11TH ANNUAL UNDERGRADUATE RESEARCH SYMPOSIUM

AUGUST 4, 2022 | 1:30 - 3:30 PM

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Welcome to the 2022 Undergraduate Research Symposium!

The Vanderbilt Institute of Nanoscale Science and Engineering and the Chemical Biology/Chemistry REU are pleased to present the 11th Annual VINSE Undergraduate Research Symposium.

Vanderbilt University's mission lies in the quest to bring out the best in humanity—pushing new ideas into the frontiers of discovery, challenging the limits of what's possible and working diligently in the service of others. Giving undergraduates 10 weeks of immersive research opportunities allows them to gain the skills and experience to accomplish that mission.

Our symposium features the work from students in the following programs:

- VINSE NSF-REU
- Chemical Biology-Chemistry NSF REU
- VINSE Tech Crew
- VUSE Summer Research Program
- Beckman Scholars

Thank you for attending!

Summer 2022 VINSE NSF-REU and Tech Crew

1 LAUREN HUBERT
University of Rhode Island
VINSE NSF-REU (Wilson)

2 DAVID MANKARIOS
Vanderbilt University
VINSE Tech Crew

3 HUNTER DAVIS
Tennessee Technological University
Chemical Biology-REU (Walker)

4 HANNAH BHAKTA
Valparaiso University
Chemical Biology-REU (Stone)

5 MICHAL PEREZ
Vanderbilt University
SUGRE (Valentine)

6 ESABELLA POWERS
Grand Valley State University
Chemical Biology-REU (Cliffel)

7 THIAGO ARNAUD
University of Florida
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8 CALE LOCICERO
Louisiana State University
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Vanderbilt University
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10 CHIAD ONYEJE
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11 SARAH HOURIHAN
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13 ALEC JONES
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14 CAROL HE
Vanderbilt University
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15 TREY THEOBALD
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16 GIANNA PAIER
SUNY Binghamton University
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17 CHRISTINA TROLL
University of Notre Dame
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Vanderbilt University
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University of Central Florida
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Emory University
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23 ANTONY PENG
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Northwestern University
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25 SARAH SIMAN
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26 LAVONTE SAUNDERS
Vanderbilt University
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27 MADELINE HERWIG
Augustana College
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Vanderbilt University
VINSE Tech Crew

VINSE & Chemical Biology REU Ice Cream Social

1 – Lauren Hubert | VINSE NSF REU

Synthesis of Tunable Protein-Polymersome Conjugates for Enhanced Targeting of Cancerous Tissues

Lauren A. Hubert[1], Payton T. Stone[2], Dr. Blaise R. Kimmel[2], Dr. John T. Wilson[2]
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[2]*Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN 37235*

Protein-polymersome conjugates have the potential to impact the field of immunoengineering leading to improved therapeutics via precise targeting and systemic monitoring. Here, we synthesized a library of diblock copolymers consisting of a first, polyethylene glycol (PEG) block, and a pH-responsive second block comprised of Dimethylaminoethyl methacrylate (DMAEMA) bound to an alkyl methacrylate chain. We subsequently utilized a rapid micro-mixing technique (flash nanoprecipitation) to generate an array of polymersomes. Polymer properties including second-block molecular weight and alkyl chain length were varied to optimize a polymeric nanocarrier capable of delivering therapeutics intracellularly. The polymer array was characterized based on size, cytotoxicity, encapsulation efficiency, potential for endosomal escape, hemolysis, and pH responsiveness to help reveal the polymer composition yielding the optimal polymersome. The tuned nanocarrier was then functionalized with an azide group on the PEG first block to enable future conjugation of immunotherapeutics.

We next synthesized a plasmid, encoding for a fusion protein containing mCherry and an antibody fragment for affinity targeting of an upregulated cancer antigen (GD2). We selectively ligated a single bicyclononyne (BCN) functional group onto the C-terminal of the fusion protein using an engineering Sortase A ligase in order to covalently link our fusion protein onto the azide-linked polymersome by strain-promoted alkyne-azide cycloaddition (SPAAC).

Our protein-polymer conjugate was confirmed via flow cytometry and fluorescence microscopy. The presence of mCherry will enable a future pilot study using *In Vivo* Imaging Systems (IVIS) to visualize the specific pathways taken by the protein-polymersome conjugates after systemic administration. Traditionally, polymersomes lack the ability to be systemically traced or target specific areas for intracellular delivery which limits their effectiveness as nanocarriers. Further, this study provides the basis for the future exploration of polymersomes linked to selectively ligated proteins allowing for enhanced functionality of these nanocarriers in biomedical applications.

Bio. Lauren Hubert is a rising junior, chemical engineering major on a pharmaceutical-focused track at the University of Rhode Island. She received the prestigious Thomas M. Ryan Scholarship from URI allowing her to become one of the seven members of the inaugural class of Ryan Scholars studying at the University with a full scholarship. She has completed 2 semesters of undergraduate research under Dr. Daniel Roxbury working on *in vitro* studies with a specific class of nanomaterials: single-walled carbon nanotubes. In that time, she has successfully applied for and obtained the $(URI)^2$ Undergraduate Research Grant and was published in ACS Applied Materials & Interfaces with the project titled: “Aggregation Reduces Subcellular Localization and Cytotoxicity of Single-Walled Carbon Nanotubes.” Over her two complete years at URI she has made the Dean’s List all four semesters, she was elected for an E-board position in the Sigma Gamma chapter of the professional engineering co-ed fraternity Theta Tau, and she has maintained memberships in both the American Institute of Chemical Engineers (AIChE) and the Society of Women Engineers (SWE). She hopes to continue working in the field of immunoengineering as she continues with undergraduate research and eventually pursues a PhD in chemical engineering.

2 | David Mankarios | VINSE Tech Crew

The Fabrication of Plasmonic Bull's Eye for Imaging Enhancement and Nano Tweezers

David Mankarios[1,2], Chuchuan Hong[3], Justus C. Ndukaife[3,4]
[1]*Department of Biological Sciences, Vanderbilt University, Nashville, TN*
[2]*Department of German, Russian, and East European Studies, Vanderbilt University, Nashville, TN*
[3]*Department of Mechanical Engineering, Vanderbilt University, Nashville, TN*
[4]*Department of Electrical and Computer Engineering, Vanderbilt University, Nashville, TN*

The capturing of microparticles is critical to many Nano-based biomedical endeavors and calls for a tweezing device that can operate on such a scale. A plasmon is to plasma as a photon is to light while a polariton is a quasi particle made up of a photon and an electron. A surface plasmon has less energy than a bulk plasmon and exists at the interface between two materials where the dielectric function changes signs across the interface. Using a Surface Plasmon Polariton (SPP), or the sum of all vectors parallel to the metal substrate through the oscillation of the surface plasmon on a planar surface, an electric field is induced both inside and outside the metal. With the patterning of a grating on this metal substrate, the excitation of the SPP is enabled as a photon is shot at it with an equivalent wavelength and frequency, dispersing energy. Using Physical Vapor Deposition (PVD) through the Multimode Deposition Chamber, clean glass samples (compressed SiO_2) have approximately a 5 nm layer of chrome and a 80 nm layer of gold deposited on them. This substrate is then taken to the Focused Ion Beam-Scanning Electron Microscope (FIB-SEM) where a 16.6 μm by 16.6 μm Bull's Eye Grating is patterned onto it. The Bull's Eye Grating allows for subwavelength optics in microscopy beyond the diffraction limit through the use of SPPs, creating imaging enhancement. The consequential electric field can likewise potentially be used for nano tweezing in future endeavors and thus produces Nano tweezers for the trapping of microparticles.

Bio. David Mankarios is a rising Sophomore at Vanderbilt University majoring in Biological Sciences and German. He joined VINSE during the summer of 2022 as part of the Tech Crew program for undergraduate students. As a member of the Tech Crew, David keeps up the cleanroom while also helping users with their research. David is currently conducting research under a graduate student, using advanced machinery such as the Focused Ion Beam Scanning Electron Microscope to fabricate a Plasmonic Bull's Eye grating. In his free time, David likes to read and play soccer. He has a love for languages and intends to bring the underlying connection of empathy and connection found in these cultural differences to his future work in clinical environments.

3 | Hunter Davis | Chemical Biology/Chemistry NSF REU

Computationally Guided Antibiotic Discovery from Natural Products of Streptomyces

Hunter Davis[1], Allison Walker, PhD[2]
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[2]*Department of Chemistry, Vanderbilt University, Nashville, TN*

As more pathogens become resistant to current antibiotics, there is an increasing need for new antibiotics. Traditionally this was done by high throughput screening of natural products, but this method alone has become uneconomical. As a result, the number of antibiotics discovered per year has decreased. In response to this issue, one strategy is to use computational means to identify active metabolites. Such methods include the use of: antiSMASH to predict biosynthetic gene clusters, machine learning for activity prediction, GNPS to identify analogs through molecular networking, and MZmine for comparison of mass spectra to known compounds. The goal of this study is to validate these methods on *Streptomyces noursei* and *Streptomyces yunnanensis*. This genus is of interest due to its reputation as a producer of bioactive metabolites. Solid and liquid cultures of the bacteria were extracted and screened for antibacterial activity against *Bacillus subtilis*. There is evidence to support the presence of up to four novel antibacterial compounds. The mass spectral data do not provide known matches when compared to multiple databases. Despite the lack of structural data, a list of potential masses can be produced for one of the compounds while an incomplete peptide sequence can be made for another. The results of this study demonstrate that it is possible to fulfil the need for new antibiotics more efficiently with a computationally guided approach.

Bio. Hunter Davis is a rising senior at Tennessee Technological University majoring in biochemistry & cell and molecular biology. He began his exposure to the field of biochemistry during high school with an internship focused on the development of monoclonal antibodies. His most significant research experience as an undergraduate at TTU has been the involvement with topoisomerase inhibition towards cancer therapy in the Jiang Lab.

4 | Hannah Bhakta | Chemical Biology/Chemistry NSF REU

Replication Bypass of N-(2-Deoxy-D-*erythro*-pentofuranosyl)-urea Adducts by Human DNA Polymerase η

Hannah Bhakta[1,2], Rachana Tomar[2], Michael P. Stone[2]

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[2] *Department of Chemistry, Vanderbilt University, Nashville, Tennessee 37235, USA*

DNA can be damaged by many natural sources, and can lead to cancer, neurological diseases, and aging. N-(2-Deoxy-D-*erythro*-pentofuranosyl)-urea adducts are formed by oxidative damage done to guanine or thymine. Human DNA polymerase η ("hpol η") is known to aid in error-free replication when the duplex contains a damaged nucleotide. We made the urea-adducted 12-mer deoxyoligonucleotide sequence from a thymine glycol-containing template and annealed it with a 5'-FAM-labeled primer sequence. Next, we performed replication assays with purified hpol η after incubating with the urea-modified DNA duplex and verified the correct nucleotide insertion opposite the modified base. In this preliminary study of urea adducts, we used gel electrophoresis in an effort to confirm this insertion of the dNTP opposite the urea lesion.

Bio. Hannah Bhakta is a rising junior at Valparaiso University majoring in biochemistry and minoring in Spanish. At her home university, she works under Dr. Jeffrey Pruet to synthesize *Argemone mexicana*-inspired antimicrobial products, and she has been working on this project for three semesters now. Bhakta has presented at the Indiana Academy of Science as well as colloquiums and symposiums at Valparaiso University. She is also a recipient of the Edith S. Lessor Memorial Scholarship for excellence as a woman in the field of biochemistry. At Vanderbilt University through the Chemical Biology REU, she has pursued structural biology research in the Stone Lab to further understand the capabilities of human DNA polymerase η.

5 | Michal Perez | SUGRE

Realizing Silicon Nitride (Si_3N_4) Based Metasurfaces for Visible Spectrum Applications

Michal Perez[1], Chibuzor Fabian Ugwu[2], Elena Kovalik[3], Jason Valentine[2]

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[2]*Department of Mechanical Engineering, Vanderbilt University, Nashville, TN*

[3]*Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, TN*

The study of metasurfaces is a highly dynamic field with ever expanding applications in holograms, invisibility cloaks, lab-on-fibers, metalenses, and much more. Metasurfaces are optically thin films composed of sub-wavelength structures that can be used to manipulate phase, amplitude, and polarization. Many state-of-the-art metasurface devices revolve around silicon or metallic nanostructures. These materials limit applications to frequencies below the visible spectrum due to high absorption losses. Silicon nitride is a promising material for visible spectrum based metasurfaces given its wide energy band gap, efficient scattering abilities, low loss, and ease of fabrication. The purpose of this project was to develop fabrication procedures for silicon nitride metasurfaces operating in the visible spectrum. Four different plasma-enhanced chemical vapor deposition (PECVD) processes of silicon nitride involving ammonia, silane, and nitrogen gas, were developed and optimized to produce various optical properties (high refractive index, low loss). The highest index film was produced with $n \approx 2.05$, and the film with the smallest extinction coefficient was produced with $k_{max} = 0.00016$— while being nearly lossless at $\lambda > 475$ nm. Additionally, a selective reactive ion etching process (RIE) using sulfur hexafluoride and fluoroform was developed to yield high aspect ratio silicon nitride nanoarrays.

Bio. Michal Perez is a rising junior at Vanderbilt University in the Valentine lab majoring in chemical and biomolecular engineering with minors in chemistry and nanoscience and nanotechnology. He joined the VINSE technical crew in the summer of 2021 and his interests include developing and improving fabrication processes used in the VINSE cleanroom.

6 | Esabella Powers | Chemical Biology/Chemistry NSF REU

Microfluidic Electrochemical Biosensors for Simultaneous Multianalyte Detection

Esabella R. Powers[1], Pragun Tuladhar[2], David E. Cliffel[2]

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[2]Department of Chemistry, Vanderbilt University, Nashville, TN 37235, United States

Monitoring electrolytes within biological fluids can provide vital information about homeostasis and cellular metabolism. Electrolytes are typically analyzed from urine, blood, sweat, etc. using solid contact electrodes. However, current techniques do not allow for continuous monitoring, low volume measurements, and multianalyte detection. In this work, a screen-printed electrode (SPE)-based potentiometric sensor for potassium ion detection under laminar flow was developed. An ion selective membrane was added to the platinum working electrodes of an 8-channel SPE enclosed in a microfluidic chamber. Ion selective membrane formulation, conducting polymer layer, and electrode conditioning parameters were optimized for linear range, sensitivity, and selectivity. Potentiometric data was collected by a CHI 1440 potentiometer. The potassium sensor gave a linear response between 58 µM–25 mM KCl in phosphate buffered solution and had a sensitivity of 71.88 ± 5 mV decade^{-1}. A poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonate) (PEDOT: PSS) conducting polymer layer was investigated to enhance selectivity in the presence of other cations. The potassium sensor will ultimately be a part of a combined potentiometric and amperometric detection platform capable of simultaneously measuring dynamic concentrations of ions and small molecules. In the future, this sensor will be used for continuous monitoring of various biomarkers from tissue cultures to assess the progression of disease or toxicity.

Bio. Esabella “Esa” Powers currently attends Grand Valley State University in Allendale, Michigan. She is studying biomedical sciences and chemistry. At Grand Valley, Esa performs physical chemistry research with Dr. George McBane. The research investigates collision broadening coefficients between differing gases at different pressures spectroscopically. Esa is a member of the National Society of Leadership and Success and the chemistry club. Esa has made the Dean’s list each semester attending Grand Valley and is the recipient of both the Grand Valley Award of Excellence and Faculty Scholarship. Recently, she was awarded the ACS Physical Chemistry Division of Undergraduate Award and Biomedical Science Graduate with Distinction.

7 | Thiago Arnaud | VINSE NSF REU

Filterless Infrared Chemical Sensing with Narrowband Thermal Emitters

Thiago S. Arnaud[1,2], Guanyu Lu[2], Mingze He[2], Ryan Spangler[3], Josh Nordlander[3], John-Paul Maria[3], Joshua D. Caldwell[2]

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A plasmon polariton is a quasiparticle made from the coupling of a photon with coherently oscillating free carriers. A TAMM plasmon mode is where a plasmon polariton is induced between a distributed Bragg reflector (DBR) and a conductive surface, which provides a significant reduction in spectral linewidth. Here, we implement a machine-learning algorithm to inversely design the structure of the aperiodic DBR and the carrier concentration of the doped CdO, an n-type semiconductor that we use as the conductive layer to support the TAMM plasmon. Due to the tunability of these structures, they can be designed for narrow absorption and thus, thermal emission peaks at arbitrary spectral position, linewidth and amplitude. This attribute allows for the design of selective infrared sources for chemical sensing, which targets the emission to match the vibrational mode of a desired molecule. Commercially, chemical sensing techniques are limited to one target molecule per device due to the dependence of a bandpass filter to eliminate other frequencies where molecules not of interest absorb. By implementing a TAMM-emitter-based sensor, we demonstrate its viability for filterless non-dispersive infrared sensing featuring an increase in discrimination for a molecule of interest. Two TAMM emitters were designed, fabricated and tested; one for CO_2 and another for CO gas sensing while having a low and indiscriminate absorption of the other when present. From plotting the ratio of power decrease due to gas absorption as a function of concentration, the TAMM demonstrated a more accurate sensitivity for concentrations of CO_2 than a blackbody with a bandpass filter.

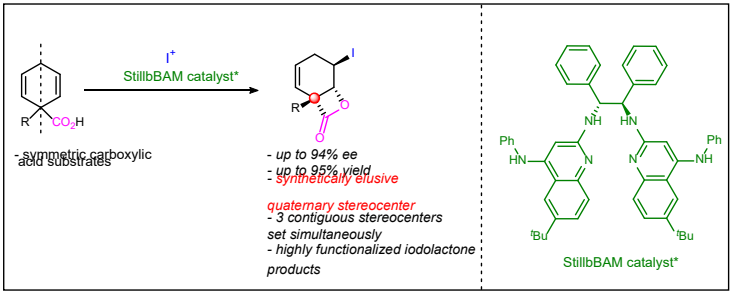
Bio. Thiago Arnaud is a rising junior from Miami, Florida. He studied at Florida International University as a Mechanical Engineer with FIU's Presidential Merit Scholarship and Florida's Bright Futures Academic Scholar. He switched majors to Physics due to his curiosity to understand fundamental concepts. He is now enrolled at University of Florida for a Bachelor of Science in Physics. In the Summer of 2021, he participated in the VINSE REU under Dr. Joshua Caldwell on a robust method of thermal imaging. He is working again with Dr. Caldwell this summer to learn more of the skills and research concepts that will prepare him for a successful graduate student career.

8 | Cale Locicero | Chemical Biology/Chemistry NSF REU

Enantioselective Desymmetrizations of Carboxylic Acids Using Chiral Proton Catalysis

Kalisankar Bera[1], Matthew T. Knowe[1], **Cale M. Locicero**[1], and Jeffrey N. Johnston[1]
[1]*Department of Chemistry and Institute of Chemical Biology, Vanderbilt University*

Within the field of asymmetric catalysis, desymmetrization reactions present themselves as valuable opportunities to build stereochemical complexity from simple prochiral starting materials. Despite the utility of these reactions, desymmetrizing halolactonizations are few, perhaps due to the difficulties associated with controlling the nucleophilicity of the carboxylate and activation of the halonium ion while achieving group-selective (*Z*-alkene) differentiation. Herein we report the enantioselective desymmetrization of cyclohexadiene carboxylic acids using chiral proton catalysis. The resulting β-lactones contain an all-carbon quaternary stereocenter and are formed in high selectivity.



The reaction products are purified by chromatography, structurally characterized using spectroscopic methods, and analyzed for enantiomeric enrichment using chiral HPLC. The ultimate goal of this endeavor is to advance the limits of organocatalysis by addressing a synthetically challenging chemical transformation that can access stereochemically complex building blocks for applications toward syntheses of biologically and pharmaceutically relevant small molecules.

Bio. Cale Locicero is an Astronaut, Goldwater, and American Chemical Society Scholar and is an Ogden Honors College Senior pursuing a B.S. in chemistry at Louisiana State University. He is President of the Student Affiliates of the American Chemical Society and Vice President of Faculty Relations of the LSU Research Ambassadors. Cale is a research assistant in the Kartika Group, where he develops novel organic reactions for the production of medicinally relevant chemical structures with special emphasis on the creation of all-carbon quaternary stereocenters. Additionally, Cale is a 2022 NSF-REU student in the Johnston Lab in the Vanderbilt Chemical Biology REU Program. He performs research in enantioselective chiral proton catalysis with a focus on alkene desymmetrization reactions. From September 2020 to February 2021, he performed research under Professor Adam T. Melvin in the LSU Cain Department of Engineering and created microfluidic concentration gradient generators to test synergistic combinations of antibiotics against E. coli biofilms. Cale has experience in nuclear magnetic resonance spectroscopy, infrared spectroscopy, gas chromatography-mass spectrometry, chromatographic techniques, microfluidics, soft lithography, 3D printing, bacterial culture, and computer programming. In his free time, he enjoys reading scientific literature on various topics, hiking, and programming.

9 | Laura Bertolami | VINSE Tech Crew

Optimization and Characterization for Precise Electron Beam Lithography Patterning

Laura Bertolami[1], Tao Hong[2]

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[2]*Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, TN*

Nanoscience is steadily becoming more prevalent in research due to its wide applications to everything from pharmaceutical drug delivery to solar cell fabrication. One recent application is the ability to tailor light into individual colors using metasurfaces that function as conventional optical filters. Metasurfaces have structures smaller than the visible light spectrum, which are very useful in optical research because of their ability to filter light passing through the metasurface to produce color. However, these metasurfaces have a challenging and time-consuming fabrication process that requires immense precision and excessive trial and error to achieve the desired color. I have focused on optimizing the liftoff process, which includes calibrating the thickness of the bilayer photoresist layers and ensuring a metal deposition perpendicular to the metasurface structures. By fine-tuning the fabrication process and including a characterization by machine learning to match the color of the metasurface to distinct patterning dimensions, we can potentially reduce the characterization time and increase the reproducibility to streamline metasurface production. This will allow for true color production without the use of dyes and pigments. This is useful in nanophotonics and has potential as a lens for color identification.

Bio. Laura Bertolami is a rising Junior at Vanderbilt University majoring in Chemical Engineering and minoring in Chemistry. She is from Lafayette, California. As a member of the VINSE Tech Crew, she works predominantly in the VINSE Cleanroom and under the mentorship of Tao Hong. She is also an active member of Vanderbilt Student Volunteers for Science, a student organization focused on encouraging science middle school students of the Nashville metropolitan area. She is also an oboist in the Vanderbilt University Concert Band.

10 | Chiad Onyeje | VINSE NSF REU

Utilizing Microfluidics to Optimize the Formulation of Antioxidant Microparticles

Chiad Onyeje[1], Blake Hanan[2], Carlisle DeJulius[2], Craig Duvall[2]

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Reactive oxygen species (ROS) are a key driver of inflammation in degenerative diseases, and treatment strategies targeting ROS overabundance have shown promise in many studies. Sulfide-containing polymers (polysulfides) can scavenge ROS and can be formulated into drug-loaded microparticles for disease treatment. The classical method for particle formulation utilizes a bulk oil-in-water emulsion technique, with the polymer being introduced dropwise with the oil phase into the water phase. However, this technique is difficult to control and typically results in particles with large size variability. Thus, the introduction of microfluidic devices as a formulation process aims to provide a new method of polysulfide microparticle generation that can quickly and effectively produce batches at a controllably consistent size.

We have developed an in-house fabrication method utilizing customizable etched channels on a glass slide base. We flow the oil and water phases while harnessing droplet microfluidics to produce microparticles. This project focused on optimizing the flow rate and pressure in the device for particle production. We also tested various oil phase solvents (dichloromethane, chloroform, and ethyl acetate) for compatibility with the device. Finally, we compared the reactivity of microparticles formulated from two polysulfide derivatives in the presence of ROS via an overdosage of hydrogen peroxide (a common reactive oxygen species), demonstrating that the composition of the microparticle directly affects the rate of scavenging.

Bio. Chiad Onyeje is a biochemical engineering student at the University of Maryland, Baltimore County (UMBC). He currently attends the school as a member of the prestigious Meyerhoff Scholars program in its 31st cohort. Throughout his college career, Chiad has been delving deep into the research of the biological & chemical sciences. His projects have included a microscopy study on the brain tissue of ferrets performed before entered college, a concurrently running study on the development of nanoparticles to seal traumatic internal bleeding, and the currently presented development of microfluidic devices for microparticle formulation. His desire to seek out new horizons and understand the quickly growing field of nanotechnology has even led to a review paper's publication early last year.

Performing research at his home university of UMBC, The Johns Hopkins University, and now Vanderbilt University are testaments to his dedication towards seeking out answers in a field where questions begin. He is currently seeking new avenues to explore the biochemical and biomedical applications of engineering research, such as graduate school Ph.D. programs.

11 | Sarah Hourihan | Beckman Scholar

Significant song and genetic differences between subspecies of the dark-eyed junco

Sarah Hourihan[1], Nicole Creanza[1]

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Following the Last Glacial Maximum that occurred approximately 18,000 years ago, the dark-eyed junco (*Junco hyemalis*) songbird experienced rapid phenotypic diversification. Presently, there is an array of subspecies occupying known regions across North America. Each subspecies bears distinct plumage colors and patterns. In our study, we included the six widely recognized subspecies. As a result of territory separation and mating within subspecies, we hypothesize that there are significant song and genetic differences between the subspecies. Birdsong is a learned behavior, with juveniles learning their songs from an adult conspecific tutor. Birdsong is used in species recognition, mate attraction, and territory defense. If the subspecies' songs differ significantly, song may be accelerating the rate of reproductive isolation between the subspecies, which could ultimately lead to speciation. Learned behaviors such as birdsong can allow species to adapt and evolve faster than what genetic evolution allows. Given the subspecies' distinct plumage and possible song differences, we were curious whether those differences are reflected in the subspecies' genetic differentiation. We parsed and analyzed song recordings from digital citizen-science repositories, genetic data from NCBI, and known location coordinates of dark-eyed juncos to better understand the current evolutionary landscape of the dark-eyed junco species complex. We found significant song and genetic differences between the subspecies, which suggests that 1) the subspecies are different in ways additional to plumage and 2) the subspecies could be becoming more distinct.

Bio. Sarah Hourihan is a rising junior at Vanderbilt University. She is studying Biological Sciences and Music (clarinet), with a possible minor in Data Science. Last summer, she began researching with the Creanza Lab as a Pre-MARC Summer Research Fellow to study the evolutionary effects of learned behaviors such as birdsong. In January 2022, she was named a Vanderbilt University Beckman Scholar, supported by the nationally recognized Arnold and Mabel Beckman Foundation. On campus, she is involved with the Spirit of Gold Marching Band, Asian-American Student Association, Nashville Navigators, FirstVU, and Blair School of Music wind symphony. In the future, she hopes to pursue her passion for research through graduate studies.

Achieving Phase Purity in Nickel Sulfides

Roxanne Hinojosa[1,2], Jeremy Espano[2], Alexandra Koziel[2], Janet Macdonald[2]
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There are seven known phases of nickel sulfide: vaesite, millerite, NiS, godleskvite, Ni_7S_6, polydymite, and heazlewoodite. Understanding how to obtain one phase over the other would allow for more reproducible, synthetic control as well as obtain more diverse materials for a wider range of applications such as catalysis and semiconductors. Here we aim to obtain each allotrope of nickel sulfide in its phase pure form by using various chemical tools and methods to manipulate the synthesis of these phases. By changing the ratio of precursor to nickel (II) stearate, the solvent, the substituted thiourea used in the reaction, the time of the reaction, and the injection temperature, we were able to obtain vaesite in its pure form, millerite, NiS, and polydymite. By systematically changing these aspects of the synthesis, we were able to understand how the nucleation and transformations of these phases happen, such as the transformation of vaesite to polydymite, and the co-nucleation of millerite and NiS. Using this knowledge will enable the synthesis of uncommon and rare phases of the nickel sulfide family.

Bio. Roxanne Hinojosa hails from Lewisville, Texas, and is a rising sophomore at the University of Oklahoma-Norman majoring in Chemical Engineering and minoring in Computer Science. While she attended Marcus High School in Flower Mound, Texas, she was a part of the National Honor Society, Spanish Honor Society, Science Honor Society, and was an athlete on the cheer team for all four years. Currently, she is a teaching assistant and tutor in the Diversity and Inclusion program at the University of Oklahoma where she assists in the education of culturally and socio-economically diverse freshmen. In her free time, she enjoys partaking in social events hosted by the Society of Women Engineers.

13 | Alec Jones | Chemical Biology/Chemistry NSF REU

Improving Iridium-Catalyzed Borylation via Ligand Iteration

Alec P. Jones[1,2], Nicole Brandau[2], and Nathan D. Schley[2]
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Hydrocarbon borylation chemistry has emerged as a premier method of carbon-hydrogen bond activation in recent decades, but more recently alkane (sp^3) C-H borylation has emerged as a promising method to functionalize inexpensive chemical feedstocks into useful, valuable, and more complex chemical building blocks. Simple linear hydrocarbons like *n*-octane which constitute a major fraction of crude oil deposits can be upgraded into more valuable products. The intrinsic selectivity of the borylation process for terminal positions provides access to linear α alcohols, acids, and related derivatives which have greater value than branched products derived of other methods. The Schley Group has found that dipyridylarylmethane ligands which coordinate with iridium ions to form catalysts for borylation give particularly high yields compared to previous catalysts. One of the most efficient ligands yet identified includes a single fluorine substituent found to be essential for high activity. Our current studies aim to build on this finding by exploring related ligand derivatives which may shed light on the role of fluorine substitution in controlling alkane borylation activity and lead to improved performance for future iridium-catalyzed borylation processes. Air-free chemistry techniques and equipment, including a Schlenk line and inert-atmosphere glove box were used to synthesize these ligands.

Bio, Alec Jones is a recent graduate from Motlow State Community College. Having begun his studies in Biology, he plans on attending Middle Tennessee State University to complete his Bachelor of Science. In his final semester at Motlow, he received the Chemistry Department Award for outstanding performance. This undergraduate research experience at Vanderbilt University has fervently ignited his passion for synthetic chemistry, which he hopes to apply to his future career opportunities.

Insights into Coarse-Grained Stratum Corneum Lipid Simulations

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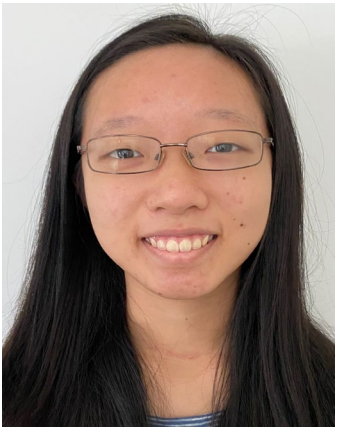
The stratum corneum (SC) is the outermost layer of the skin and serves as the primary barrier against external penetrants and water loss. It has a brick-and-mortar structure; the "bricks" are corneocytes (dead skin cells), and the "mortar" is lipid lamellae consisting primarily of ceramides, cholesterol, and free fatty acids in an equimolar ratio. The primary pathway for diffusion is through the lipid lamellae, so the SC barrier function is highly dependent on the lipid structure and organization. Unlike experiments, simulations provide a highly controlled molecular view of the lipid matrix and can assist in studying relationships between lipid composition, structure, and organization. These insights further our understanding of healthy and diseased skin structure, which can provide a framework for designing topical treatments that restore and manipulate the barrier to allow for drug delivery. To understand the SC structure, we implement coarse-grained (CG) molecular dynamics simulations to self-assemble lipid multilayers. Through these simulations, we examined the minimum number of lipids required to form stable layers. Additionally, the ceramides we examined varied in the level of hydroxylation in their head group chemistry. We were able to understand how changing the hydroxyl groups correlates with structural property data and the lateral and lamellar packing. Finally, we tested our CG model by comparing directly to experimental work. Through our understanding of ceramide head group packing, we studied the role of lipid tail length in experimental diseased and healthy skin mixtures.



Bio. Carol He is a rising sophomore majoring in Computer Science at Vanderbilt University. She is from Marion, AL and is a National Merit Scholar. Since January 2022, she has researched in the Walker and McCabe Labs at Vanderbilt University to learn more about the biological and chemical applications of computer and data science. When Carol is not writing Python scripts and analyzing data for research, she is a developer at Change++ (a club that codes for nonprofits), helps out on the mechanical team at Vanderbilt Robotics, and works on small coding projects with friends.

15 | Trey Theobald | VINSE NSF REU

Identifying Early Developmental Neurotoxicity Modeled in a Cerebral Organoid System

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Pregnant individuals are typically excluded from traditional clinical trials due to ethical and safety concerns for the fetus. This lack of data leads to challenges in managing the health concerns of the expectant patient while also protecting the developing fetus from neurologically damaging medications. To be able to effectively understand how certain medications impact fetal neurodevelopment, alternative screening methods for neurotoxicity are essential. Here, we provide a scalable, human specific model for neurological drug toxicity screening using human induced pluripotent stem cell derived cerebral organoids that model the growth and layering of the developing fetal brain. In control organoids, neural progenitors ($SOX2^+/PAX6^+$) comprised the center of the tissue while mature neurons ($ßIIIT^+/TBR1^+$) formed the outer surface. We tested gabapentin for neurotoxicity using folic acid and valproic acid as controls to verify the sensitivity of our system. Size and shape characterization over 30 days revealed that folic acid and gabapentin drug concentration did not affect the growth kinetics of organoids while organoids dosed with valproic acid exhibited a decreased growth rate at a concentration of 10 mM. Secondary cell titer assays revealed decreased viability in organoids with high concentrations of valproic acid, confirming the size characterization. Preliminary spinning disc confocal imaging indicated that organoids dosed with 10mM valproic acid exhibited few $ßIIIT^+$ cells. Future development of our high throughput screening organoid model will provide an ethical and efficient method of evaluating neurotoxicity for early developmental and fetal populations.

Bio. Trey Theobald is a sophomore in the Honors Program at Ohio Wesleyan University majoring in biochemistry. Trey is a sprinter and thrower on the track team and was named Ohio Wesleyan's 2022 Most Outstanding Freshman. He is active in the health science community on campus and serves as the treasurer of the Ohio Wesleyan Health Sciences Club. This summer Trey is working in Dr. Ethan Lippmann's lab with his graduate student mentor Andrew Kjar to develop an early developmental neurotoxicity screening technique using cerebral organoids. Trey would like to thank Andrew, Dr. Lippmann, and the rest of his research team for their guidance and direction throughout the summer. The collaborative nature of the VINSE program has inspired Trey to pursue the possibility of future research. Finally, Trey is grateful for the experience he has had this summer with the VINSE staff as well as the rest of his cohort both within and outside of the laboratory.

16 | Gianna Paier | VINSE NSF REU

Using Machine Learning with Porous Silicon to Determine IgG Concentrations in Human Serum

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The importance of accurate, robust, and cheap disease diagnostics has proven to be essential in modern society. However, many diagnostic techniques are only available in a clinical setting with trained personnel and expensive, bulky instruments, including the quantification of different protein levels in human serum. Elevated levels of certain serum proteins can indicate a variety of diseases. In this work, we investigate a new approach using a porous silicon material, optical reflectance measurements, and machine learning analysis, which could enable point-of-care serum protein testing. Porous silicon (PSi), fabricated by electrochemically etching nanoscale pores into silicon wafers, is a promising material to form the basis for small, cheap, and robust diagnostic tests. Physical properties of PSi pores, such as size and shape, can be tuned by changing the etching current density and duration. This determines how different molecules selectively enter and adsorb in the pores, which can be quantified by measuring shifts in optical reflectance spectra. Here, we explore which pore sizes most effectively separate Immunoglobulin G (IgG), one of the most abundant serum proteins, spiked in a healthy human serum control. We found that a current density of 80 mA/cm^2 best discriminated IgG from other serum proteins, both in terms of optical response magnitude and kinetics. At the highest etching current density investigated (100 mA/cm^2), which gives the largest pores, sensor response to IgG spiked serum was no different to the control, likely due to surface saturation. At the lowest studied current density (60 mA/cm^2), which gives the smallest pores, there was negligible difference in response, since IgG is too large to enter the majority of the pores. To further refine the initial design of our sensor, we will study other characteristics that effect pore selectivity such as solvent pH and hydrophobicity. Data from the optimized PSi sensor will be fed into a machine learning algorithm to quantify IgG in serum. This approach can provide a convenient solution to many medical diagnostic challenges in the doctor's office, or even at home.

Bio. Gianna Paier is a rising senior studying biomedical engineering with a concentration in biomedical devices at Binghamton University. Gianna spent her summer in the Weiss lab at Vanderbilt researching the development of point-of-care medical devices using porous silicon. In fall 2021, Gianna was inducted into Alpha Eta Mu Beta, the biomedical engineering honors society, and Tau Beta Pi, the engineering honors society. She will be acting as the secretary for Tau Beta Pi in the coming academic year. She was the Vice President of the Biomedical Engineering Society (BMES) for the past 2 years and was elected to be President for next year. Gianna is also an active member of Alpha Omega Epsilon, having been their historian, outreach, sisterhood, and professional chair. Gianna has also been a peer tutor through the Educational Opportunity Program (EOP) for the last year. She was a physics lab teaching assistant during the fall 2020 and spring 2021 semesters, where she led the class by performing scientific demonstrations and answering questions to cultivate students' interest in the field. She is also excited to be a course assistant for the biomedical instruments and devices lab this coming semester under the guidance of Ammar Abdo. Gianna plans to pursue her PhD in biomedical engineering after she finishes her undergraduate education. She is grateful for her experience, and the people she met this summer for the support that guided her towards this decision.

17 | Christina Troll | Chemical Biology/Chemistry NSF REU

Investigation of the XPA-RPA Interaction in Nucleotide Excision Repair

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Nucleotide excision repair (NER) is an essential process by which cells repair bulky DNA lesions. NER requires the action of multiple proteins, including both Xeroderma Pigmentosum Complementation Group A (XPA) and Replication Protein A (RPA). XPA and RPA both interact with the DNA as well as with one another via two interacting regions with differing affinities. While there are various mutations in XPA that can cause lower NER activity, the mechanism remains unknown. Several NER-deficient mutations of interest are located in one of the RPA-interacting regions of XPA. This work seeks to test the hypothesis that XPA mutation reduces interaction with RPA and causes NER defects. Recombinant wild type XPA protein as well as the XPA mutants M113I and D114Y were expressed and purified. Isothermal Titration Calorimetry (ITC) was performed to test the binding affinity of purified XPA and RPA. Using this technique, the dissociation constant (K_D) was determined. By comparing the K_D values of XPA mutants to the K_D value of wild type protein, it was possible to test whether the XPA mutants have altered RPA binding affinity. Preliminary analyses have revealed that single point mutations are not sufficient to significantly alter the XPA-RPA binding affinity, which suggests that the reduced NER activity associated with these XPA mutants should be attributed to another factor.

Bio. Christina Troll is a rising senior biochemistry major at the University of Notre Dame in Notre Dame, Indiana with minors in bioengineering and real estate. There, she performs biochemical research under the guidance of Dr. Katharine White. She studies the consequences of increased intracellular pH (pHi) on the polarization of the Golgi apparatus and subsequently, single cell migration using the light activatable optogenetic tool Archaerhodopsin. This fall, Christina will be presenting this research at the American Chemical Society conference. In addition to research, she seeks to aid other students by working as an undergraduate teaching assistant and is involved with the Chemistry/Biochemistry Club and the Graduate School Student Club. She made Dean's List in the Fall of 2021 and will graduate with Honors upon completion of her thesis this spring.

18 | Esther Ayoade | VINSE Tech Crew

Fabrication of Microfluidic Devices with Integrated Sensing Capabilities for Electrophysiology Retina Studies

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Microfluidics allows for the precise flow of small quantities of liquids through micro-scale channels. It reflects the unique properties of these fluids which would not be normally seen in macroscopic channels. These systems are developed following photolithographic processes that utilize the exposure of ultraviolet light onto a photosensitive material to pattern a design onto a substrate. Microfluidic devices are used for biomedical applications including organ-on-a-chip technology and the formation of nanoparticles for drug delivery. My goal is to implement various techniques— metal deposition, photolithography, and soft lithography— to fabricate two different microfluidic devices for electrophysiology studies of *ex vivo retinal tissues*. Electrophysiology is the study of electrical activity within biological cells. The first device combines microfluidics with electrical sensing technology to probe and sense extracellular electrical neuronal activities in mice retinas. The second device uses a low flow rate of liquid and an elevated pressure within chambers to measure intracellular calcium levels of retinal ganglion cells. Both devices that I fabricated are essential in further understanding illnesses related to neural activities within mice retinas.

Bio. Esther Ayoade is a rising junior majoring in Biology and Medicine, Health, & Society and minoring in Spanish on the pre-medical track. She originates from Laurel, Maryland and joined the VINSE Tech Crew in the summer of 2022. Along with assisting VINSE cleanroom users to operate machinery, Esther does photolithography using the Mask Aligner to fabricate microfluidic devices. She also specializes in mask fabrication using the Photoplotter. In high school she was captain of the cheerleading team and a member of marching band as a clarinetist. Now, she is on the board for Vanderbilt University Theatre (VUT), an active member of Project C.U.R.E, and a dancer on Nilaja Amari Dance Troupe.

Composite Films of Photosystem I Proteins with Substituted Polyanilines

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[2]*Department of Materials Science and Engineering, University of Central Florida, Orlando, FL*

Photosynthesis is one of the most critical processes in nature, sustaining a wide array of living organisms by converting sunlight into chemical energy. The process of oxygenic photosynthesis relies heavily on four multi-subunit protein complexes, with one of these being Photosystem I (PSI). PSI proteins are photoactive, have a nearly perfect quantum yield, and bear electron-hole splitting capabilities at the P700 active site, but their lack of overall conductivity limits applications in solar conversion systems. Researchers have mixed PSI with various conducting polymers, including polypyrrole, polyaniline, and poly(ethylenedioxythiophene), to generate composite films that circumvent the challenge of poor conductivity. Still, these conducting polymers are mostly water-insoluble, are challenging to incorporate with PSI in an aqueous-based process, and have energies that may not align well with PSI's active sites. In this work, we report the polymerization of two substituted anilines—p-anisidine and o-anisidine—in the presence of PSI in aqueous solution to form conducting polymer-protein composites. Since these are methoxyanilines, their processability in water as both monomers and polymers is greatly improved over the more common conducting polymers noted above. These composites can be easily drop-casted onto an electrode to form photactive, conductive films. Infrared spectroscopy shows that the final composite film contains both polymer and protein at a ratio that depends on the monomer-to-protein ratio in the polymerization solution. Contact angles were used to show that the composite film becomes more hydrophilic with increased ratio of polymer to protein. As ongoing work, the level of conjugation and intermolecular attraction between the protein and the resulting polymer will be examined using analytical ultracentrifugation, SDS-PAGE, and photoelectrochemical measurements of protein-polymer films. We will also examine if PSI can photooxidatively grow these polymers in a solution at neutral pH.

Bio. Emily Martinez is a rising junior at the University of Central Florida in Orlando, FL. She is majoring in Materials Science and Engineering and is also pursuing a minor in music, an area which she has been passionate about since childhood. She is a Florida Bright Futures Academic Scholar, a National Hispanic Scholarship recipient, and has been on the Principal's List for all 4 semesters she has attended university. Outside of the lab, she demonstrates leadership in UCF's choir ensembles, being the vice president of the chamber choir. She additionally contributes to her community as a member of the Society of women engineers (SWE) at UCF as well as being in the Burnett Honors College. At her home institution, she is a part of the NSF's Partnerships for Research and Education in Materials (PREM) program as a research intern studying photocatalytic materials; in this program, she is gaining experience in research while also performing outreach activities to foster an appreciation for STEM and scientific research in younger students. She aims to go to graduate school to study chemical engineering and ultimately work in the renewable energy industry.

20 | Yingrong Chen | Chemical Biology/Chemistry NSF REU

Developing Structure-based Drug Discovery Methods at the BCL-Rosetta interface

Yingrong Chen[1], Benjamin Brown[2], Jens Meiler[2,3]

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Computational modeling of protein-small molecule interactions can be used to study biological activities and facilitate small molecule drug discovery. Rosetta is a software package primarily used for macromolecular structure simulation and structured-based drug design. In contrast, the Biochemical Library (BCL) is a ligand-based chemoinformatic toolkit focusing on small molecules. Integration of BCL into Rosetta enables simultaneous manipulation of protein pockets and small molecules, and, therefore, allows researchers to develop more complex drug discovery protocols that are currently unavailable in the computer-aided drug discovery (CADD) field.

However, the current BCL-Rosetta interface is limited to performing structure-based chemical structure perturbations. Thus, this project aims to expand the BCL -Rosetta integration to enable additional tasks, such as small molecule alignment, chemical property prediction, and neural network-based binding energy estimation. Utility methods are developed to convert between Rosetta Pose and BCL FragmentComplete objects. Then, BCL applications are wrapped into Rosetta Movers and SimpleMetrics to enable modular access. Ongoing effort in this project will lead to the development of state-of-the-art protocols for small molecule drug design, such as methods for free energy perturbation. In the long term, this project will enable more accurate protein-small molecule interaction modeling in biological research and broaden the scope of computer-aided drug discovery to satisfy unmet research demands.

Bio. Yingrong Chen (also goes by Momo) is a rising junior from Emory University majoring in Chemistry and Computer Science. She is passionate about developing and applying computational methods to chemical and biomedical problems. This summer, she works on computer-aided drug discovery software with Benjamin Brown at the Meiler Lab. Back at Emory, she has also worked with protein dynamics in Alzheimer's Disease and molecular dynamics simulation of psoriasin protein structure.

21 | Nicholas Pugh | VINSE NSF REU

Heat Transfer by Surface Phonon Polaritons in Silicon Carbide Nanowires

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Understanding thermal transport at the nanoscale level is crucial for maintaining the safe operation of modern electronic devices. It is well-established that electrons and phonons are the major energy carriers for thermal transport in metals and semiconductors/insulators, respectively. Recently, it has been suggested that surface phonon polaritons (SPhPs) could contribute to thermal transport in polar thin films and nanowires. SPhPs are energy carriers resulting from optical phonons coupling with surface electromagnetic waves. In this study, to evaluate the contribution of SPhPs to thermal transport, measurements of the thermal conductivity of a silicon carbide (SiC) nanowire were performed using a microthermal bridge method. Measurements of the thermal conductivity of the same sample with different suspended lengths, 22 μm 11 μm respectively, were first carried out. The overlapping thermal conductivity indicated negligible contact thermal resistance. Then, we introduce SPhPs into the SiC nanowires with the electron-beam induced deposition of platinum to probe the effect of SPhPs on thermal transport. A thermal conductivity enhancement of ~2% was obtained at room temperature. The enhancement becomes larger at low temperatures and eventually reached ~12% at 30 K. The temperature dependent behavior may originate from the stronger loss in SPhP propagation at elevated temperatures. This study provides experimental evidence of SPhP contribution to thermal transport in polar nanowires and inspires a revisit of the effect of EBID treatment on thermal transport in polar materials.

Bio. Nicholas Pugh is a rising sophomore attending the University of Maryland, Baltimore County (UMBC) as a mechanical engineering major. At UMBC, Nicholas is a member of the 33rd cohort for the Meyerhoff Scholars Program and a member of the Honors College. He has been placed on the Dean's list for the Fall 2021 and Spring 2022 semesters at UMBC for academic achievements. Nicholas is also a member of the American Society for Mechanical Engineers (ASME) and the National Society of Black Engineers (NSBE). This summer Nicholas is participating in a ten-week research experience at Vanderbilt University in Dr. Deyu Li's Lab studying nanoscale thermal transport. He is excited to continue his research career in the upcoming years and prepare a path toward obtaining his Ph.D.

Synthesis of an AAT donor to enable access to bacterial glycans

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[2]*Department of Chemistry, Vanderbilt University, Nashville, TN*

Bacterial exopolysaccharides possessing zwitterionic charge motifs (ZPSs) are known to modulate the cellular immune system. AAT (2-acetamido-4-amino-2,4,6-trideoxy-D-glucopyranose) is a rare deoxy-amino sugar previously found within the repeating unit of ZPSs isolated from several different bacteria. Recently, a ZPS was isolated from *P. vulgaris* and is composed of AAT and two D-ribitol phosphate (D-Rib-ol-5-P) residues. Thus, we initiated a synthesis campaign to target the O-polysaccharide repeating unit to elucidate its role in immune modulation.

Bio. A rising senior from Raleigh, North Carolina, Myaisha, is majoring in Biochemistry at High Point University. At her home institution in North Carolina, her undergraduate research focuses on the synthesis of biologically active compounds. She is a student instructor for organic chemistry and co-founder of a student ambassador program aimed at prospective students interested in natural sciences. In addition to being the Vice President of the American Chemical Society student chapter on her campus, she is involved in nearly every instrumental ensemble on her campus. The clarinet player plans to attain a Ph.D. in chemistry and work on a total synthesis project. As for her career, she ultimately hopes to work in drug development for the pharmaceutical industry.

23 | Antony Peng | Beckman Scholar

Synthesizing Unnatural Metal Selenide Nanocrystal Phases

Antony R Peng[1], Eric A Ho[2], Janet Macdonald[1]

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This study develops a mechanistic understanding of the role of solvent and ligand conditions in phase control of copper selenide nanocrystal synthesis and seeks to draw comparison against a similar cadmium selenide system. ^{1}H NMR and ^{77}Se NMR were used to study how commonly used solvents and coordinating ligands alter the dodecyl selenol (DDSeH) and didodecyl diselenide (DD_2Se_2) reactants *in situ* at varying synthetic temperatures. DDSeH was highly reactive; alkenes were prone to selenol addition, carboxylates were susceptible to selenoesterification, amines released H_2Se gas. Wet solvent or ligand led to oxidation of DDSeH to DD_2Se_2, which remains unaltered by solvent and ligand chemistry. The NMR studies were correlated with the phases that resulted in syntheses of nanocrystalline copper selenides, in which berzelianite, umangite, or a metastable hexagonal phase was produced, as identified by X-ray diffraction. Formation of the rare hexagonal Cu_2Se phase was facilitated by reaction conditions that utilized the slower decomposing DD_2Se_2 reagent or long-chain saturated amine ligands. The trapping of this metastable phase shows a linear dependence upon the alkyl chain length of these saturated amine ligands. Additionally, the formation of the hexagonal phase was facilitated by lower (155 °C) synthetic temperatures to avoid thermal conversion of the hexagonal product into the thermodynamically preferred cubic berzelianite. These results indicate that slow reaction kinetics facilitate formation of metastable phases. This is supported by heated x-ray diffraction experiments of cadmium selenide, which exhibits similar phase conversion behaviors independent of ligand chain length.

Bio. Antony Peng is a rising third-year senior student at Vanderbilt University majoring in Cognitive Studies and Chemistry. Both a National Merit Scholar and Arnold & Mabel Beckman Scholar in chemistry, he joined the Macdonald group in the summer of 2021, beginning his work investigating phase control of copper selenide nanoparticles via *in situ* reactions with commonly used ligands and solvents. Currently, his research focuses upon understanding the role of reaction kinetics and thermodynamics in phase control of both copper and cadmium selenide nanoparticles. Beyond his work in the Macdonald lab, he is also working with Dr. Jessika Boles to investigate the efficacy of post-bereavement services provided to families at the Vanderbilt University Medical Center.

Controlling Light Propagation at the Nanoscale in Confined Molybdenum Trioxide (MoO_3) Nanobelts

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Light is comprised of electromagnetic waves characterized with defined frequencies and wavelengths. The wavelength determines the length scale of the light and is dependent upon the material through which it propagates. Due to the long free-space wavelengths associated with infrared (IR) light, the realization of nanoscale optical components is challenging, with flat and sub-diffractional optical components promising advances in imaging, communications, sensing, and light sources. The nanoscale confinement of this long-wavelength IR light can be achieved through the formation of polaritons – excitations in materials that result from the interaction of light and coherently oscillating charges. Polaritons exhibit much smaller wavelengths in the materials that support them, enabling us to achieve subdiffractional control of light and overcome some of these challenges. Of the numerous types of polaritons, hyperbolic polaritons exist in highly anisotropic materials, where the dielectric permittivity tensor is opposite in sign along different crystal axes. In these materials, such as molybdenum trioxide (MoO_3), the polaritons can only propagate along certain in-plane directions at any given frequency. Here, we seek to enable the propagation of polaritons along the normally "forbidden axis" within MoO_3, which occurs within specific spectral bands. From electromagnetic simulations, such propagation is anticipated to become allowed within narrow MoO_3 nanobelts (< 500 nm width). We aim at experimentally verifying this. We first fabricate narrow MoO_3 samples with the focused ion beam, an instrument which irradiates a sample with heavy ions to mill away material. Then, we carry out scattering-type scanning near-field optical microscopy (s-SNOM) experiments to visualize the propagation of polaritons, including the wavelength and direction. Such work furthers our fundamental understanding of polaritons in complex anisotropic materials and enables us to work towards advance wave-guiding and on-chip photonics and sensing applications in IR optics.

Bio. Levi is a rising junior at Northwestern University, studying materials science and Integrated Science (an honors, interdisciplinary program that covers math, biology, chemistry, and physics). At Northwestern, she has participated in research in Professor Hersam's nanoscale group, working within the field of 2D materials. She was awarded the McCormick Undergraduate Research Grant last summer, as well as awards for her coursework, including the Outstanding Materials Science and Engineering (MSE) Sophomore award in Materials Science, the Excellence in Mathematics by a First Year award, and numerous High Honors (4.0 GPA in the academic quarter) recognitions. Levi is also a member of Northwestern's Division I Fencing Team. As a part of this team, she has fenced at NCAA regionals, has worked with coaches and staff as a part of their Leadership Council, and has engaged with the community by introducing fencing to a local group called Girls Play Sports. Levi plans to pursue graduate school in materials science, with a strong interest in the various applications of this field, including the areas of energy and sustainability.

25 | Sarah Siman | VUSRP

Understanding the Durability of Iron Oxide Silica Bonds in Anishinaabe Cliff Face Paintings

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The Anishinaabe people, native to the area surrounding the Great Lakes, possess unique artwork that has lasted over 2,000 years. Unlike most Paleolithic rock paintings, these hematite (α-Fe_2O_3) paintings are on cliff faces that are constantly exposed to weathering from rainfall and lake water. Unfortunately, the Anishinaabeg have lost the knowledge needed to prepare the pigments to create these paintings. This project aims to understand the chemistry behind the durability of the cliff face paintings, and eventually present the Anishinaabe people with reproducible methods to prepare the paint. It is hypothesized that the durability is from the formation of the Fe-O-Si bonds between the surfaces of the cliff (silica, SiO_2) and the pigment, hematite. Here, the roles of pH, suspension environments and paint deposition methods are explored in order to observe their effects on the fugacity of the applied pigments. Paint suspensions are applied to microscope slides comprised of silica; a standardized way to simulate rainfall and test the strength of the Fe-O-Si bonds has been developed. When waterglass (sodium silicate) was added to the suspension, stronger adhesion of the pigment to the microscope slide was observed. These results suggest that silica may have been present in the pigment mixture itself, rather than only on the cliff surface. Going forward, natural reagents with high silica concentrations will be investigated.

Bio. Sarah Siman is a sophomore majoring in Chemical Engineering at Vanderbilt University. She is a Cornelius Vanderbilt Scholar from Miami, FL, and is currently conducting research in the Macdonald Lab in the Department of Chemistry. When she is not in the lab, Sarah is proposing and funding student-created sustainability projects as the Assistant Green Fund Coordinator for Students Promoting Environmental Awareness and Responsibility (SPEAR).

26 | Lavonte Saunders | VINSE Tech Crew

Solar Cell Nanofabrication for Science Education and Outreach

Lavonte Saunders[1], Elena Kovalik[2]

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[2]*Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, TN*

This project describes the process of solar cell nanofabrication for increasing scientific literacy surrounding energy consumption and sustainable power through outreach lessons. During these lessons, rural students at the middle and high school levels learn about the role cleanrooms play in developing nanotechnology by making and testing their own solar cell devices. The fabrication process involves the coating of a doped polymer onto a silicon substrate, deposition of aluminum, and patterning the metal into an electrode. However, small fabrication tolerances mean that students' cells often short circuit and fail upon testing, hindering the learning experience. To mitigate this, two problematic steps in the fabrication process were identified and improved. During the spin coating step, it was identified that the samples need to be transferred immediately to a hot plate to keep the doped polymer from congealing. Incorporating this method, it was then identified that an oversized electrode design was causing short-circuiting. A new electrode pattern was then designed to prevent short-circuiting and improve electrical contact during testing. Cells made using the current and proposed fabrication techniques were then evaluated, with the modified technique samples showing greater photoresponse. Further work needs to be done to determine the optimal amount of doped polymer and explore differing electrode patterns to further enhance the photoresponse of the cell.

Bio. Lavonte Saunders is a Biochemistry and Mathematics Junior who joined the VINSE Tech Crew in the summer of 2022. He specializes in creating solar cells within the cleanroom of VINSE, which requires the use of physical vapor deposition and photolithography. Outside of Tech Crew, Lavonte is an organic chemistry tutor, student ambassador for Immersion Vanderbilt, and a course assistant for math. Lavonte is excited to continue carrying out his undergraduate career at Vanderbilt, in addition to gaining new experiences to help him in the world.

27 | Madeline Herwig | Chemical Biology/Chemistry NSF REU

Deletion of Translational Slippery Sites in CFTR Changes Expression Levels in a Mutation Dependent Manner

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Slippery sites are specific nucleotide sequences in mRNA that affect the rate of ribosomal translation. These sites cause the ribosome to "slip", resulting in a frameshift in the reading frame of the ribosome. These sites have recently been discovered in the transcript of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) the causative mutated protein in Cystic Fibrosis (CF) a lethal, monogenetic disease. CFTR is a membrane protein expressed in epithelial cells. It is an anion channel protein that is responsible for the transport of chloride and sodium ions. The most common mutation of CFTR is the deletion of phenylalanine 508 (F508del) and 90% of CF patients have at least one allele containing this mutation. Notably, slowing translation speed increases F508del expression. However, the relevance of these identified slippery sites in CFTR and their effect on its translation is largely unknown. Here, we used affinity purification mass spectrometry to quantify protein interactors between wildtype CFTR and F508del with and without these slippery sites conserved. We hypothesize that there will be differences in interactors between the conserved slippery site and deleted slippery site.

Bio. Madeline Herwig grew up in Geneva, Illinois and is a rising senior at Augustana College studying Biochemistry and Public Health. Throughout her undergrad, she has worked in Dr. Pamela J. Trotter's lab investigating the biochemical relevance of glutamine dehydrogenase in *Yarrowia Lipolytica*, a nonconventional yeast model. After completing her undergraduate studies, she hopes to continue her education and pursue a PhD in Chemical Biology. Outside of the lab, Madeline enjoys playing her violin, singing, and spending time with her family and friends.

28 | Sarah Shibuya | VINSE NSF REU

Selective Functionalization of Leukocyte Subpopulations with E-Selectin Liposomes

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Metastasis occurs when cells break off a primary tumor and enter the blood stream. This process can create secondary tumors at distant sites. To combat metastasis, an antimetastatic therapy uses the protein TNF-related apoptosis inducing ligand (TRAIL) to initiate apoptosis in circulating tumor cells (CTCs) in the blood stream. Liposomes with the protein E-Selectin (ES) attach to leukocytes in the bloodstream and are used as vessels to transport TRAIL to CTCs. Here, we investigate the influence that ES has on the binding of liposomes to subpopulations of leukocytes, specifically monocytes and granulocytes. Through flow cytometry analysis of monocytes and granulocytes from healthy patient blood, the concentrations of fluorescent ES-liposomes bound to the surface of these cells were investigated. It was found that as the average number of ES per liposome increases, the greater occurrence that liposomes are bound to granulocytes. The number of ES yields no correlation on the effect of liposome-monocyte binding. The influence of the liposome component DSE-PEG was also investigated. When DSPE-PEG was removed from the liposome fabrication process, a specific subpopulation of higher fluorescence in flow cytometry measurements indicated more efficient binding to granulocytes. Imaging using fluorescence microscopy visually confirmed the binding of liposomes without DSE-PEG to leukocytes using a DiI lipid dye and DAPI nuclei dye. A population of granulocytes did not bind to these liposomes, while most were bound to them in abundance, indicating there may be selective binding to specific types of granulocytes. There was little to no binding to monocytes with 0 ES, but with ES present, binding was found to occur to select monocytes. High binding to platelets was found in both leukocyte populations. The investigation of this topic can yield better results in the utilization of liposomes as a delivery system for TRAIL in antimetastatic therapies.

Bio. Sarah Shibuya is a rising sophomore at Rose-Hulman Institute of Technology from Portland, Oregon. She is majoring in biomedical engineering with a focus in biochemistry and molecular biology. Sarah is a Commitment Scholar and a part of the Noblitt Scholars Program. She belongs to the Biomedical Engineering Society, the Society of Women Engineers, and is a player on the Rose-Hulman Women's Soccer Team. She earned her Silver Award through Girl Scouts and continues to be a part of scouting through the Alpha Phi Omega service fraternity. In her free time, she loves to crochet, read, and enjoy nature. Looking into the future, Sarah plans to attend graduate school to study biology or biomedical engineering.

29 | Irina Samsonova | Chemical Biology/Chemistry NSF REU

Benchmarking Configurational Entropy of Small Organic Molecules: Maximal Entropy Approach

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Free energy computation is vital to computational modeling of proteins and protein-ligand interactions for drug design and discovery. The accurate computation of entropy, i.e., the central component of free energy, presents a big challenge to the community. This work develops an approach for calculating the configurational entropy of small organic molecules and benchmarks computational prediction against experimental observation. Conformational entropy is calculated using the Maximum Information Spanning Tree (MIST) approach with the molecular topology determined by the maximal entropy method. Translational, rotational, and momentum terms are added to the computed configurational entropy for comparison with the experimental values. This work is a preliminary benchmark and can be further developed to treat macromolecular systems, such as peptides, proteins, or a protein-ligand system. As the next step, we will also employ a deep generative model to enable entropy calculations for QM systems. These studies will lay the foundation for entropy-based functional molecule design and discovery.

Bio. Irina Samsonova is a rising Junior at the University of Missouri. She is currently working on completing a Bachelor of Science in Chemistry with ACS Certification as well as a B.S. in Physics and a Certificate in Computational Physics. Irina has worked in computational chemistry at Mizzou for 2 years and has also worked as a teaching assistant for 1 year. After completing undergraduate studies, she plans on attending Graduate school for Physics and pursuing theoretical and computational Physics.

30 | Andrea Valero | VINSE NSF REU

Using a Microtrack Platform to Determine the Effect of Reactive Oxygen Species on Confined Migration

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Tumor heterogeneity remains a clinical challenge in cancer treatment as it drives differential responses of cancer cells subpopulations to various environmental cues. Both mechanical cues, such as confinement, and metabolic cues, such as levels of metabolic intermediates like reactive oxygen species (ROS), have been shown to promote cell invasion and migration. To understand the role of heterogeneity in breast cancer cell behavior, we previously sorted MDA-MB-231 triple negative breast cancer cells (MDA) into highly (MDA+) and weakly (MDA-) migratory subtypes and assessed their differential response to metabolic cues. We found that treatment with high doses of the ROS activator, tertbutylhydroperoxide (TBHP), significantly decreased speed in both subtypes, in contrast with previous reports. Here, we aim to better understand how ROS production contributes to breast cancer cell migration. To investigate the effect of ROS, collagen microtracks were formed using polydimethylsiloxane (PDMS) stamps to mold collagen into tunnels that mimic the tumor matrix. Parental MDA-MB-231 cells seeded into the microtracks and cells were treated with 25 μM, 50 μM, and 75 μM concentrations of TBHP and migration speed was assessed. We observed that when treated with 25 μM TBHP, a fraction of the parental cells slightly increased migration velocity, suggesting that ROS may have differential effects on different cell subtypes at low doses. Metabolic dysregulation is a primary driver of metastasis and understanding the contribution and influence of ROS on breast cancer cell migration is pivotal to understanding how to target metastasis.

Bio. Andrea Valero is a rising sophomore studying chemical engineering at the University of Texas at San Antonio. She has research experience in neurodegenerative diseases, wind energy optimization, drug delivery systems, and cancer cell migration. Her passion for research have earned her a position in the ESTEEMED, a NIH/Federally-funded program that helps freshman and sophomore-level trainees develop as scholars and scientists. During her freshman year, she became an undergraduate researcher under the supervision of Dr. Gabriela Romero, where she works independently in the experimentation and data analysis of polymers for drug delivery. At her home institution, she exerts a leadership role as the Senator for the College of Engineering and as part of the Presidential Student Advisory Council. Additionally, she is part of Society of Women Engineers and the UTSA SACNAS Chapter. Due to her academic achievement, she has earned her a place on the Dean's List and as a Klesse Scholar. This summer, she is working under the supervision of Jenna Mosier and Dr. Reinhart-King to understand the behavior of breast cancer cells and the effect of reactive oxygen species on confined migration. Her professional aspirations are to obtain a PhD and become a biomedical innovator.

31 | Sarah Driscoll | VINSE Tech Crew

Graphene Electrode Transistor Fabrication for Retina Electrophysiology Studies

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Graphene has drawn significant attention since it was first isolated because of its unique mechanical and electrical properties. It now offers promising potential for biosensing devices because of its high charge carrier mobility and superior sensitivity. This emerging technology can be applied to physiological studies of the retina to understand the action potentials for neuronal sensing by placing a mouse retina on graphene electrode transistors. These complex devices were fabricated in the VINSE cleanroom using photolithography, metal deposition, and synthesizing and transferring graphene. To concentrate the fabrication process into one location, there needs to be a reliable procedure for synthesizing graphene in the cleanroom. The goal was to learn how to make graphene in labs outside of the cleanroom and master this process to diagnose the chemical vapor deposition furnace inside the cleanroom. Through meticulous inspection of this machine, the vacuum pressure of the system was successfully lowered from 33 millitorr, the lowest recorded pressure of the system, to 17 millitorr. This was accomplished by performing leak checks, changing out pieces of the connection system, and adding parafilm to all connections. At this point it has been determined that there is no leakage in the system, rather the capacity of the vacuum pump itself is being reached. Further investigation into the pump system will be needed to achieve the preferred pressure to grow graphene.

Bio. Sarah Driscoll is a Chemical Engineering sophomore who has been on VINSE Tech Crew since the summer of 2022. She specializes in growing graphene in the chemical vapor deposition furnace and photolithography for microfluidic and electrical applications. Her favorite part of the job is chatting with cleanroom users about their projects to better understand the world of nanoscience. Outside of Tech Crew, Sarah is a part of many campus organizations. She is a member of Theta Tau where she served as the care chair, the American Institute of Chemical Engineers where she served as the Freshman Representative, and is active in the Nashville Navigators. Sarah has been on the Dean's List for all of her semesters at Vanderbilt. She is very excited to carry out the rest of her undergraduate degree at Vanderbilt and utilize her experience in Tech Crew to continue to learn and grow both academically and professionally.

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