine-metal interaction. Additionally, future work may focus on adsorption onto other atoms within the perovskite structure, as well as onto different materials and surfaces.



Bio. Nandana Venkitesh is a rising sophomore studying mechanical engineering at the University of California, Los Angeles. She has completed an externship at LA-based sustainability startup Miravel, and at UCLA, she is a member of the Formula SAE racing team and Bruin Spacecraft group, where she explores her interest in energy storage. She is a recipient of the Steinbach Endowed Scholarship, awarded by UCLA's Henry Samueli School of Engineering.

Immunostimulatory Extracellular Vesicle Vaccine for Activation of Immune Responses

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[2]*Interdisciplinary Materials Science Program, Vanderbilt University*
[3]*Department of Biomedical Engineering, Vanderbilt University*
[4]*Department of Chemical and Biomolecular Engineering, Vanderbilt University*

Extracellular vesicles (EVs) are lipid-based nanoparticles secreted by cells that facilitate the intracellular delivery of biochemical cargoes. EVs are also promising drug delivery carriers as they can be modified and leveraged for an array of treatments. One novel application is the addition of an adjuvant to the EV surface to promote immune activation and antigenicity. To accomplish this, HEK293SF-3F6 cells expressing a fusion of the model antigen ovalbumin (OVA) and the EV-associated protein BASP1 underwent metabolic glycoengineering via N-azidoacetylmannosamine-tetraacylated (Ac4ManNAz) to produce OVA+ EVs with surface azide functionalization. The EVs were then conjugated to a modified version of the stimulator of interferon genes (STING)-agonist diABZI containing a dibenzo cyclooctyne (DBCO) reactive handle using strain-promoted azide alkyne cycloaddition (SPAAC). The efficacy of the diABZI-conjugated EVs was tested *in vitro* using bone marrow-derived dendritic cells (BMDCs) and compared to that of free diABZI. Results showed a significant increase in antigen presentation and upregulation of BMDC activation markers compared to free diABZI. Interestingly, BMDCs treated with EV-diABZI conjugates secreted significantly more TNF-α than BMDCs treated with diABZI alone. This suggests EV-diABZI conjugates are capable of shifting cytokine secretion from the interferon regulatory factor (IRF) pathway to another immune related pathway, NF-κB, which is conventionally activated by toll-like receptor (TLR) signaling. More investigations are needed to determine the signaling mechanism and downstream implications of this phenomenon. Overall, EV-diABZI conjugates demonstrated efficient BMDC activation and antigen delivery *in vitro*, suggesting that this platform may serve as an effective cancer vaccine. Future studies aim to optimize this technology for *in vivo* applications.

Bio. Hannah Crane is a chemical engineering undergraduate at the University of Pittsburgh in Pennsylvania. For her Vanderbilt University research experience, she was placed in Dr. John Wilson's ImmunoEngineering Lab alongside graduate student mentors Jack Loken and Hayden Pagendarm. "My dream is to help research and develop novel biotechnology in my future career", Hannah says, "and working on EV based therapeutics in the Wilson Lab has been a great introduction to cell-based manufacturing for me." Throughout the summer with VINSE, Hannah worked to develop and test a potential extracellular vesicle (EV) based cancer vaccine while growing her knowledge in drug delivery, immunology, molecular chemistry, and experimental design. She plans to use these new skills when she returns to her research on liposome and nanoparticle conjugation at Pitt.

7 | AUDREY BIRDWELL | Chemical Biology REU

The Elicitor-Regulator Relationship between Chloramphenicol and JadR2 for Secondary Metabolite Discovery and Novel Therapeutics

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Bacteria communicate by secreting secondary metabolites in their environment. In a laboratory setting, these secondary metabolites can be analyzed for their bioactive properties such as antibiotics. This research is essential due to the rise in antimicrobial resistance (AMR). AMR remains one of the top threats to global health resulting in millions of infections and thousands of deaths annually. A particularly challenging aspect of novel drug discovery is that secondary metabolite production in bacteria is highly regulated. For example, JadR2 is a DNA binding protein that regulates antibiotic production in Streptomyces venezuelae through binding of its promoter region. Interestingly, in the presence of the drug chloramphenicol (CAM), JadR2 releases from DNA and allowing transcription to occur. We are particularly interested in elicitors (CAM) and regulators (JadR2) of secondary metabolism. To establish CAM and JadR2 as an elicitor regulator pair, we heterologously expressed a Streptomyces promoter with GFP and JadR2 in E. coli. In hopes of discovering novel therapeutics from bacterial secondary metabolites, my project is interested in establishing a method for identifying elictor-regulator pairs through the known relationship between chloramphenicol (CAM) and JadR2 in Streptomyces venezuelae.

Bio. Audrey Birdwell is an upcoming senior at Lipscomb University in Nashville, TN. She is majoring in molecular biology and Spanish with a minor in chemistry. She actively participates in Lipscomb's student life by serving as student ambassador president of Lipscomb Admissions, president of TriBeta Biological Honors Society, vice president of Alpha Chi National Honors Society, and student representative on the Honors College student council. Aside from student life, Audrey has also worked in Dr. Joshua Owen's research lab for three years as an undergraduate researcher. Dr. Owen's research lab investigates a gut-derived metabolite o-valerobetaine and its inhibitory properties on mitochondrial fatty acid oxidation in cancer cells. Currently, she is leading her own research project partially funded by the TriBeta Research Grant awarded to her in the fall of 2023. She has presented her research at Lipscomb University's Student Scholars Symposium in 2023 and 2024. This summer, Audrey was chosen to participate in the Chemical Biology NSF REU at Vanderbilt University. Here, she works as an undergraduate researcher in Dr. Allison Walker's natural product discovery lab.

Smartphone compatible detection of drug resistant bacteria using enzyme-linked immunosorbent assay

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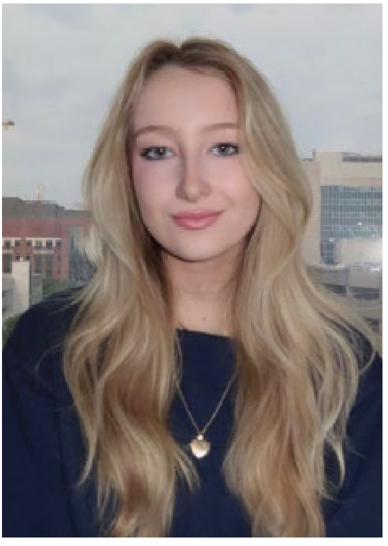
Multidrug-resistant bacteria, such as A. Baumannii and S. Aureus, can cause injured or immunocompromised military personnel to pass away. Personnel are often infected during treatment efforts in their own austere healthcare environments. To allow for surface detection of such bacteria, a rapid diagnostic test can be made by utilizing ELISA sandwich assays and gold nanoparticles. By immobilizing the primary antibody to the test paper, secondary antibodies electrostatically labeled with gold ions can sandwich the antigen if it is present on the tested surface. When gold nanoparticles come into contact with 3,3',5,5'-Tetramethylbenzidine (TMB), a blue-green color change occurs. This color change would indicate a successful sandwich assay aka detection of the antigen. If the primary antibody can be printed onto nitrocellulose paper, lateral flow assay technology should allow the color change from test results to display machine-intelligible barcodes that can be scanned by smartphones for a cost-effective detection system. To achieve this, sandwich assay trials must first show successful color change on nitrocellulose paper without a printer. Acidic buffer was used to immobilize the primary antibody to nitrocellulose squares followed by milk blocker aimed to prevent non-specific binding. The nanozyme was synthesized by combining the secondary antibody, acidic buffer, and chloroauric acid. Impurities were removed using dialysis cassettes and the solution displayed color change upon contact with TMB and TMBZ/H2O2 showing successful gold aggregation. Yet upon addition of the nanozyme to the squares, no color change was observed when TMB was dropped post rinse. The current procedure has not yet proved successful. Based on analyzing past data, color change might not be visible under current conditions due to low antibody concentration.



Bio. Fiona Power is a third-year undergraduate neuroscience student at the University of Miami. With an interest in the intersection of biochemistry and technology, Fiona aspires to continue her education beyond the undergraduate level with a focus in neural engineering. In her free time, she is actively involved in her university's Red Cross initiative and works with grade school students to aid in academic comprehension.

9 | GRACE HEILMANN | Chemical Biology REU

Determining Protein-Protein Interactions of SARS-CoV-2 Mac1 Domain

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SARS-CoV-2 has been responsible for the death of over 7 million individuals. All coronavirus strains contain a highly conserved macro domain (Mac1) within nonstructural protein 3 (nsp3) that can bind and remove ADP-ribose modifications. The Mac1 domain is responsible for removing ribosylation performed by poly-adenosine diphosphate-ribose polymerases (PARPs) which activate the interferon response (IFN), a cell signaling pathway that mounts an antiviral response. By altering a single amino acid within the Mac1 domain that is responsible for hydrogen bonding and critical for function, we hypothesize that the protein-protein interactions will differ between the wildtype (WT) and the mutant Mac1 as the interactions may be substrates for Mac1 deriboyslation activity. Site directed mutagenesis was used to change arginine at position 40 to alanine, which has been shown to reduce deribosylation efficacy of Mac1. Mass spectrometry was used to determine the protein-protein interactions of the WT Mac1 domain and the mutated Mac1 domain (N40A). Over 50 interactors of Mac 1 were identified after performing mass spectrometry, 2 of which were previously identified interactors of nsp3. These interactors are associated with other post-translational modifications as well as cell stress pathways and may infer future drug targets for coronaviruses.

Bio. Grace Heilmann is a senior majoring in Biology at the University of North Carolina Greensboro. Grace's academic excellence has been recognized by being on the chancellor's list since 2022 and receiving biology specific scholarships such as Burrell Biology scholarship and Ms. McIver scholarship. These scholarships are awarded to individuals in the top 5% of their major. She started undergraduate research her sophomore year working on resensitizing glioblastoma cells to cancer therapies. Grace's future career goals are to pursue a PhD in cancer biology. When Grace is not working in the lab, she is mentoring students in UNCG's Academic Achievement Center. Grace spends her time coaching students on how to study and transition to a university setting. Grace was awarded student employee of the year in April of 2024 because of her dedication to student success. Grace is currently participating in Vanderbilt's Chemical Biology REU under Dr. Lars Plate working on proteomics of SARS-CoV-2.

Investigating the Electrical Properties of Metal/GaN Interfaces

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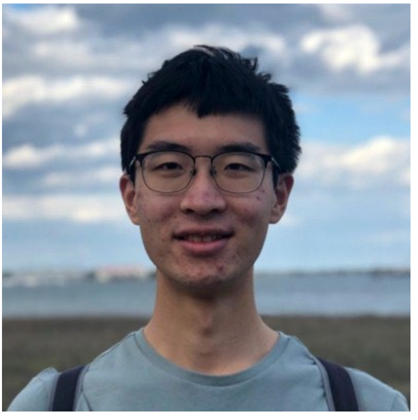
[1]*Department of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA*
[2]*Department of Electrical and Computer Engineering, Vanderbilt University, Nashville, TN*
[3]*Interdisciplnary Materials Science, Vanderbilt University, Nashville, TN*

Gallium Nitride (GaN) possesses extraordinary physical properties including a wide and direct bandgap and a high breakdown voltage. GaN-based power devices have shown great potential. One fundamental building block of these devices is the interface between the metal stack and semiconductor layer (GaN), which forms two types of contacts: Ohmic and Schottky. The former exhibits linear current-voltage (I-V) characteristics in both directions, while the latter has a rectifying behavior that only permits current to flow in one direction. This study aimed to optimize these two behaviors through various metal stacks and processing parameters and extract doping level in different GaN substrates. This study utilized both n-doped and p-doped GaN grown on sapphire and Qromis engineered substrates. For Ohmic contacts, the specific contact resistance and sheet resistance were measured using Circular Transmission Line Measurement (CTLM), and it was found that annealing the Pd/Pt/Au stack to p-GaN at 500℃ for 1 minute improved the contact resistance from 0.15 to 0.04 $\Omega\cdot cm^2$. For Schottky contacts, some Schottky diodes exhibited a rectifying behavior with a low leakage current around 10 nA, while others displayed higher leakage current. The high leakage current made it challenging to conduct capacitance-voltage (C-V) measurements and extract a reliable doping level. C-V measurements were conducted on Schottky diodes with low leakage and linear Ohmic contact on Qromis wafers, and a doping level of $5*10^{15}$ cm^{-3} was extracted. A third type of I-V behavior was also observed where current flows in both directions, but Ohm's law was not obeyed. To investigate this behavior, temperature-dependent I-V measurements are ongoing.



Bio. Tianqi Sun is a rising fifth-year student at Georgia Institute of Technology with a major in Materials Science and Engineering and a minor in Computational Data Analysis. This summer, he is researching at Vanderbilt University, where he is working on electrical characterization of metal/GaN contacts. At Georgia Tech, he is currently working as an undergraduate research assistant in Dr. Lauren Garten's research group on electrical characterization of the ferroelectric properties of sputtered AlScN. He also served as the X-Ray equipment Technical Officer and Summer Fellow at the Materials Innovative and Learning Laboratory in MSE at Georgia Tech.

11 | JENNA JANG | VINSE Tech Crew

Enhancing Reactive Ion Etching Control with Real-Time Laser Interferometry

Jenna Jang[1], Benjamin Schmidt[2]
[1] Department of Neuroscience, Vanderbilt University
[2] Vanderbilt Institute of Nanoscale Science and Engineering, Vanderbilt University

Accurately etching thin films is crucial in fabricating microelectronic devices for creating nanoscale features and ensuring desirable device performance. Deep Reactive Ion Etching (RIE) is a widely used etching technique in the VINSE cleanroom that operates based on fixed times. However, this time-based approach often fails to deliver consistent results as the etch rate could vary from numerous factors such as material properties and environmental conditions. These variabilities lead to over-etching where the process etches beyond the targeted layer, damaging the sample and hindering device performance. Additionally, under-etching could leave residual material that interferes with the intended design of the device. This project aims to optimize the etching parameters for the Oxford PlasmaPro100 Cobra instrument by incorporating real-time monitoring techniques such as laser interferometry. The goal is to establish a precise correlation between the changes of reflected light intensity and etch depth by analyzing interference patterns. Time-based etch rates could be compared with interferometry data to validate the etch process. By developing a robust protocol, real-time monitoring will improve the precision and reproducibility of the etching process that will ultimately ensure a higher quality of fabricated devices.

Bio. Jenna Jang is a rising junior majoring in Neuroscience who joined the VINSE Tech Crew in the summer of 2024. She joined the Tech Crew to learn more about nanofabrication and expand her interests in creating flexible, transparent brain computer interfaces. Her favorite part of the cleanroom is the autonomy to learn new tools and friendliness of VINSE users. She is excited to learn more about the diverse research projects done in VINSE and provide assistance. Outside the cleanroom she is involved in the Vanderbilt Undergraduate Research Journal and likes to explore local coffee shops in her free time.

Modulating the Infrared Response of 2D Materials for Nanophotonic Applications

David Flores[1], Jeb Buchner[2], Saurabh Dixit[2], J. D. Caldwell[2]
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The confinement of infrared light into deep sub-diffraction volumes enables nanophotonic devices for various applications, including molecule sensors for environmentally polluting molecules and biomolecules, as well as integrated photonic circuits. This work focuses on confining IR light in the form of light-matter waves called phonon polaritons (PhPs), which has been demonstrated in hyperbolic 2D materials. The propagation direction of PhPs can be controlled by stacking slabs of biaxial 2D hyperbolic materials, like MoO3, at different twist angles. Additionally, confinement of PhPs can be improved by incorporating a metallic thin film beneath these materials, creating ‘image’ PhPs. In this work, we explore the intersection of these advancements, demonstrating both directional control and superior confinement by observing the behavior of image PhPs in twisted MoO3 structures. Using a dry release transfer method, we fabricated single and twisted (θ=60°) MoO3 structures atop a TiO2 dielectric spacer on a gold coated substrate. We observed PhPs in these structures by using scattering-type scanning near-field optical microscopy (s-SNOM) and found significant confinement of IR light (about 1/60th of free space wavelength). We validated our experimental findings with numerical simulation models that show strong agreement. We experimentally demonstrate unprecedented variation in PhP propagation in both twisted and semi-suspended MoO3 structures, associated with changes in twist angle and effective dielectric permittivity, respectively. These findings open avenues for the devices used for molecular sensing and integrated photonic circuits. Ongoing efforts include fabrication of more twisted structures at different angles between 0° and 90°.

Bio. A proud Honduran national and Canadian citizen, David Flores is a rising third-year Millennium Scholar at Penn State University, studying Materials Science and Engineering. David’s research experience includes inverse design of high entropy alloys using machine learning (Penn State) and simulating the structure of sustainable Li-ion cathode materials (Northwestern University). David is the Secretary for Penn State Society of Hispanic Professional Engineers, and an HSF and ACS Scholar. Following his pursuit of graduate studies, David aims to leverage the power of startups to facilitate the implementation of cutting edge science in emerging economies.

Synthesis of Diastereo- and Enantioselective Catalysts for Aza-Henry Reactions

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The focus of this research is to synthesize diastereo- and enantioselective catalysts for aza-Henry reactions to expand the scope of substituents that can be further used in peptide synthesis. The products of the aza-Henry reactions can then be used to conduct Umpolung amide synthesis (UmAS), developed by the Johnston Lab. Two catalysts, H,[4]PyrrolidineQuin-BAM (PBAM) and Adamant-AmA (AmA), were produced via a 3-step and 5-step synthesis, respectively, involving a Buchwald-Hartwig amination and microwave radiation. Air and moisture sensitive reagents are required, facilitating the need for degassing and drying methodology. (*R,R*)-AmA and (*R,R*)-PBAM were successfully synthesized and further used in enantioselective aza-Henry reactions to create alpha-bromo nitroalkanes via reduction of the nitroalkene. The product of these reactions will then be used towards UmAS, reacting with the aid of electrophilic iodine and stoichiometric base to form an amide.

Bio. Cait is originally from Mobile, AL and is currently completing her undergraduate studies at Oglethorpe University in Atlanta, GA. She is majoring in chemistry, with a special interest in organic synthesis. During the summer of 2023, she conducted research at UF Scripps where she synthesized a small bioactive ligand that had the potential to reverse the phenotypes of certain neurological disorders. She is the Co-President of Sigma Zeta Honor Society, Secretary of Chemistry Club, Treasurer of Data Club, a member of The National Society of Leadership and Success, along with being a chemistry lab assistant and being a member of the Gabriel lab at her university. Her plan after she graduates this fall is to get accepted into a graduate program and start earning an organic chemistry PhD. She hopes to eventually go into the pharmaceutical industry and work in drug discovery, specializing in medicinal chemistry.

The effects of shear stress on BMEC cytoskeleton alignment

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The blood-brain barrier (BBB) is a semi-permeable membrane comprised of brain microvascular endothelial cells (BMECs) that protect the central nervous system from harmful substances and pathogens. The BBB traits are not just a result of BMECs, but from a dynamic relationship with their microenvironment, including blood flow dynamics. Blood flow produces a tangential force across the vessel endothelium known as shear stress. The dynamic nature of blood flow significantly influences the properties of BMECs, but there are conflicting reports in the scientific literature regarding the effects of shear stress across different BMEC lines *in vitro*. Resolving these discrepancies is fundamental to advancing our understanding of the BBB and improving the reliability of research in this field.

To address this discrepancy, a high throughput cone-and-plate device (MoCAP) capable of imitating the hemodynamic in vivo environment was engineered to expose brain endothelial cell lines to varying shear stress conditions. Utilizing the MoCAP device we subjected three common cell lines (primary, immortalized, and induced pluripotent stem cell-derived BMECs) to low (0.6 dyn/cm^2) and high (10 dyn/cm^2) levels of continuous and pulsatile shear stress. Cells were then fixed with 4% paraformaldehyde and immunofluorescent staining was performed. Immunofluorescent staining of the actin cytoskeleton revealed that all three cell lines align perpendicularly to the direction of fluid flow regardless of shear stress magnitude and flow pattern. In addition, while the mean cell angle remained unaffected, the cell aspect ratio was significantly altered across cell lines.

The study presented here helps clarify some of the conflicting reports regarding the effects of shear stress across multiple BMEC lines. Ultimately, it allows for a better understanding of the neurovascular microenvironment which can help identify new therapeutic targets to strengthen the BBB and protect the brain.

Bio. Kissamy Georges is a rising sophomore at the University of Massachusetts Dartmouth studying Bioengineering. For her Vanderbilt University research experience, she has been placed in Dr. Ethan Lippmann's lab alongside post-doctorate mentor Dr. Daniel Chavarria. Kissamy aspires to be a clinical lab technician as she enjoys studying the intersection between biology, chemistry, and technology. Outside of doing research, some of Kissamy’s hobbies include: dancing, crocheting, and jewelry making.

Optimizing Indium Tin Oxide for Flexible, Transparent Neural Probes

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Extracellular microelectrode arrays are a widely used and critical technique for transducing brain signals. More recently, optical approaches have also been developed to read and write neural activity through imaging and optogenetic stimulation, respectively. However, conventional metal and silicon-based recording electrodes are opaque and light sensitive, making them largely incompatible with optical techniques. Here, we seek to optimize the design of a highly transparent, polymer-based neural probe capable of recording single-neuron activity. To acquire single-spike resolution neural recordings, an implanted sensor must be near the size of a single cell (<50 um diameter) while maintaining a low (<1 MOhm) electrochemical impedance at neurophysiological frequencies (~1 kHz). Furthermore, to avoid producing light artifacts during optical stimulation or imaging, the implantable probe must be as transparent as possible. Given these two objectives, we have designed a neural probe consisting of indium tin oxide (ITO)—a transparent conductor—surrounded by insulating layers of biocompatible Parylene C. We specifically characterized the effects of ITO deposition thickness and electrode diameter on electrochemical impedance, in addition to the tradeoffs of these parameters with transparency. We found thicknesses even up to 150 nm to be sufficiently transparent for optical modalities. Surprisingly, we also observed a non-linear relationship between ITO thickness and transparency at light wavelengths relevant for optogenetic stimulation. Thicker ITO layers exhibited a higher transparency at 460 nm, counterintuitively suggesting that thick ITO is more optimal for optogenetic applications. The more challenging design constraint we encountered was electrochemical impedance. In our experiments, we found that even thick ITO samples with large recording sites have a high electrochemical impedance at 1 kHz. These results suggest that while ITO is a promising candidate for transparent neural probes, it may need to be paired with traditional conductors such as Au and Pt for achieving single-unit recordings in vivo.

Bio. Thaissa Peixoto is a rising senior at Johns Hopkins University majoring in Electrical Engineering and Psychology. At Vanderbilt, she has worked in the Gonzales Lab, cultivating her interest in neural engineering research. Her background lies in analog design for Biomedical Engineering research, and she hopes to continue working in the intersection between hardware and the brain.

How Modifying Power Changes the Optical and Conductive Properties of RF Magnetron Sputtered Indium Tin Oxide Films

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Magnetron sputter deposition is a physical vapor deposition process in which gas particles are ionized in a vacuum chamber and bombard a target material, scraping off nano-sized pieces that are "sputtered" onto a substrate. This process is commonly utilized for fabricating transparent, conductive thin indium tin oxide (ITO) films that are employed in a variety of applications, such as touch screens, displays, and more! When depositing ITO, adjusting the radio frequency (RF) sputtering power affects the transparency and conductivity of the resulting film. This is significant because better electrical conductivity and greater transparency is optimal for most applications. Currently, in the Vanderbilt Institute of Nanoscale Science and Engineering (VINSE) Cleanroom, users deposit ITO with a set of default parameters that have not yet been optimized to achieve the desired film characteristics for their specific applications. As a solution, this project aims to formulate a detailed ITO deposition guide. To accomplish this, ITO was deposited at a thirty and sixty minute duration using the AJA ATC-2200 Sputter Deposition Chamber at five different power settings. Measuring conductivity, resistance, and transmittance of the samples has suggested that power could be positively correlated with conductivity and negatively correlated with transparency. Further analysis through scanning electron microscopy has also revealed a change in the morphology of ITO film structure at higher power settings. Initial results imply that using less extreme parameters will result in a smoother film with an optimal balance between quality optical and electrical properties. In the future, more testing can be conducted to analyze the effects of adjusting chamber pressure or heating the substrate during deposition to broaden the reference guide.

Bio. Vivian Ma is a rising sophomore at Vanderbilt University studying Computer Science and is a recipient of the Hudson Honors Scholarship and National Merit Scholarship. She started working with VINSE in the summer of 2024 as a part of the Undergraduate Technical Crew. In the cleanroom, Vivian specializes in sputter deposition and is currently analyzing how various power settings affect the quality of indium tin oxide (ITO). She also really enjoys photolithography ("creating fun patterns"), microfluidics, and scanning electron microscopy. Her favorite part of this summer has been meeting and working with the amazing VINSE team!

17 | NICHOLAS GRAY | VINSE REU

Vanadium dioxide-integrated valley photonic crystals for topological control of light

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As computational technology needs increase, the demand for faster, smaller, and more robust devices faces the challenge of fundamental physical limitations. Much like semiconductors influence the flow of electrons to transmit information, photonic crystals manipulate the propagation of light, offering tight directional control and defect resistance. Furthermore, the precise fabrication of photonic crystals allows for integrated optical circuits with dimensions comparable to the wavelength of light. The unique band structure topology of valley photonic crystals allows for robust control of light based on its valley degree of freedom, leading to switchable optical paths and tight light propagation. In this work, we present preliminary fabrication techniques for vanadium dioxide-integrated valley photonic crystals and demonstrate through simulation their ability to tightly control light propagation and create switchable optical paths on a single chip. A hexagonal grid of alternating vanadium dioxide and germanium pillars were fabricated using electron beam lithography, electron beam deposition, and sputter deposition. This technology has significant potential applications in quantum information science and neural networks, where it can enhance the encoding and manipulation of information through multiple optical paths within integrated circuits.

Bio. Nick is a rising fifth-year at West Chester University pursuing a degree in physics. Nick's research has spanned several labs at his university, where he first conducted simulations of nanostructure interactions. He now performs research measuring and studying the emission spectra of LEDs. He recently coauthored a paper, "The e/m experiment: Student exploration into systematic uncertainty," which details methods for reducing experimental uncertainties in a common undergraduate physics experiment. Outside of academics, Nick is involved in the Society of Physics student, serving formerly as his chapter's secretary and treasurer, and the Friars' Society, a community-service organization serving the greater West Chester area. He is an avid pianist, having formerly majored in music, and enjoys running and biking. He plans to pursue a Ph.D. in physics or materials science researching photonic structures and their use in quantum information science.

Photopolymerization of Pyrrole Thin Films

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The photosystem I (PSI) protein complex has near 100% internal quantum efficiency. Biohybrid solar devices now use PSI to harvest light energy. Previous work showed that PSI has the ability to photopolymerize monomers such as pyrrole, forming a conductive polymer to effectively wire the protein. Our investigation into this photopolymerization focuses on thin film growth and specifically the effect of photopolymerization time on the resulting polymer film. To further develop this wiring methodology, photopolymerization was carried out by submerging PSI films in monomer solution and illuminating for a specified time. Photochronoamperometry (PCA) was performed to analyze the photoactivity of the resulting films, and profilometry was utilized to characterize the thickness. Other characterization methods such as SEM, TEM, STEM EDX, and IR were also carried out to further investigate the polymer films. The PCAs showed that peak current density did not significantly increase or decrease over photopolymerization illumination time from 4 to 48 hours, but film thickness did increase over time. SEM imaged the surface morphology of the films, showing network changes from columns to spheres over time. PSI and pyrrole were confirmed to be in the films by their signatures in IR and STEM EDX. The isolated composite spheres have potential for furthering PSI/nanoparticle applications leading to biohybrid energy conversion.

Bio. Allison Portaro is a rising senior in the University of Louisville Honors Program majoring in Chemistry with a track in Biochemistry. She is a Henry Vogt Scholar (2021-2025) who has received the Tilford and Vicki Riehl Scholarship (2023) and the Freshman Honors Scholarship (2022) from the Department of Chemistry. She is also a member of the Kentucky Academy of Science, the Society of Undergraduate Chemistry Students, and tutors General Chemistry courses. At UofL she conducts biochemical research on the anticancer properties of *Salvia* (sage) and its effects against breast cancers. Allison is currently completing an NSF-funded REU in Chemical Biology at Vanderbilt University. She graduates in May 2025 and plans to pursue a PhD in Chemistry.

19 | KENDALL KELLY | VINSE REU

Optimizing Bioadhesive Properties in siRNA Nanoparticles for Osteoarthritis Treatment

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Osteoarthritis (OA) is a prevalent degenerative musculoskeletal disease characterized by the deterioration of cartilage, leading to pain and inflammation within the joint. Current OA treatments primarily focus on symptomatic relief rather than a cure, highlighting the need for more effective therapeutic solutions. This study explores the potential of bioadhesive nanoparticles encapsulating short interfering RNA (siRNA) (bioad-si-NPs) as a potential therapeutic approach for OA.

To develop these bioad-si-NPs, a library of bioadhesive surfactant (surface-coating) polymers with varied aldehyde-to-polymer ratios was synthesized using RAFT (reversible-addition fragmentation chain transfer) polymerization and copper-free click chemistry to add hydrophobic lipid tails for anchoring to the nanoparticle core. The aldehyde content within the polymer chain was adjusted to determine the optimal ratio for bioadhesion, as aldehydes enable reversible bonds to form with amines present in the extracellular matrix, allowing for extended retention in the joint. The polymers synthesized were characterized with nuclear magnetic resonance imaging (NMR) and gel permeation chromatography (GPC) to evaluate the degree of polymerization (DP), aldehyde content, and molecular weight. With these polymers, nanoparticles were created using a confined impinging jet (CIJ) mixer. The size and zeta potential of the bioad-si-NPs formulated were characterized with dynamic light scattering (DLS). Lastly, the cytotoxicity of the nanoparticles was evaluated by treating ATDC5 cells with a range of doses. The characterization process yielded polymers with a DP of 50, successful deprotection of aldehydes, and molecular weights of approximately 6 kDa. The polymers formed bioad-si-NPs around 150 nm in size with a positive surface charge, and doses less than 25 nM were found to be non-cytotoxic. The synthesized bioad-si-NPs demonstrated promising properties for potential use in OA treatment. Studies are ongoing to evaluate the knockdown efficacy and bioadhesive properties of the nanoparticles.

Bio. Kendall Kelly is a rising senior majoring in Biomedical Engineering at the University of Mississippi. She is actively engaged in undergraduate research within the Interdisciplinary NanoBioScience (iNBS) Lab under the guidance of Dr. Thomas Werfel, focusing on mRNA vaccines for cancer therapies. Kendall has previously participated in the University of Mississippi's Nanoengineering REU, where she presented her summer research at the Biomedical Engineering Society (BMES) Conference in Seattle, Washington. At the University of Mississippi, Kendall holds the position of secretary in the BMES Club and is an active member of the Sally McDonnell Barksdale Honors College, the Society of Women Engineers, Tau Beta Pi, and Phi Kappa Phi. This summer, she has been placed in Dr. Craig Duvall's lab, working alongside her graduate mentor Amelia Soltes to develop siRNA nanoparticles for the treatment of osteoarthritis. After graduation, Kendall plans to pursue a PhD in biomedical engineering, with a specific focus on nanomedicine.

Augmented Reality for Kidney Stone Training

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Augmented Reality (AR) technology offers innovative ways to enhance medical training. This project explores the application of AR for training medical professionals in the diagnosis and treatment of kidney stones. The purpose of this study is to develop an AR-based training tool that provides an immersive experience, simulating real-world scenarios in the identification and management of kidney stones. The HoloLens 2 platform was used to integrate 3D models of kidney anatomy and common surgical instruments used in lithotripsy. The main results demonstrate that AR significantly improves the learning curve, with trainees achieving competency faster than with traditional methods. The conclusions suggest that AR can be a valuable supplement to existing medical training programs, providing a safe and cost-effective environment for skill acquisition. This presentation will cover the design and development process, key findings, and potential future applications in medical education.

Bio. Carisa Lynch is an undergraduate student at Florida International University (FIU) in Miami, Florida, where she is pursuing a pre-med track with aspirations of becoming an orthopedic surgeon. She recently completed an internship at Vanderbilt University, working with Maple Labs. During her internship, Carisa gained valuable hands-on experience in medical research and technology, further solidifying her passion for the medical field.

21 | RAFAEL RODAS | VINSE TECH CREW

Production of Graphene Resistors for Educational Purposes

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Since its Nobel-winning discovery in 2004, graphene has caused great excitement, this 2D material made of carbon hexagons has many properties such as high conductivity, transparency, and flexibility, making it a prime candidate for leading a revolution in electronics. Moreover, as the first 2D material ever made and how simple and hands on the historical experiment is, graphene allows for a hands-on introduction to nanoscience. As part of VINSE's commitment to educating the broader community, many high school outreach events are hosted throughout the year. These can include the opportunity for students to make their own graphene and explore its fascinating characteristics and applications. One type of electrical component we would like to showcase for these students are resistors, which help regulate the flow of current in a circuit. Previously, some samples were made for this purpose, but no longer function, in part due to physical damage sustained through student testing. My project aims to create graphene resistors that can both illustrate the importance of graphene and its properties as well as withstand the harsher handling the samples undergo when students attempt to measure the electrical characteristics of the device. To do this, new chips with varying gap sizes between the contact pads have been fabricated, such that a better yield and more consistent resistance values were achieved. These devices will allow outreach groups to explore and test more robust graphene based electronics.

Bio. Rafael is a member of the class of 2026 majoring in Electrical and Computer Engineering with a minor in Nanotechnology who joined VINSE as a user in Spring 2024 and Tech Crew in the summer of 2024. Additionally, he has also taken classes with lab components inside the cleanroom. As a member of Tech Crew, he is working on developing graphene electronics for research and procedural optimizations as well as demo samples for high school outreach events. With interests in nanostructures, semiconductors, electromagnetic properties of 2D materials, optoelectronics, and integrated circuits, Rafael jumps onto any project that presents a challenge where outside the box thinking and creative design is encouraged. As a user, Rafael is currently working on microfluidics and optical sensing as an avenue for detecting lead contaminated water in sources such as drinking fountains and faucets. He has a strong interest in pursuing both research and pedagogical positions where he can implement new techniques and help redefine how STEM is taught at all levels.

22 | ELVIS DANIEL PEREZ GALARZA | Chemical Biology REU

Investigating the Impact of Mutations on Substrate Positioning in Fluoroacetate Dehalogenase (FAcD)

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The strong and stable carbon-fluorine (C-F) bonds in per- and polyfluoroalkyl substances (PFAS), used in many industries and consumer products, has caused environmental concerns due to their resistance to degradation. A potential non-toxic and efficient method of PFAS degradation is to use enzymes. An enzyme known as fluoroacetate dehalogenase (FAcD), isolated from bacterium Rhodopseudomonas palustris, hydrolyzes the C-F bond present in a natural toxin, fluoroacetate (FAc). In this work, we used our Python software, Enzy-HTP, to explore how mutations affect substrate positioning and key residue interactions in the active site, focusing on the catalysis of trifluoroacetate (TFA) as a model system for polyfluorinated compounds. A wildtype FAcD-TFA complex was created and subjected ten randomized single-point mutations, resulting in the creation of ten FAcD-TFA variants. Classical molecular dynamics (MD) simulations of 200 nanoseconds were performed and repeated three times for the wildtype structure and each variant structure. By measuring distances between key residues and TFA in the active site, key interactions for the reaction can be analyzed. These interactions are responsible for the positioning and successful cleavage of the C-F bond. Differences in distances observed in the mutated structures compared to the wildtype structure might indicate either enhanced or reduced catalytic activity.

Bio. Elvis Daniel Perez Galarza is an undergraduate from Western Carolina University. He is majoring in Chemistry and minoring in Biology and German. He has participated in undergraduate research at Western Carolina University since his sophomore year with Dr. Channa De Silva. He has recently received an award from the American Chemical Society for his research in inorganic chemistry. He will be the secretary for the Chemistry Club next year and is very involved in the Brinson Honors College at Western Carolina University as well. Elvis has participated in another REU at UNC-Chapel Hill. He is currently working in Dr. Zhongyue (John) Yang's lab here at Vanderbilt.

23 | ANGELICA VELASQUEZ | Chemical Biology REU

Structural Analysis of Mitoxantrone Binding to AP Sites in DNA: Regarding its Chemotherapeutic Effect

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Apurinic sites (AP sites) are generated in cellular DNA by a variety of alkylating agents. Once formed, AP sites equilibrate in the deoxyribose via a transient aldehyde intermediate. Mitoxantrone (MTX), is a chemotherapeutic agent capable of treating various cancers such as lymphomas, breast cancers, and leukemias. Secondary amines present in MTX may react with the aldehyde intermediate at AP sties to form reversible AP-site conjugates (Schiff bases). The chemistry and biology of these AP site conjugates is not well understood. Our study aims to provide insights about the effects of MTX conjugation at AP sites in DNA and how it may alter the thermodynamics of the duplex, and DNA structure. We achieve this by synthesizing site-specific MTX-AP site conjugates. We purify them through HPLC chromatography and characterize it using mass spectrometry. We compare the conjugate to a corresponding unmodified DNA sequence using both thermodynamic and NMR studies. Our data reveals a 4º lower melting temperature (T_m) in the DNA containing an MTX-AP site conjugate. NMR suggests that MTX conjugation at AP sites causes localized structural disturbance to DNA. These structural changes may be responsible for the thermal destabilization of the DNA. Structural analysis serves to unveil the effects of MTX conjugation to DNA at AP sites.

Bio. Angelica is a rising third-year chemistry student from the University of Connecticut. She is gaining experience in an analytical laboratory at her home institution which focuses on the identification of organic pollutants and bioactive compounds. In the previous spring semester, she presented her poster, "Detecting the Presence of PFAS 'Forever Chemicals' in Commonly Used Infant Care Products" at UConn's Randolph T. Major Symposium, where she was awarded 3rd place in Undergraduate Poster Presentations. She has a keen interest in drug development, specifically pertaining to cancer research. In the future, she hopes to further her education in chemistry with regards to cancer therapeutics so that she can make meaningful contributions to the field.

Creating a Simple Calibration to Correct Wearable Insole Force Measurements

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Currently in biomechanics research, the gold standard for force measurement is stationary force plates that can only be used within a laboratory setting. Wearable technologies, such as sensorized insoles that use pressure sensors to measure ground reaction forces, have emerged in recent years. These types of technologies offer the potential to mobilize force measurements and because insoles can be worn in almost any shoe, there are few limitations for when they can be used. However, these wearables currently incorrectly estimate the magnitude of forces. In this study, participants completed trials on a lab-based force instrumented treadmill while wearing sensorized insoles. The insoles were worn in running sneakers and no software-based insole calibrations were performed before the trials. For the calibration, participants completed the following tasks at the beginning of each trial: standing on both feet, standing on each foot individually, and standing on both feet again. The insole calibration was created based on the force while the participant was standing on one foot. The calibration was applied retroactively to each trial. Before calibrating the insoles, the average error was 0.27 bodyweights. After calibrating the insoles, the average error was 0.10 bodyweights. This calibration decreased the insole force measurement error by 63.7%. Based on these results, the insole calibration was effective in reducing the insole force measurement error during walking trials. This means that the insoles and calibration can be used in situations when ground reaction force measurements are needed, and laboratory-based force plates are not available or suitable.

Bio. Kaitlyn is a rising junior at the University of Florida, pursuing a degree in Biomedical Engineering and a certificate in Dance in Medicine. Her experience dancing has fostered her interest in studying biomechanics and human movement. At UF, she is involved in research in the Musculoskeletal Biomechanics Lab and focuses on the biomechanical effects of carpometacarpal osteoarthritis. She also completed college-level research and a capstone project that was presented at the Max Planck Florida Institute for Neuroscience as part of her high school studies at FAU High School. This summer, she joined Dr. Karl Zelik's lab in CREATE as part of the VUSE Summer Research Program and is studying the use of wearable insoles to measure tibial forces. Outside of research, Kaitlyn is a Peer Advisor for the UF College of Engineering, a member of the UF Chapter of the American Society of Biomechanics, and volunteers with GEMS – an organization that promotes STEM education in elementary-aged girls in Gainesville. After graduation, she hopes to matriculate to medical school and eventually specialize in pediatric orthopedics.

25 | ELLIOTT BALLINO | Chemical Biology REU

Investigations into NHC-difluoroborane Precursors for Novel Transformations with *π*-Systems

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Boron centered radicals are useful in numerous synthetic applications including reduction and polymerization reactions. Generally, boryl radicals are nucleophilic in nature; however, a recent discovery by Subervie describes the generation of the first electrophilic boryl radical from a *N*-heterocyclic carbene (NHC) difluoroborane precursor. Initially we sought to harness this radical for novel transformations with electron-rich π-systems. Preliminary results demonstrated that this electrophilic radical can functionalize a silyl enol ether. We believe alternative NHC- and amine difluoroborane radicals could facilitate these transformations with improved efficiency. Therefore, we seek to develop a library of these difluoroborane precursors. We hypothesize that these radicals react regioselectively with radical acceptors like indoles, which will form the foundation for future research.

Bio. Elliott Ballino is a rising senior with a chemistry major and mathematics minor at the University of Scranton. He is the recipient of multiple scholarships and awards at the University of Scranton. He has been a peer tutor in chemistry and mathematics for the past two years and will serve as a General Chemistry Graduate Assistant in the fall.

26 | LISA SEBASTIAN | VINSE REU

Etch, Release, and Transfer of GaN Transistors

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Gallium Nitride (GaN) High Electron Mobility Transistors (HEMTs) have emerged as next generation devices for RF and microwave applications. Due to the material properties of GaN, this semiconductor exhibits superior performance and efficiency when compared to silicon. However, GaN HEMTs lack the well-established logic function capabilities of silicon CMOS technology. This has led to a recent push for the integration of GaN HEMTs with CMOS technology, aiming to combine the advantages of both materials. Micro Transfer Printing presents a unique solution to the incompatibility between the two fabrication processes. With this technique, GaN HEMTs and CMOS can be fabricated separately and then combined. In this work, we demonstrate the successful transfer of GaN HEMTs from a Qromis Substrate Technology (QST™) wafer to a silicon wafer. The project began with testing devices fabricated on a QST™ wafer. Then, a plasma etch process was engineered to create deep trenches in the QST™ wafer, exposing a buried silicon layer. A XeF_2 gas based etch was developed to selectively remove the silicon layer beneath the devices, releasing them from the substrate. Micro Transfer Printing parameters were optimized, enabling individual devices to be transferred from the source substrate to the target silicon wafer. Various adhesion layers on the target wafer were tested to improve the bonding of the device to the new substrate. Electrical measurements were taken again after the transfer process, revealing minimal changes in device performance. GaN HEMTs were successfully etched and released from a QST™ GaN substrate and transferred to a new substrate, confirming the viability of Micro Transfer Printing for the heterogeneous integration of GaN HEMTs with CMOS technology.

Bio. Lisa Sebastian is a rising senior at Rose-Hulman Institute of Technology majoring in NanoEngineering and minoring in Electrical and Computer Engineering. Her introduction to research occurred as a rising high school junior through the Air Force LEGACY program at Wright Patterson Air Force Base (WPAFB). Over four summers at WPAFB, she developed a passion for working in the cleanroom and an interest in III-V semiconductor fabrication. Additionally, Lisa gained experience at HRL Laboratories, where she probed wafers to obtain device characteristics and analyzed device performance. At Rose-Hulman, Lisa is actively involved in research, developing a process to sputter Indium Tin Oxide thin films. This summer, Lisa was grateful to be a part of the Vanderbilt Institute for Nanoscale Science and Engineering (VINSE) REU program in the Ebrish lab, where she has enjoyed working on processes to successfully transfer devices between substrates. After graduating from Rose-Hulman, Lisa plans to pursue a PhD in Electrical Engineering, specializing in III-V semiconductor device fabrication.

27 | TUONG NGUYEN DINH CAT | Vanderbilt Summer Intern

Synthesis and Characterization of Novel Hexagonal Copper Gold Selenide ($Cu_2Au_5Se_3$) Nanoparticles

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The synthesis of novel nanocrystals with desired compositions and properties is an essential prerequisite to developing nanoscale devices such as solar cells, semiconductors, and radiation detection devices. Building onto existing research, this project refined a four-step synthesis of novel hexagonal copper gold selenide ($Cu_2Au_5Se_3$) nanoparticles. Hexagonal wurtzite-phase cadmium selenide (CdSe) nanocrystals of size 5 - 10 nm were synthesized and grown to around 100 nm in the presence of $CdCl_2$ and oleylamine. The CdSe particles were exchanged with copper to form copper selenide (Cu_2Se), then partially exchanged with gold to form $Cu_2Au_5Se_3$, utilizing air-free cation exchange techniques. The growth of the particles was monitored *in-situ* with ultraviolet-visible spectroscopy (UV-Vis); the crystal phase was characterized with powder X-ray diffraction (pXRD); the morphology and size were imaged with transmission electron microscopy (TEM); and the elemental distribution and stoichiometric ratios were determined using scanning transmission electron microscopy - energy dispersive X-ray spectroscopy (STEM - EDS). pXRD of the final product indicated a novel crystal pattern not matching anything previously reported in the literature, and the EDS data revealed the presence of copper, gold, and selenium. The size and consistent morphology of the particles were also confirmed with TEM and UV-Vis. Future progress towards control of the purity of the wurtzite phase of the $Cu_2Au_5Se_3$ and elucidation of the crystal structure using three-dimensional electron diffraction (3DED) - which would be permissible given the large particle sizes - would greatly contribute to the understanding of the specific characteristics and potential uses of the particles.

Bio. Tuong (Kathleen) Nguyen is a rising junior at Franklin & Marshall College, where she is pursuing a double major in Chemistry and Biochemistry & Molecular Biology, with a minor in Anthropology. This summer, she worked on synthesizing novel copper gold selenide nanoparticles in the Macdonald Lab at Vanderbilt. At her home institution, she developed two independent research projects in the lab of Dr. Kate Plass: one focusing on selenium and tellurium anion exchanges on copper indium sulfide nanorods as part of the Hackman Summer Research Scholars Program; and her current project on the effects of tellurium exchange and cadmium exchange on copper vacancies in chalcocite copper sulfide nanorods. Her work has been presented at the Primarily Undergraduate Nanomaterials Cooperative (PUNC) and the Middle Atlantic Regional Meeting of the American Chemical Society. Tuong has also been the event coordinator of her college's American Chemical Society Student Affiliates (ACSSA) chapter; worked as a teaching assistant in many chemistry and biology courses and as a lab assistant in a marine ecology lab; and had experience volunteering in computational chemistry research.

Alternative Ligand Metalation Strategies for Alkane Borylation

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Our lab has focused on some of the most challenging substrates for linear hydrocarbon transformations. These substrates are simple alkanes (e.x. n-octane) and are a major chemical feedstock which results from the refinement of petroleum. Hydrocarbons are abundant, cheap, but inherently unreactive, as they lack functionality and only contain carbon-carbon bonds and carbon-hydrogen bonds. It is interesting that catalysts have been developed to react with these molecules; they also show very high selectivity for the terminal $-CH_3$ groups over internal methylenes ($-CH_2$). We have previously identified 2,2'-dipyridylarylmethanes as a highly performing ligand class for undirected alkane borylation (a transition metal catalyst replaces a C-H bond with a C-B bond). Using our novel ligand class, our lab has successfully isolated cyclometalated species of iridium. We plan to expand this chemistry to other transition metals. To do so, we aim to discover new precatalyst candidates across different transition metals by developing a versatile cyclometalation strategy. The newly synthesized aryl bromide ligand precursor (L28/L31) will enable us to access cyclometalated species via transmetalation. After further research, we have successfully isolated, characterized, and crystallized a cyclometalated aryl zinc (Ar-ZnBr). Through transmetalation, we hope to use this Ar-ZnBr to access new potential transition metal precatalysts for alkane borylation and beyond. Early evidence provides potential success of our preliminary transmetalation with ruthenium and rhenium. We are in the process of developing new ligands and stabilized organozinc species for metal-catalyzed reactions. Next steps include optimizing transmetalation conditions and the evaluation of potential applications for isolated metal complexes.

Bio. Montana Price is a rising junior at Tennessee Tech University. She recently graduated with an associate degree in chemistry from Volunteer State Community College near her hometown of Hendersonville, TN. She is currently interning in the Schley Research Lab working on developing a cyclometalation strategy that will enable the exploration of other transition metals to identify and isolate precatalyst candidates. She plans to venture out into forensic pharmacology and conduct research that helps advocate for women's health.

Hypertension worsens ovariectomy-induced bone loss in aged mice

Priya Soma Mathiy[1], Elizabeth M Hennen[2], Sasidhar Uppuganti[3], Santosh Thapa[4], Elizabeth Rendina-Ruedy[4], David G. Harrison[4], Jeffry S. Nyman[2,3]
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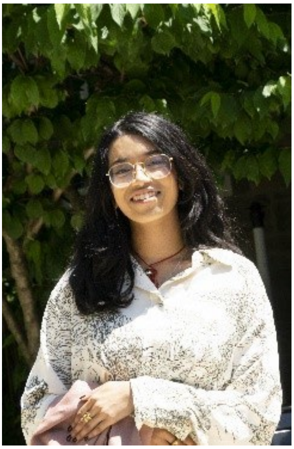
Hypertension (HT) leads to high blood pressure, impacting all bodily systems in ways not thoroughly researched. Estrogen, a hormone proven to support bone density and prevent HT, lead to women being more likely to experience fragility fracture following menopause. This study uses an ovariectomy (OVX) model of menopause-related osteoporosis to determine whether HT interacts with estrogen withdrawal to decrease bone strength. We hypothesize ovariectomized, hypertensive, aged mice will experience worse loss of bone mass and strength than OVX alone or HT alone. C57Bl/6J mice were ovariectomized or underwent sham surgery at 52 weeks-of-age and then given subcutaneous osmotic mini-pumps at 56 weeks-of-age, infusing buffer (Veh) or angiotensin II solution 490 ng/kg/min. Thus, providing 4 groups: Sham-Veh, Sham-HT, OVX-Veh, and OVX-HT (n≥11/group). Infusions lasted 6 weeks before euthanasia when bones and blood were assessed.

Cortical femoral mid-diaphysis and trabecular sixth lumbar vertebra (L6) were analyzed using micro-computed tomography (μCT) and mechanical testing (three-point-bending and compression, respectively). Additionally, serum ELISAs for biomarkers P1NP and CTX-1 were utilized to quantify the osteoblast-osteoclast relationship. Results support estrogen withdrawal from OVX surgery is necessary for angiotensin II-induced hypertension to decrease bone mass and strength. Bone Mineral Density is impacted by OVX conditions with less force needed to fracture L6 after 4 weeks of estrogen withdrawal and 6 weeks of hypertension. Likewise, the femoral mid-diaphysis requires less force breaking cortical bone in OVX-HT conditions vs. OVX-Veh. This suggests post-menopausal hypertension contributes to osteoporosis. Further study is needed to observe bone mineralization and quality in this model.



Bio. Priya S. Mathiy is a rising senior at Penn State University, majoring in Biology and Health Humanities with a minor in Religious Studies. Priya has presented research at Weill Cornell and has won 1st twice within her division at Penn State Abington in Humanities and in Biochemistry. She intends to continue an award-winning study in gastrointestinal stromal tumor cells this fall and to present nationally. Outside of academics, Priya serves as a medical assistant for an OB/GYN office and enjoys kickboxing and trying new foods.

Determining Insulin Aggregation Kinetics and Dipeptide Terminal Capping Effects Using 2D IR Spectroscopy and Amide I Transition Dipole Strength

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Vibrational spectroscopy uses infrared, near-infrared and Raman scattering to measure vibrational frequencies between bonded atoms. Two-dimensional infrared spectroscopy (2D IR) is one of these spectroscopic tools with increased structural sensitivity over linear IR methods and unique cross peaks that indicate coupled modes. 2D IR is also used to calculate transition dipole strength (TDS), which quantifies vibrational coupling and delocalization of vibrational modes. TDS values are particularly useful for distinguishing spectrally similar molecules, such as polymorphs of the same peptide. 2D IR and TDS calculations are broadly applicable to peptide structure and dynamics studies in both small peptides, and complex protein systems with *β*-sheets, α-helices, and disordered proteins. In this study, 2D IR was used to investigate how sequence variations in insulin II, a mouse homologue of the human insulin gene, can affect its aggregation kinetics. The transgenic insulin (B:9-23) variants demonstrated complete aggregation into fibrils (LYLAEV mutant), partial aggregation (E21A mutant), and no aggregation (short 6.9HIP mutant) after two and a half hours. In addition, the stabilization and reduced-charge effects of post-translational protein modifications such as N-terminal acetylation and C-terminal amidation was investigated using alanine dipeptides. These precise studies of molecular interactions demonstrate the advantages of 2D IR in peptide-based studies over other linear methodologies.

Bio. Erica Hengartner is a rising senior in the University of Florida Honors Program majoring in Chemistry with a concentration in Biochemistry. She is a Florida Bright Futures Scholar (2021-2025) and has received a Jorge Mas Canosa Freedom Foundation Scholarship (2021-2025). At UF, the University Scholars Program Cancer Center funds her mechanobiology research in neuron electrophysiology and long-distance cancer cell signaling. She is also a TA for organic chemistry and is an executive board member of the student chapter of the American Chemical Society. She has completed an NSF-funded Biochemistry REU at AgroParisTech in France (2023) and is currently completing a Chemical Biology REU at Vanderbilt University. Following graduation in May of 2025, Erica aspires to pursue a PhD in Chemistry.

31 | GLADYS MARTIEZ FRANCO | VINSE REU

Developing a Microfluidic Model of the Mammary Gland Vasculature to Study Stromal-Immune Cell Interactions

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Triple negative breast cancer (TNBC) is one of the most aggressive sub-types of breast cancer. Because it lacks expression of molecular targets, current treatments are limited to chemotherapy, radiation therapy (RT), and surgery. Previous research from our lab indicates that the interactions between neutrophils and vasculature play a significant role in locoregional recurrence of TNBC. Abnormal vasculature triggered by RT initiates pro-tumor microenvironments, enabling circulating tumor cells to be recruited to the primary tumor site and ultimately leading to TNBC recurrence. Our objective is to identify targetable interactions between neutrophils and vasculature and develop a microfluidic organ-on-a-chip model that will improve the translation of our *in vitro* findings. To study these interactions *in vitro*, irradiated endothelial cells (ECs) were cultured with or without neutrophils at various timepoints post-RT. Immunocytochemistry was used to identify the changes in expression of the NF-kB proteins p65 and p100, which influence vascular remodeling and contribute to a pro-tumor microenvironment. Most notably, we identified an increase in nuclear p100 at 6 days after radiation. We also optimized the design and fabrication protocol of the organ-on-a-chip devices. We utilized polydimethylsiloxane (PDMS) and polyester membranes to fabricate the devices. Membranes were incubated with amine-PDMS linker at 37ºC for 1h or room temperature for 20m. Membranes and PDMS were plasma treated, bonded, and baked overnight at 80ºC. Irreversible bonding of the device was achieved by incubating the membrane in the linker at room temperature for 20m, allowing us to culture cells in the device. The interactions between neutrophils and vasculature will continue to be studied in the microfluidic devices. Identification of vascular remodeling mechanisms that facilitate TNBC recurrence will ultimately lead to more robust treatments and reductions in recurrence for the most vulnerable patients.

Bio. Gladys Martinez Franco is an undergraduate at Cal Poly Pomona, pursuing a B.S. in Chemical Engineering with minors in Materials Engineering and Spanish. She currently serves as a Learning Strategist with the Educational Opportunity Program (EOP) at Cal Poly Pomona, believing that empowerment and belonging are key to student success. By aiding students in developing their skills and knowledge, she fosters meaningful and independent learning. She hopes to one day give back to her community by starting a non-profit that supports low-income, first-generation students interested in STEM. As a member of the Society of Hispanic Professional Engineers (SHPE), she engages in community events, connecting with peers and sharing diverse experiences.

Optimizing PECVD Silicon Nitride Films for Advanced Electronics

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[2]*Interdisciplinary Materials Science, Vanderbilt University*

In the quest for more efficient electronics, particularly Gallium Nitride High Electron Mobility Transistors (GaN HEMTs) for high-frequency applications such as power converters, applying a thin insulating layer, known as passivation, is essential. Silicon nitride (SiN_x) is a top choice for this purpose due to its chemically inert nature, which enhances the electrical properties of devices and protects them from external contamination. This project focuses on optimizing the deposition of SiN_x films using Plasma-Enhanced Chemical Vapor Deposition (PECVD). This method uses plasma as an energy source to create these protective layers. We investigated how varying the RF power (the energy used to generate the plasma), the pressure within the deposition chamber, and the gas ratio of nitrogen and silane (the sources of nitrogen and silicon) impact the quality of the SiN_x films. We identified the optimal conditions for producing high-quality films by adjusting these key parameters. To measure the effectiveness of our SiN_x films, we first used ellipsometry to determine their thickness and refractive index. We then used these films to fabricate capacitors, assessing the performances of our deposited films as dielectrics by measuring breakdown voltage and capacitance. Once the optimal recipe is developed, it will be applied to GaN HEMTs, enhancing their reliability and efficiency which could lead to significant improvements in applications such as electric vehicles.

Bio. Winston Nfor Kanjo Ndi is a rising sophomore at Vanderbilt University, majoring in Mechanical Engineering and Mathematics. With a keen interest in nanotechnology, Winston joined VINSE's Tech crew in the summer of 2024 gaining hands-on experience in nanodevice fabrication and maintenance. He is also a research fellow in the SyBBURE, Searle Undergraduate Research Program, and will be working in Dr. Xiaoguang Dong's lab in the fall of 2024. He will focus on designing, manufacturing, and controlling miniature swarm robots, exploring their potential applications in biomedicine and biomechanics. Additionally, Winston will continue his work in the cleanroom as an Associate Tech crew member, further honing his skills in cutting-edge nanotechnology.

33 | MARGARET MARTE | VINSE REU

Improving Fiber-to-Chip Edge Coupling Efficiency using Inverse Taper Waveguides

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The study of photonic integrated circuits, which use light instead of electric current to carry information on chip, is essential for advancing low-power, high data rate computing technologies. Currently, most photonic integrated circuits rely on off-chip laser sources that must be coupled to on-chip photonic components. In this work, we study inverse taper waveguides, which are light-guiding structures specifically designed to reduce coupling losses when off-chip laser light transmitted through an optical fiber is coupled to on-chip photonic components. We demonstrate through simulations and experiments that appropriately designed inverse taper waveguides can reduce fiber-to-chip coupling losses by more than 3 dB compared to conventional straight couplers. The inverse taper, which narrows at the edge of the chip, reduces the effective index of the on-chip waveguide by delocalizing some of the optical mode of the substrate. This delocalization allows the waveguide effective index to more closely match that of the optical fiber, leading to a higher coupling efficiency. The importance of both inverse taper design and implementation tolerances for achieving high coupling efficiency will be discussed. The enhanced coupling efficiency of the inverse taper waveguides is important for future quantum information and on-chip signal processing applications.

Bio. Maggie Marte is a rising senior at Clemson University majoring in Physics with a minor in Mathematical Sciences. Maggie's research has primarily been studying the electrical properties of piezoelectric materials at cryogenic temperatures. Maggie was also a teaching assistant for the Summer Quantum Engineering Internship Program, and she is a 2024 Goldwater Scholar and Astronaut Scholar. Outside of her research, Maggie serves as the Vice President of the Society of Physics Students Clemson Chapter, and she is involved in the Women in Physics organization. Additionally, Maggie is a member of the Clemson Club Gymnastics team. After receiving her degree from Clemson, Maggie plans to pursue a Ph.D. in condensed matter physics. Professionally, she hopes to conduct research in academia or a national lab on materials and devices for quantum technology applications.

Recreating the Preparation of Anishinaabe Rock Art: Investigating Silica-Hematite Bonding

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Anishinaabe rock paintings depicting various animals, spirits, and humans commonly overlook lakes and rivers in the northern midwest and southern Canada. These paintings are exposed to extreme weathering by wind and water, and yet, they have survived for centuries. This rock art is culturally significant to the Anishinaabeg, but the knowledge of how to prepare this type of art has been lost due to the Iroquoian wars of the eighteenth century and the cultural genocide of the nineteenth and twentieth centuries. The return of the knowledge of the rock painting method used by the Anishinaabeg would positively impact their still-active culture. Previous studies found that the art consists of a hematite (α-Fe_2O_3) pigment layer attached to a silica rock surface. We attempt to replicate the chemistry of this paint in a sol-gel-type reaction involving hematite, silica slides, and catalytic base. Because the methods must be accessible to Anishinaabe painters, hydroxide was sourced from plant ash lye. Since previous research has found the pigment layer to be rich in silicon, various culturally-significant plants were analyzed for their silicon content with inductively coupled plasma optical emission spectroscopy (ICP-OES). We find bulrush (*Schoenoplectus acutus*) and sweetgrass (*Hierochloe odorata*) to be probable lye sources due to their relatively high silicon content that is accessible through simple ash quenching and extraction. Additionally, we find highly-concentrated lye to be essential to pigment-binding. Future work will test paint on granite surfaces as well as simulate groundwater silica seepage to determine paint resiliency in natural conditions.

Bio. Noah Durlam is a rising senior chemistry major at Valparaiso University. He has researched medicinal organic synthesis with Dr. Jeffery Pruet and currently researches nanoplastic formation and solubility with Dr. Julie Peller. He is a recipient of Valparaiso University's Undergraduate Award for Achievement in Physical Chemistry and the ACS Award in Inorganic Chemistry. He is a member of the Phi Lambda Upsilon National Honorary Chemical Society, Beta Sigma chapter. This summer, he received an REU from Vanderbilt Institute of Nanoscale Science and Engineering (VINSE) to study methods of recreating Anishinaabe rock art with Dr. Janet Macdonald.

35 | Allison Wightman | Chemical Biology REU

Understanding Regioselectivity Trends in Ca2+-Mediated Functionalization of Monosaccharides

Allison Wightman[1,2], Valentina Guidi[2], Yunkai Hua[2], Daria Kim[2]

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Glycans are involved in vital signaling functions and cell-cell recognition. However, the molecular mechanisms that underpin these crucial cellular processes are still poorly understood. Our research aims to develop new methods for the precise structural perturbation of glycans through monomer-selective and regioselective transformations of monosaccharides and glycans. Conventional approaches to regioselective carbohydrate modification involve lengthy protection, activation, deprotection sequences that are impractical in application to biological glycan modification. However, single-step site-selective transformations may be possible by leveraging the metal-chelating and/or hydrogen-bonding abilities of sugar residues. Our lab has developed a C2-selective acetylation of methyl-mannopyranoside in the presence of $CaCl_2$, which occurs in 10 minutes at a quantitative yield. This reaction is not only entirely regioselective at the C2 position, but also exhibits substrate-dependent reaction rates that strongly favor mannopyranosides. Our ongoing work aims to clarify the factors which influence the selectivity profile of this reaction. Mechanistic understanding of this process may expand the substrate scope to other monosaccharides and achieve more complex transformations, such as glycosylation to generate complex polysaccharides.

Bio. Allison Wightman grew up in Philadelphia before moving to Grinnell, Iowa to pursue her B.A. degree in Chemistry at Grinnell College. At her undergraduate institution, Allison is involved in investigating the microwave synthesis of α-substituted chalcones under neat reaction conditions under the mentorship of Prof. Stephen Sieck. She is currently participating in the REU program in chemical biology at Vanderbilt University working with Prof. Daria Kim. She expects to graduate from Grinnell College in May of 2025 with a B.A. in Chemistry and then continue her education in graduate school for organic chemistry.

Computational Study of Malononitrile-Based Carbanions for CO2 Capture

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As climate change accelerates, scientists are reevaluating carbon capture and sequestration methods to address the adverse effects of rising atmospheric CO_2 levels. A promising approach involves task-specific ionic liquids (TSILs) for CO_2 removal, which demonstrate significant potential due to their high chemical absorption and CO_2 holding capacity. Among these, malononitrile-based carbanions—organic compounds featuring two cyano (CN) groups attached to a central methylene group—can form reactive negatively charged species that interact effectively with CO_2. In this study, we computationally investigated 11 different malononitrile-based carbanions, each with varying functional groups, to assess their potential for CO_2 capture. The carbanions were computationally analyzed in three stages of bonding with CO_2: physisorption, carboxylate formation, and carboxylic acid formation. Density functional theory (DFT) simulations were conducted using Gaussian and modeled with GaussView 6, providing insights into the electronic structures and interactions of these compounds. The findings indicate that the $CH_3SO_2CHF^-$ carbanion, which incorporates both fluorine and sulfate substituent groups, formed the most stable and spontaneously reactive compounds with CO_2. This conclusion is supported by its Mulliken charge distribution and enthalpy changes. These results suggest a strong potential for TSILs in atmospheric CO_2 removal and lay the groundwork for further research in this area.

Bio. Dhemi Mislenkov is a rising third-year student in a 4+1 dual-degree, double major program studying chemistry at Saint Mary's College and chemical engineering at the University of Notre Dame. At Saint Mary's College, she is an active member of the Drummond Lab, studying non-aqueous redox flow batteries as a potential for the future of renewable energy storage. More specifically, she studies organo-metallic complexes using the ligand tetra-2-pyridinylpyrazine and its iron complexes. Further, at Saint Mary's, she serves as the vice-president of their American Chemical Society Chapter, as well as the Co-Chair for the Student Committee on Research Expansion. At the University of Notre Dame, she is a member of the Grand Challenges Scholars Program, as acknowledged by the National Academy of Engineering. She hopes to pursue a future in materials science and engineering, as she believes that it is the natural intersection between her passions in both chemistry and chemical engineering.

37 | Yukie Chang | VUSE Summer Research Program

Bundle-wise Functional Connectivity Density and Fractional Amplitude of Low-frequency Fluctuations Reveal Declines in White Matter Function and Associations with Aβ, Tau, and Cognition

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Neurophysiological changes associated with Alzheimer’s disease (AD) begin decades before clinical symptoms emerge, a stage known as preclinical AD. Growing evidence indicates structural abnormalities in white matter (WM) in preclinical AD, yet functional abnormalities in WM remain inadequately understood. To explore WM functional abnormalities in preclinical AD, resting-state functional magnetic resonance imaging (rs-fMRI) data of 344 participants from the Alzheimer's Disease Neuroimaging Initiative was utilized to evaluate bundle-wise functional connectivity density (FCD) and fractional amplitude of low-frequency fluctuations (fALFF). The two metrics assess the strength of connection between WM bundle and whole-brain GM regions, and the spontaneous activity of WM bundle, respectively. To mitigate site/scanner effects on the metircs, ComBat harmonization was applied. Permutation tests (n=5000) on each harmonized metric for each bundle was performed to determine differences in FCD and fALFF in preclinical AD relative to controls, adjusting for sex, age, and education using multiple linear regression. Linear correlations of the metrics with pathological biomarkers and cognitive scores were assessed using a general linear model. Multiple compasions were corrected via false discovery rate. Preclinical AD exhibited reduced FCD and fALFF in specific WM bundles compared to controls ($p < 0.05$). These reductions were associated with poorer cognitive performance and higher levels of Aβ and tau accumulation ($p < 0.05$). This study, to the best of our knowledge, is the first to examine both bundle-wise FCD and fALFF in preclinical AD using a large, multi-site, cross-sectional dataset, suggesting potential clinical applications of these metrics for detecting preclinical AD with rs-fMRI.

Bio. Yukie Chang is a senior at Pomona College in Claremont, CA, pursuing a double major in neuroscience and computer science. She has been recognized as a Grew Bancroft Scholar (‘21-‘25), an AMGEN Scholar (‘23), and a Pomona College Scholar (‘21). Yukie’s research interest involves applying her knowledge from both fields to advance studies in neurodegenerative diseases, especially Alzheimer’s and Parkinson’s diseases. Beyond academics, she serves as the student liaison for Pomona’s Department of Neuroscience and enjoys organizing hackathons with peers.

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