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Summer Undergraduate Research Expo

August 11, 2022
McNamara Alumni Center
Memorial Hall
4:00-6:00pm



Undergraduate Poster Presentations Listed Alphabetically by Presenting Author

Presenters should be at their posters at the following times:

4:00 - 5:00 even numbered posters

5:00 - 6:00 odd numbered posters

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| 1. | <p>Ebubechukwu Agwaramgbo <i>Affinity Maturation for B7-H3 Binders</i> Advisor: Ben Hackel Sponsoring Program: MRSEC Home Institution: Xavier University of New Orleans Louisiana Abstract: B7-H3, an important immune checkpoint inhibitor of T-Cell function, is a common tumor vasculature biomarker that is overexpressed in various cancers. Its overexpression is linked with tumor growth and metastasis. Ligands that bind to target antigen with high affinity and specificity could have therapeutic and diagnostic uses. Gp2 and affibody are protein scaffolds that have been previously evolved to bind B7-H3 with nanomolar affinity. Using error-prone polymerase chain reaction, affibody and Gp2 proteins will be affinity matured and engineered via yeast surface display, creating a 2.0 library. Stringent magnetic and florescent activated cell sorting techniques will sort cells for picomolar binding affinity, specificity, and stability. The proteins will be tested for functionality in the human body by undergoing thermolysin and thermostability. The top performing ligands will have low picomolar affinity to B7-H3. These proteins can be deep sequenced to better understand them.</p> |
| 2. | <p>David Ajayi <i>Investigating the mechanism of nanoparticle toxicity by tracking H2O2 production with electrochemical techniques</i> Advisor: Christy Haynes Sponsoring Program: Center for Sustainable Nanotechnology Home Institution: University of Minnesota Rochester Abstract: Nanoparticles are increasingly being applied to new technologies as their unique size-dependent properties contribute to more efficient systems. However, the use of nanoparticles hasn't come without a cost. Studies show that these engineered nanomaterials can lead to toxic effects on the life present in the environment by producing reactive oxygen species like hydrogen peroxide (H2O2). H2O2 is a powerful oxidizer that remains relatively stable in abiotic environments. However, H2O2 also has the capacity to rapidly kill cells via hydroxyl radical generation. Lithium Cobalt Oxide (LCO) and lithium nickel manganese cobalt oxide (NMC), both nanoparticles used in the fabrication of lithium-ion batteries, were tested for the generation of H2O2. Using the electrochemical techniques amperometry and cyclic voltammetry, the voltage and current of the LCO and NMC solutions were compared with a background solution of .1M potassium nitrate (KNO3), in order to track the production of H2O2 from these material in solution over 26 hours. Findings suggested that LCO leaked H2O2 into the solution overtime, with the most H2O2 being released in the first 30 minutes. H2O2 emanated from these nanoparticles could explain the mechanism for their toxicity in the environment, informing the creation of safer nanomaterials in the future.</p> |
| 3. | <p>Narcedalia Anaya Barbosa <i>Understanding polymer shear rates and their relation to molecular architectures in the Micro compounder.</i> Advisor: Frank Bates Sponsoring Program: MRSEC Home Institution: University of Texas Rio Grande Valley Abstract: The results of this research will help provide a better understanding of the processing conditions in the DSM Xplore 5 and 15 cc micro compounders. Measurements obtained in the micro compounders will be compared to those measured with an ARES-G2 rheometer for a range of shear rates, temperatures, fill volumes and polymers. The measurements can be used to evaluate the accuracy of the micro compounders and scalability between the systems. Rheometer data can aid identifying viscosity changes related to the polymer architecture and help hypothesize the impact that simple and extensional shear have when processing. Polymers used are High Density Polyethylene (HDPE) with a linear architecture, Low Density Polyethylene (LDPE) showcasing a long chain branched structure, and Linear Low Density Polyethylene (LLDPE) exhibiting the same architecture with smaller branches.</p> |

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| 4. | <p>Eliza Asani <i>Fermionic Deep Neural Networks in Quantum Embedding Calculations of the Spin-Splitting Energy of $[Fe(H_2O)_6]^{3+}$</i> Advisor: Jason Goodpaster Sponsoring Program: UMN Chemistry - CTC Home Institution: University of Alabama in Huntsville Abstract: Ligated transition metals display unique spectroscopic and magnetic properties due to transitions between multiple spin states. These spin transitions, or spin-splitting energies, are difficult to compute due to subtle electronic effects and strong electron correlation. While <i>ab initio</i> methods exist that are reasonably accurate at calculating spin-splitting energies, they are frequently too computationally expensive to perform on large transition metal complexes. An alternative is quantum embedding, which isolates specific areas of a system to be calculated using methods of differing levels of accuracy, typically density function theory in density functional theory (DFT-in-DFT) or wave function in DFT (WF-in-DFT). While this decreases the computational cost, the high-level methods of choice still compromise on accuracy in their determination of the spin-transition energies. Here, we utilize a fermionic deep neural network (DNN) for the WF method in quantum embedding calculations. These networks are accurate even within strongly correlated systems and are also easily parallelizable for an even greater reduction in computational cost. We test this system on $[Fe(H_2O)_6]^{3+}$ and discuss the comparison between the WF-in-DFT and DNN-in-DFT methods.</p> |
| 5. | <p>Monica Bandora <i>Mechanical function of stretched Vascular Smooth Muscle Cells.</i> Advisor: Patrick Alford Sponsoring Program: BME Pathways Home Institution: Morgan State University Abstract: Each year, about 50% of college and high school football players suffer concussions, which is a mild neuro-traumatic injury. One common manifestation of neurotrauma is vascular dysfunction in the form of vascular rupture. It is not yet known how trauma acutely affects individual vascular cells. Previously, in an in vitro model of head injury, we studied how stretching vascular smooth muscle cells (VSMCs) at different strain rates affects short term stress generation by VSMCs. We learned that VSMCs stretched at high strain rates produced less stress shortly after stretch than those stretched at a slower rate. It is currently not clear if this strain rate-dependence in stress persists over long time periods. Here, we use Cellular Micro-biaxial Stretching (CμBS) to apply a step change in strain to VSMCs and then track the change in stress generated by the cells for one hour. Our data suggests that the strain rate-dependent stresses observed immediately after stretch persist over the long term. This data has important implications for understanding arteries' long-term adaptation following mechanical disturbance during brain injury.</p> |
| 6. | <p>Nayan Banerjee <i>Structure-Activity-Relationship of a New Class of Domain-Selective Heterocyclic Bromodomain Inhibitors</i> Advisor: William Pomerantz Sponsoring Program: UMN Chemistry- Lando Home Institution: Indian Association for the Cultivation of Science (IACS) Abstract: Bromodomains (BRDs) are a class of evolutionary conserved epigenetic protein-protein interaction domains that bind acetylated lysine residues on histones and are responsible for transcriptional regulation and recruitment of members of the transcriptional machinery. These proteins are often dysregulated in a wide array of diseases including obesity, inflammation, cancers, viral infections, and cardiac disorders, making the study of BRD inhibitors of immense therapeutic and clinical relevance. Thiazepane-based scaffolds, recently reported by the Pomerantz lab have demonstrated unique selectivity targeting the second BRD of the bromo and extra terminal (BET) subset of these proteins. To improve upon the potency and selectivity, herein we synthesized a set of novel 7-membered heterocycles and screened them for specificity against two BET BRDs using a competitive AlphaScreen biophysical assay. We also report our synthetic progress towards a ring-expanded heterocycle and lay the foundation for directed functionalization of these new scaffolds. Future studies shall be directed towards further optimizing these molecules in an attempt to enrich the drug discovery chemical space for selective BET inhibitors.</p> |

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| 7. | <p>Jessica Beaudoin <i>Developing antimicrobial nanocrystalline cellulose filters enabled by a natural amphiphilic peptide coating</i> Advisor: Boya Xiong Sponsoring Program: MRSEC Home Institution: University of Minnesota Morris</p> <p>Abstract: Synthesized sterically stabilized nanocrystalline cellulose (SNCC) will be used as a substrate to functionalize antimicrobial peptides for removing pathogens in drinking water. Amphiphilic and cationic proteins found in the seeds of <i>Moringa oleifera</i> (MO), a tree rich in nutrients native to many tropic countries, exhibits excellent antimicrobial properties. The proteins extracted from MO seeds will be functionalized to the surface of SNCC that was synthesized from wood pulp with pretreatments. Two types of protein immobilization include covalent linkage of amines from the protein to dialdehydes of SNCC, and electrostatic sorption of the protein on SNCC oxidized to carboxylic acids. Protein concentration and the level of oxidation of the SNCC will be explored to yield sufficient protein coating that is functional after immobilization. Aldehyde content of pretreated SNCC will be measured by titrations of Schiff bases from hydroxylamine reactions with aldehyde. Morphology of protein functionalized SNCC will be visualized and measured with atomic force microscopy (AFM), scanning electron microscopy (SEM), dynamic light scattering (DLS), and contact angle (CA). Standard deadend filtration was used to assess the permeability of a filter of the protein-functionalized SNCC. The proposed research yields a sufficient and functional protein coating on filtration material for waterborne pathogen removal.</p> |
| 8. | <p>Paxton Berger <i>Soft Burrowing Robot Mechanism: Energy efficiency and force propagation</i> Advisor: Jim Van de Ven Sponsoring Program: ME Home Institution: University of Minnesota - Twin Cities</p> <p>Abstract: The exploration and development of underground infrastructure is a difficult process for heavy machinery when delicacy and precision is required. To combat this issue, projects in the past have created burrowing soft robots that act as small maneuverable devices to lead lines through areas or explore sections of earth. These robots used a hydraulic ram to push themselves through the dirt and rock. Using a cone shaped head and a large amount of force and energy they force through the material. This however causes issues as the process is incredibly power consuming. Our solution to this issue is intelligently removing material in front of the robot to lessen the density of forward material, making it easier and less energy intensive for the robot to maneuver. Our research uses a head mechanism that expands and contracts at the tip of the robot, pushing material to the side. Similar to previous designs, it is powered by a hydraulic ram. This mechanism is designed to apply maximum outward force while maintaining a lower energy profile than simply pushing directly. This technology can improve the efficiency of these borrowing processes while maintaining the necessary tunnel characteristics, and bounds of force put upon the robot.</p> |
| 9. | <p>Josselyne Berrios <i>Phase Equilibrium Study of Mixed Rare Earth Aluminate-Zirconates as Candidate Thermal Barrier Coatings</i> Advisor: David Poerschke Sponsoring Program: MRSEC Home Institution: University of California, Los Angeles</p> <p>Abstract: Thermal and environmental barrier coatings (TBC and EBC) enable turbine engines to work at higher temperatures for higher engine efficiency. TBCs provide thermal insulation with low thermal conductivity, while dense, volatilization-resistant EBCs prevent interdiffusion and reaction between the combustion environment and engine components. Rare earth (RE) zirconate or aluminate TBCs have good thermal stability and are highly resistant to corrosive environments. For this category of materials we focused on identifying phase equilibria and testing of (Gd, Y)-aluminate-zirconates. We studied their phase equilibria, including the stability of specific phases, the RE elements partitioning between these phases, and their thermal and sintering resistance for various Gd:Y ratios. In addition, as an EBC candidate, ytterbium disilicate (YbDS) was synthesized and characterized, which is a desirable material due to its reported volatilization resistance and suitable CTE for silicon carbide (SiC) based components. Future research work will focus on the interaction between (Gd, Y)-aluminate-zirconates and YbDS. The mixed multiphase samples were prepared by reverse co-precipitation method. Sintering behaviors were studied by heat treatment with various temperatures and durations. X-ray diffraction (XRD) was used to study phase constitutions; while scanning electron microscope (SEM) was used to study grain growth kinetics and microstructure evolution.</p> |

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| 10. | <p>Malachy Bloom <i>Angular Resolution of the Search for Anisotropic Stochastic Gravitational Wave Backgrounds with LISA</i> Advisor: Vuk Mandic Sponsoring Program: Physics REU Home Institution: Carleton College Abstract: Gravitational waves (GWs) provide an exciting new domain for astrophysical, cosmological, and fundamental physics exploration. With new GW detectors such as the Laser Interferometer Space Antenna (LISA) set to launch in the 2030s, there is a very strong possibility of detecting stochastic gravitational wave backgrounds (SGWBs) from a variety of sources across the millihertz GW frequency band. In this work, we investigate the angular resolution of anisotropic SGWB searches with LISA by simulating and analyzing anisotropic SGWB signals using the Bayesian LISA Pipeline (BLIP). We use a spherical harmonic basis and a full-width-half-max method to characterize this angular resolution. We find that the number of spherical harmonic components used to conduct the search is the dominant contributor to angular resolution, but other factors may have smaller, yet non-negligible effects.</p> |
| 11. | <p>Raviya Careem <i>Understanding the structural basis of small molecule inhibitors of M. tuberculosis DosS</i> Advisor: Ambika Bhagi-Damodaran Sponsoring Program: UMN Chemistry- Lando Home Institution: State University of New York at Oswego Abstract: Tuberculosis (TB) is an infectious airborne disease caused by Mycobacterium tuberculosis (Mtb) that mainly affects the lungs. Mtb growth is inhibited when the bacteria is engulfed by macrophages into granulomas, causing Mtb to become dormant in the host cell. In the presence of hypoxic conditions, the DosS/DosR regulatory system is responsible for the upregulation of the dormancy genes. When sensing the change in oxygen level, DosS undergoes autophosphorylation transferring the phosphate group to the DosR regulator, which then binds to the DNA regulon and upregulates ~50 genes dormancy genes essential for dormancy survival. Therapeutics has proven to be ineffective when treating dormant TB. The DosS/DosR regulatory system can be inhibited by introducing small molecule inhibitors that bind to the GAF-A domain on the DosS sensor. In this work, the inhibitor-bound GAF-A domain was crystallized using the hanging drop crystallization method to elucidate the overall structural changes of the inhibitor-bound protein. This knowledge would then be used for further drug modification and discovery.</p> |
| 12. | <p>Erika Cerna Arroyo <i>The Effect of Lipid Phase Behavior on F127 Polymer Binding to Liposomes</i> Advisor: Dr. Tim Lodge Sponsoring Program: UMN Chemistry- Lando Home Institution: University of Rochester Abstract: PEO-PPO block polymers interact with phospholipid bilayers and can have a stabilizing effect on cell membranes under stress. The stabilization mechanism remains unknown but previous studies have found that a wide range of cell signaling pathways are upregulated and down regulated. Liposomes are useful membrane models because they can be prepared with custom compositions to probe the effect of different membrane components on polymer-lipid interactions. Previous research has shown that ternary mixtures with saturated lipids, unsaturated lipids, and cholesterol lead to phase coexistence. In this work, we leverage published ternary phase diagrams to explore the impact of lipid phase behavior on the binding of Poloxamer F127 to different membrane compositions of phosphatidylcholine, palmitoylsphingomyelin, and cholesterol. Unimodal liposomes were prepared with vesicle extrusion diameter of 50 nm. Dynamic light scattering was used to validate the prepared liposomes, and pulse-field-gradient NMR was used to quantify the amount of F127 bound to the liposomes. We observed that the addition of cholesterol significantly reduced polymer binding to the liposomes relative to the POPC control. Addition of PSM also decreased binding non-monotonically. Compositions with L_d/L_o/S_o coexistence showed maximal binding of polymer, possibly because phase boundaries on the lipid bilayer present attractive binding sites.</p> |

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| 13. | <p>Adriana Chapa <i>Improving the Dispersion of Silicon/Silicon Dioxide Quantum Dots</i> Advisor: Vivian Ferry Sponsoring Program: MRSEC Home Institution: The University of Texas Rio Grande Valley Abstract: Luminescent Solar Concentrators (LSCs) are devices that can generate renewable electricity and are composed of a transparent waveguide which is coated with a luminescent solution. Silicon Quantum Dots (Si QDs) are semiconductor nanocrystals that broadly absorb UV light and photoluminesce near-infrared light. Si QDs can suit LSC applications as they are nontoxic, are made from an abundant element, and have succeeded in renewable energy technology. We use nonthermal plasma to synthesize Si QDs, but as-synthesized, Si QDs have a high defect density. A silicon dioxide (SiO₂) shell can protect the Si QD core and reduce the defect density. Unfortunately, Si/SiO₂ nanoparticles still agglomerate due to the nonpolar silicon hydride and polar silanol surface groups that prevent dispersion in either polar or nonpolar solvents. This work focuses on developing a method for the Si/SiO₂ QDs to stay in a stable, homogeneous mixture. This study varied different aspects of the dispersion by experimenting with different ligands, pH levels, and solvents. We characterized the solutions by using FTIR, UV-Vis, and PL spectroscopies. We concluded that using PEG-Silane as a ligand in an acidic environment with a polar solvent led to a stable, homogeneous mixture with a high photoluminescence intensity.</p> |
| 14. | <p>Alicia Chen <i>Hybrid Additive Manufacturing for Precise Drug Delivery</i> Advisor: Michael McAlpine Sponsoring Program: ATP-Bio Home Institution: New York University Abstract: Proper spatial and temporal presence of biochemical signals are necessary for eliciting changes in cell behavior, such as differentiation and migration conducive to tissue development. However, precise drug delivery in artificial tissue constructs with respect to space and time remains a challenge. To better stimulate biochemical cues, we developed a system wherein near infrared-programmable drug capsules are placed via robotic-control into a 3D printed hydrogel. Drug capsules are made using a custom-fabricated microfluidic system, and hydrogels are printed via Direct Ink Writing (DIW) into a microparticle support bath (Lee et al). This study specifically focused on optimizing hydrogel printing speed as well as subsequent precision placement of the capsules. By testing varying printing speeds between 10 mm/s and 17.5 mm/s, we found an optimized speed where the construct thickness is accurate to computational design. Additionally, capsule placement speeds between 10 mm/s and 20 mm/s result in minimal movement of the capsule, reinforcing precise delivery. With accurate hydrogel 3D printing and programmable capsule placement, we made major improvements towards constructing a tissue-engineered system which possesses enhanced spatiotemporal presence of biochemical cues. For future direction, this system can be used for a variety of applications including cryoprotective agent delivery.</p> |
| 15. | <p>Ainsley Clark <i>Pressure-induced Transition of M₂X Compounds into Topological Insulators</i> Advisor: Turan Biroli Sponsoring Program: MRSEC Home Institution: University of California, San Diego Abstract: Topological insulators are materials which have electronic properties leading to the mobility of electrons being limited to the surface of the material. Zintl phase materials of the form M₂X (M = Ca, Ba, Sr, and X = Sn, Ge, Pb) have been the subject of limited prior research due to their potential to transform from topologically metallic materials into topological insulators, but the full extent of the conditions that cause this transition is not yet studied. In this experiment, the role of pressure on the transition of M₂X compounds from topologically metallic to topologically insulating materials will be analyzed. Specifically, density functional theory will be used to calculate the band structure of M₂X materials under various pressures. This will allow for a determination of the wave function of these types of molecules. Once the wavefunction is known, the materials can be analyzed further to determine whether they form nontrivial topology under pressure, indicating whether they are topological insulators. It is anticipated that increased pressure will induce the transition of M₂X materials into topological insulators, and in demonstrating this, a greater understanding of the electronic properties of M₂X materials will be gained.</p> |

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| 16. | <p>Sydney Cole <i>Development of (+)-3-Carene based Monomers for Polyurethanes</i> Advisor: Jessica Lamb Sponsoring Program: Center for Sustainable Polymers Home Institution: The University of Southern Mississippi Abstract: The shift to renewable and bio-sourced feedstocks is critical to easing the impact plastic production and use has on the environment. Polyisocyanates, a primary component of polyurethanes, are derived from chemical warfare agent, phosgene. Due to the hazardous nature of polyisocyanates, they have been heavily regulated in Europe, expediting the need for an alternative feedstock to continue the production of polyurethanes. One such feedstock is turpentine oil, a waste product from the pulp-industry. (+)-3-carene, a primary component of turpentine oil, has been chosen for its advantageous stereochemistry and structural properties. (+)-3-carene exhibits potential as both a refuse-derived and a chemically circular bio-feedstock for the development of polyurethanes. To obtain chemical circularity we have focused on regioisomerism of the molecule. Synthetic pathways have been studied to develop a new (+)-3-carene derived oxazolidinone monomer via diastereoselective epoxidation, regioselective ring opening of epoxide, and carbamate cyclization.</p> |
| 17. | <p>Evan Danielson <i>Block copolymer additives for polyolefin recycling</i> Advisor: Frank Bates Sponsoring Program: Center for Sustainable Polymers Home Institution: Miami University of Ohio Abstract: Polyethylene (PE) and isotactic polypropylene (iPP) are two of the most produced plastics in the world. However, the two polyolefins are immiscible, resulting in PE/iPP blends with poor mechanical properties. It poses a challenge to recycling as plastic waste streams often contain mixtures of PE and iPP that cannot be separated easily. Block copolymers (polymers consisting of chemically distinct polymer blocks) are potential compatibilizers, improving interfacial adhesion between the two polymers, and producing blends with competitive mechanical properties.</p> <p>In this study, we synthesized PE–polyethyl(ethylene) (PX) block copolymers from butadiene and evaluated their ability to compatibilize PE/iPP blends. Tensile testing showed a dramatic increase in blend toughness with the addition of 1 wt% PE-PX triblock copolymer. Further investigation using atomic force microscopy and scanning electron microscopy show decreased domain size and strong interfacial adhesion upon adding the block copolymer to the blend. We propose that the triblock copolymer is able to toughen PE/iPP blends through co-crystallization in the PE phase as well as the entanglements between the PX block and the iPP phase. Overall, these results demonstrate a potential opportunity to produce competitive recycled plastic materials using only mechanical processes.</p> |
| 18. | <p>Katherine Del Cairo <i>Monitoring Lipotoxicity in Yeast with Fluorescent Microscopy</i> Advisor: Elias Puchner Sponsoring Program: Physics REU Home Institution: University of Texas at Austin Abstract: The unfolded protein response (UPR), an intracellular signaling pathway, helps restore homeostasis in the cell when misfolded proteins accumulate in the endoplasmic reticulum. When the UPR fails, it leads to cell death and its repeated failure has been linked to contributing to diseases such as cancer and diabetes. To understand the UPR the cells must be succumbed to stress; one approach to activate the UPR is to overload the cell with lipids, causing lipotoxicity. Most of the research how lipotoxicity triggers the UPR has been done in mammalian cells. This study proposes to examine how the UPR will react within yeast cells when induced with lipotoxicity. We do so by doing live imaging of the yeast cells through fluorescence microscopy. When the UPR is turned on in yeast cells, it activates the stress sensor protein called Ire1 which clusters on the endoplasmic reticulum. Ire1 is a green fluorescent protein, whose clusters will emit a strong light signal upon stress, providing information on the UPR activity. From these measurements, we hope to understand how specifically fatty acids, both saturated and unsaturated affect the unfolded protein response in yeast cells.</p> |

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| 19. | <p>Holly Den Hartog <i>Remdesivir and Remdesivir Analogs Inhibit the Transcription of the SARS-CoV-2 Genome</i> Advisor: Natalia Tretyakova Sponsoring Program: UMN Chemistry- Heisig Gleysteen Home Institution: University of Minnesota Abstract: The Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) is an enveloped, single-stranded virus with an RNA genome. The replication and transcription of its genome is dependent upon RNA-dependent RNA polymerase (RdRp), which is central to the viral replication machinery of SARS-CoV-2. Coronavirus RdRp is highly error-prone, and recognizes several nucleotide analogs (NAs) as viral substrates. NAs are structurally similar to natural nucleotides, which allows them to be incorporated in RNA. They eventually hinder the function of the RdRp, causing chain termination and inhibiting viral replication. NAs are thus promising agents to fight viruses with RNA genomes, such as SARS-CoV-2. Remdesivir, a nucleotide prodrug that is an analog of adenosine triphosphate (ATP), initially showed effectiveness against the Ebola virus, and this effectiveness made it an early candidate to combat COVID-19. In this work we are investigating the effect of remdesivir and four analogs of remdesivir on RNA replication by using gel-based primer extension assays. We hypothesize that RdRp-mediated RNA replication will be halted upon the incorporation of remdesivir and remdesivir analogs into the nascent viral RNA.</p> |
| 20. | <p>Victor Drewanz Gnani Ernesto <i>Effects of the Copper-Titania Interface in UiO-66 on the Selective Hydrogenation of CO₂ to Methanol</i> Advisor: Matthew Neurock Sponsoring Program: UMN Chemistry - CTC Home Institution: Rollins College Abstract: Metal-organic frameworks (MOFs) are porous materials comprised of metal oxide nodes connected by organic linkers that offer unique tunability and have shown promise in catalyzing the hydrogenation of CO₂ potentially offering novel strategies for green-house gas emissions. UiO-66 is a MOF comprised of ZrO₂ clusters linked by 1,4-benzenedicarboxylic acid units. Previous results show that UiO-66 impregnated with Cu nanoparticles demonstrate high catalytic activities and selectivities for CO₂ hydrogenation. This is thought to be the result of bifunctional metal-Lewis acid sites that form at the Cu/ZrO₂ interface where both sites cooperatively drive the adsorption and hydrogenation of CO₂. In an effort to design more active materials, we examine the influence of Lewis acidity on the CO₂ reduction activity of UiO-66 by replacing a Zr atom with a more Lewis acidic Ti atom. The effect of this substitution on CO₂ hydrogenation were examined by carrying out density functional theory calculations on Cu-UiO-66 (Ti) models. The calculations examine the elementary steps for the hydrogenation of CO₂ and explore the role of hydrogen availability and metal-coordination on MOF's reactivity. The Ti interface shows lower CO₂ activation due to size and high node coordination. Lower coordination on titanium showed stronger CO₂ adsorption and high reactivity.</p> |
| 21. | <p>Claire Dwyer <i>Position Measurement Improvement for the LDMX Hadronic Calorimeter</i> Advisor: Jeremiah Mans Sponsoring Program: Physics REU Home Institution: Vassar College Abstract: Observations of experiments suggesting the presence of dark matter, including via study of the cosmic microwave background, combined with the lack of observation of dark matter in larger colliders motivates a search for dark matter in the sub-GeV region. The Light Dark Matter Experiment (LDMX) is a future experiment to be based at SLAC whose design is a candidate for detecting this light dark matter. LDMX utilizes a missing-momentum approach, and uses a hadronic calorimeter as a veto against backgrounds. A test beam campaign was run in April 2022 at CERN with one aim being to optimize the hadronic calorimeter. The calorimeter utilizes bars which detect incident particles but does not record the position of each hit. As a result, position resolution is limited to an assumption that the hit occurred at the center of the bar. In this investigation, test beam data using muon runs was considered for several runs where the bars were displaced progressively further from the initial position by a known distance. Analysis of the recorded time of arrival for these hits in conjunction with their pulse information was then assessed to develop a methodology for determining more precisely where the hit occurred.</p> |

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| 22. | <p>Erin Eason <i>Incorporation of Heteroatoms in the TriDDA Net [4+2] Cycloaddition</i> Advisor: Tom Hoyer Sponsoring Program: UMN Chemistry- Lando Home Institution: College of the Holy Cross Abstract: The Diels Alder reaction has been coined one of the most powerful synthetic techniques. The cycloaddition allows chemists to access a variety of quite complex organic scaffolds. The work of this project aims to expand the substrate scope available via a specific derivative of the Diels Alder reaction, the TriDDA reaction. The tridehydro-Diels-Alder reaction is a net [4+2] cycloaddition involving a pendant alkyne or nitrile, ene, and an allene intermediate. Previous Hoyer lab work has investigated the mechanism of the TriDDA reaction and provided access to a variety of carbon-based aromatic compounds. The current work aims to incorporate heteroaromatic moieties into the di-yne substrate in attempt to provide access to organic frameworks used as the building blocks for complex pharmaceutical molecules. In tandem, we have also modified the di-yne linker to evaluate electronic effects on allene formation.</p> |
| 23. | <p>Justus Fagan <i>Dynamic pH and Temperature Kinetic Measurements During In Vitro Protein Synthesis Reactions</i> Advisor: Vincent Noireaux Sponsoring Program: Physics REU Home Institution: Austin College Abstract: TXTL is a cell-free protein synthesis platform with the potential for many biomedical applications. During the Summer of 2022, research was done on measuring the pH and temperature kinetics in the TXTL, Tool Box 3.0, platform. 2',7'-bis-(2-carboxyethyl)-5-(and-6)-carboxy-fluorescein (BCECF) is a blue-green fluorescent pH probe that is highly sensitive to pH fluctuation and is optimal for TXTL reactions due to having a pKa close to the physiological pH. To acquire precise measurements of pH, a ratiometric calibration is performed using a resolute in-house constructed buffer, S30c. 5-Carboxytetramethylrhodamin (TAMRA) is a red fluorescent quenching dye in response to temperature. TAMRA calibration involves manipulating the programming of a microplate reader to measure fluorescent intensity at independently set temperatures. Accurate pH and temperature measurements may give insight into a more in-depth understanding of the physical properties that are involved in transcription-translation reactions.</p> |
| 24. | <p>Nitza Falcon-Cruz <i>Formation of Block Copolymer Micelles in Ionic Liquids via Cosolvation</i> Advisor: Timothy Lodge Sponsoring Program: MRSEC Home Institution: University of Puerto Rico at Humacao, Puerto Rico Abstract: Block copolymers self-assemble to form different micellar nanostructures in a solvent that is selective to one of the polymer blocks. Block copolymer micelles have been applied in drug and gene delivery, catalysis, and industrial applications, such as the modification of lubricants' viscosities. However, the mechanism through which micelles form and achieve equilibrium is not well understood. The goal of this project is to study the formation of diblock copolymer micelles in ionic liquids using the cosolvent method. The model consists of 1,2-polybutadiene-b-poly(ethylene oxide) block copolymers, an ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C2MIM][TFSI]), and a cosolvent, tetrahydrofuran or dichloromethane. The samples were prepared by dissolving diblock copolymers in a mixture of equal weight proportions of cosolvent and ionic liquid. Dynamic light scattering measurements were performed to determine the hydrodynamic radius of the micelles at various stages that were controlled by decreasing cosolvent composition by evaporation. Results show that cosolvent physical properties play an important role in the starting point of micelle formation. Inverting the method by adding cosolvent, instead of evaporation, yields the same path for annihilation as for the formation of the micelles. This study will help us to better understand the mechanism behind block copolymer micelle formation and equilibration.</p> |

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| 25. | <p>Alejandra Felix <i>Pre-Clinical Benchtop Model to Assess Lung Viability and Therapies</i> Advisor: Paul Iazzo Sponsoring Program: ATP-Bio Home Institution: University of Southern California Abstract: Patients in need of a lung transplantation are placed on what has been dubbed the "mortality waitlist" because the criteria for a lung graft is very restrictive and many patients do not receive the donation in time. Addressing this issue, ex vivo lung perfusion (EVLP) is a method to assess marginal lungs to increase the number of available grafts. Previous research has shown that increased edema is related to worse graft dysfunction. In addition, there has been a lack of research observing edema consistently over time in donor lungs using EVLP. The goal of this study was to understand the edematous response of the lungs when placed on EVLP. Five sets of porcine lungs underwent EVLP using porcine whole blood as the perfusate. Lung edema was assessed using a load cell attached to an Arduino scale sensor that measured lung weight about every 40 seconds. We observed that the curve reflecting lung edema changes depending on some conditions i.e., the presence of glucose and the administration of nitroglycerin to maintain perfusion of the lungs. These results highlight the need to monitor how fluid changes over time in the lungs throughout EVLP.</p> |
| 26. | <p>Emily Foley <i>Simulations of compact binary merger events in preparation for forthcoming LIGO observing runs</i> Advisor: Michael Coughlin Sponsoring Program: Physics REU Home Institution: Wake Forest University Abstract: With the fourth LIGO observing run (O4) scheduled for March of 2023, rapid search and identification measures for electromagnetic counterpart signals to binary neutron star mergers (BNS) are of utmost importance. In this work, we present updated simulations on the order of 10^6 compact binary merger events for O4 and O5. We use updated PDB merger rates, projected sensitivity thresholds, and improved signal to noise ratios (SNR) of the LIGO-Virgo-KAGRA detector network. We find that our simulations are in agreement with O3 public alerts, and predict 17^{+35}_{-13} BNS, 10^{+18}_{-8} neutron star-black hole (NSBH), and 46^{+33}_{-23} binary black hole (BBH) detections in O4. Finally, we generate lightcurves from simulated injections of BNS merger events, and evaluate their detectability by the ZTF and Rubin observatories.</p> |
| 27. | <p>Ally Garza <i>Tuning degradation and drug release in thermoresponsive hydrogels</i> Advisor: Michelle Calabrese Sponsoring Program: MRSEC Home Institution: University of Texas Rio Grande Valley Abstract: While oral antibiotics are the current standard treatment for middle ear infections, such administration has numerous harmful side effects. Alternatively, recent efforts have turned to biocompatible gels that can be injected directly into the ear, reducing side effects, and improving ease of administration in children. This work focuses on Poloxamer 407 (P407), a water-soluble, non-ionic triblock polymer that is commonly utilized as a pharmaceutical ingredient. With an increase in temperature, P407 chains in water arrange into spherical micelles. With further temperature increase, these formulations gel as the micelles pack into ordered structures. This gelation can be exploited to design drug-loaded formulations that can be injected at room temperature and then gel near body temperature. This work evaluated the rheological and structural changes in P407 gels upon addition of clinically relevant small molecules with the ultimate goal of forming an injectable gel that adheres to the eardrum to treat ear infections. Here, polymer assembly as a function of temperature and small molecule content was characterized using rheology, small-angle X-ray scattering, and differential scanning calorimetry. In addition, a Franz diffusion cell was used to show that these gels remain stable throughout the course of delivery.</p> |

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| 28. | <p>Allison Gatz <i>Synthesis of 2,2-LI-HOPO for Lanthanide Separation</i> Advisor: Valerie Pierre Sponsoring Program: UMN Chemistry- Lando Home Institution: Loyola University Chicago Abstract: Lanthanides are a group of metals, found in ores exclusively as mixtures of elements, which have a variety of nuclear, catalytic, and technological applications. Previous methods utilized to separate lanthanides are inefficient due to excess solvent use and lack of selectivity. A ligand can be employed to separate these mixtures because of Lewis-acidity differences across the lanthanide series. The 2,2-LI-bisHOPO ligand was selected as the ligand of interest because of its predicted high selectivity for lanthanides with smaller ionic radii and ability to easily be covalently immobilized on a solid support. This ligand was synthesized using a five-step method employing the commercially available 6-hydroxypicolinic acid. Moreover, lanthanide-ligand complexes have an affinity for phosphate, making the 2,2-LI-bisHOPO ligand a means of phosphate removal in biological and aquatic systems.</p> |
| 29. | <p>David Geeganage <i>Comprehensive Laboratory Evaluation of the Sensirion SPS30 Low Cost Particulate Matter Sensor</i> Advisor: David Pui Sponsoring Program: ME Home Institution: Macalester College Abstract: The health risks posed by particulate matter (PM) in the air have increased the need for spatially dense air quality monitoring in urban areas. However, research grade particle measurement instruments are extremely expensive, making them unusable for large scale air quality monitoring. Low cost PM sensors (</p> |
| 30. | <p>Karan Gill <i>Total Synthesis of Eburnamonine through a Pd-catalyzed Asymmetric Cyanoamidation reaction</i> Advisor: Chris Douglas Sponsoring Program: UMN Chemistry- Lando Home Institution: Carnegie Mellon University Abstract: The <i>Aspidosperma</i> alkaloid (+)-eburnamonine is a relevant target for enantioselective total synthesis due to its potency as a cerebral vasodilator and anti-tumor drug. We have proposed an efficient, 11-step, enantioselective synthesis of (+)-eburnamonine. We present our synthetic pathway that features reactions with reproducible yields and relatively mild conditions. Our synthesis highlights a palladium-catalyzed asymmetric cyanoamidation reaction, which intramolecularly forms a lactam with an all-carbon quaternary stereocenter by C–CN bond activation. The synthesis of the cyanoamidation starting material features a CuI-catalyzed carbometalation of propargyl alcohol, a Johnson–Claisen rearrangement, carbonyl diimidazole (CDI) coupling with tryptamine, lithium aluminum hydride (LAH) reduction, and cyanoforylation of the resulting secondary amine by in situ preparation of carbonyl cyanide from tetracyanoethylene oxide (TCEO) and dimethyl sulfide.</p> |
| 31. | <p>Amiya Gupta <i>Neural Networks for Modeling of Combustion Systems</i> Advisor: Suo Yang Sponsoring Program: ME Home Institution: University of Florida Abstract: Combustion mechanisms are complex and highly stiff systems are computationally expensive and time consuming to model and control. The novel reduced-order neural ODE (RONODE) methodology, composed of a stiffness-reduced nonlinear autoencoder and a neural ODE model, has been shown to greatly decrease the computational cost and time required to model steady and unsteady 0-D reactions and steady 1-D reactions. The focus of this research is to extend this model for higher-dimensional data. Laminar counter diffusion flame simulations were run using the OpenFOAM CFD solver coupled with the Cantera Chemical Kinetics library. The RONODE model was then applied to this higher-dimensional data to determine the appropriate parameters for reducing stiffness and optimizing the efficiency and accuracy of the solution.</p> |

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| 32. | <p>Kobi Hall <i>Optimization of Medium Scale Electrostatic Precipitators</i> Advisor: Christopher Hogan Hogan Sponsoring Program: ME Home Institution: Columbia University Abstract: In Heating/Ventilation/Air Conditioning (HVAC) systems, fibrous filters are commonly used to prevent the spread/release of hazardous particles such as soot or viruses. These filters involve a considerable pressure drop, making filtration energetically expensive, especially for indoor air cleaning applications. Electrostatic precipitators (ESPs) can be used in place of traditional filters, allowing the collection of particulate matter while also, depending on the application, being more energy efficient. By applying a voltage high enough (>10 kV) to sustain corona discharge, the ESP simultaneously charges and collects particles via electrostatic attraction over a wide range of particle sizes ranging from ~10 nm up to ~10 μm. The unipolar charging process within an ESP is poorly understood, especially at different particle sizes, leading to many inefficient ESPs on the market. Obtaining the bidimensional size and charge distribution of particles can inform decisions about ESP design optimization. Such distribution is measured here for spherical potassium chloride particles using a tandem differential mobility analyzer setup. Preliminary results show clear peaks of particle number concentrations that reduce in intensity and shift towards larger electrical mobility as the ESP voltage increases. We also observed that charge distribution may vary considerably as a function of particle size.</p> |
| 33. | <p>Peter Hartford <i>Development of Multi-view 3D Particle Tracking System for Measuring Pollen Transport in Atmosphere</i> Advisor: Jiarong Hong Sponsoring Program: UROP/URS Home Institution: University of Minnesota Abstract: Pollen transport in the atmosphere is a crucial process involved in the cross-pollination of plant species. In addition, such processes can yield significant implication on public health as the presence of certain pollens can lead to discomfort or even severe risks for people with allergies or other respiratory disorders. Therefore, an enhanced understanding of the fundamental mechanism behind pollen transport can improve our modeling strategies and corresponding regulatory practices for various applications in agriculture, ecology, and public health domains. However, there is a significant lack of experimental data showing detailed pollen transport kinematics in the atmosphere due to the technical challenges involved in the field measurements of this phenomenon. In this work, we develop an imaging-based measurement system using four-synchronized cameras controlled through a Wi-Fi network and demonstrate its capability to capture 3D tracks of pollens emitted from a Cottonwood (<i>Populus deltoides</i>) tree in a volume on the order of ~64m³. Our system can be extended for measurements in a broad range of transport phenomena of other particle types (e.g., snow drift, sand dune migration, sea spray generation).</p> |
| 34. | <p>Genevieve Herron <i>Polysaccharide Derived Crosslinkers for use in Thermoset Polymer Networks</i> Advisor: Theresa Reineke Sponsoring Program: Center for Sustainable Polymers Home Institution: Middlebury College Abstract: As plastic waste continues to enter the environment, developing biobased materials that can replace traditional plastics has become a rapidly growing field of study. Thermosets are a type of plastic that are a network of crosslinked molecules. To explore a library of possible polysaccharide derived crosslinkers, several differently-sized saccharides were chosen as starting points of functionalization. An enzyme-driven esterification of trehalose that produces a thiol functionalized trehalose has shown encouraging results. Analysis by ¹H NMR showed promising peaks which indicate that substitution of the primary hydroxyl groups has occurred. The thiol-functionalization was chosen for its reactivity and use in "click" chemistry. An allylated trehalose has also been synthesized for investigation into its uses as another crosslinker. A larger polysaccharide, β-cyclodextrin, shows potential for a rigid crosslinker due to its cyclic structure. Functionalization of the β-cyclodextrin uses a one-pot switchable solvent method to synthesize an allyl carbonate β-cyclodextrin. Future work with these materials would involve crosslinking a thiolated trehalose and allyl carbonate β-cyclodextrin into a network.</p> |

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| 35. | <p>Vy Huynh <i>Synthesis, Microstructure Stability, and Phase Behavior of Al-Containing Refractory Multi-Principal Element Alloys</i> Advisor: David Poerschke Sponsoring Program: MRSEC Home Institution: The University of Washington Abstract: Refractory multi-principal element alloys (MPEAs) have the potential for high-temperature applications due to their increased yield strength at elevated temperatures compared to other commonly used alloys. MPEAs are composed of at least five elements with 5-35 at% concentrations each. Those consisting of refractory metals are usually BCC solid solutions and the addition of aluminum can lead to precipitation of a higher strength B2 phase. The B2 phase forms coherently to the BCC solid solution and the resulting microstructures have been shown to provide superior combinations of yield strength and ductility under 1000 °C compared to BCC alloys. Five alloy compositions ($Al_{0.25}NbTaTiZr$, $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$, $AlMo_{0.5}NbTa_{0.5}TiZr$, $Al_{0.75}NbTi_3VZr_{1.5}$, $Al_{0.75}Hf_{0.5}Nb_{0.5}Ti_2VZr$) were fabricated by arc melting and annealed at 1200 or 1400 °C to form solid solution phases. The MPEAs were subsequently annealed at 600 °C to grow the precipitating phases. The samples were characterized by XRD, SEM, and EDS to identify the phases and microstructures. Analysis revealed that only $Al_{0.25}NbTaTiZr$, $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$, $AlMo_{0.5}NbTa_{0.5}TiZr$ formed cross-hatched patterns composed of a BCC and a B2 phase, while the other two exhibited a single BCC phase. After the 600 °C anneal, only $AlMo_{0.5}NbTa_{0.5}TiZr$ retained the cross-hatched pattern, whereas the microstructures changed, or different phases appeared for the other MPEAs.</p> |
| 36. | <p>Rachel Itow <i>Isothermal Ice Formation Kinetics of Cryoprotective Agents</i> Advisor: John Bischof Sponsoring Program: ATP-Bio Home Institution: University of California, Riverside Abstract: With the cryopreservation of biological tissues, cryoprotective agents (CPAs) are frequently implemented, as CPAs are chemical agents capable of reducing ice formation and promoting vitrification when cooling to cryogenic temperatures. CPAs play a critical role in cooling since the formation of ice crystals in biological tissues can result in physical damage through tearing and changes in solute concentrations in cells. However, high concentrations of CPA are toxic and interfere with the future growth and development of cells. The type of CPA, its concentration, and the method for cooling are all factors that contribute to the degree of ice formation within cells. In addition, phase change within solutions of potential CPAs needs to be well understood. The thermodynamics of phase change for CPAs can be analyzed using Differential Scanning Calorimetry (DSC). This study utilized DSC to examine ice formation kinetics in CPA solutions at fixed cryogenic temperatures. Specifically, 46 wt. % Propylene glycol (PG) aqueous solutions were cooled to varying temperatures from -40C to -46C. We show the Avrami rate constants for this CPA.</p> |
| 37. | <p>Salman Jaitheh <i>Synthesizing Carbon Dots For Binding Per -and Polyfluorinated alkyl substance (PFAS)</i> Advisor: Christy Haynes Sponsoring Program: Center for Sustainable Polymers Home Institution: University Of Minnesota Abstract: Per and polyfluorinated alkyl substances (PFAS) have been widely used in industries for coatings and as a water repellent. However, exposure to PFAS are suspected to result in adverse health effects in humans. For this reason, is important for us to have effective remediation methods for removing PFAS from the environment. Current remediation methods for PFAS, such as ion resin exchanges, are frequently costly and require a lot of energy. Our goal is to deploy a sustainable method for remediating PFAS from the environment by enhancing plant uptake (phytoremediation) of PFAS through carbon dots (CDs). We are designing CDs with an affinity for PFAS by using amine rich precursors which will form cationic CDs to sorb anionic PFAS. We have synthesized CDs using a kitchen microwave with different ratios of glucose and L-arginine. A 1:15 ratio of glucose to L-arginine results in CDs with an average size of 49 nm and a zeta potential of +5.237mV. We are continuing to tune the size and charge to optimize the interactions between PFAS and CDs.</p> |

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| 38. | <p>Bhavnes Jangid <i>Calculation of Barrier Heights using Multiconfiguration Pair-Density Functional Theory: Assessment of the Performance of On-Top Density Functionals</i> Advisor: Donald G. Truhlar Sponsoring Program: UMN Chemistry - CTC Home Institution: Accurately describing the barrier heights of chemical reactions is a central problem of theoretical chemistry. A special difficulty is encountered in the case of reactions involving open-shell systems such as radical reactions, transition metal complexes with broken bonds, or molecular systems composed of nearly degenerate states, also known as multi-reference (MR) systems. Multiconfiguration pair-density functional theory, MC-PDFT, is an affordable MR approach in which the total energy is obtained using MCSCF kinetic energy (T), density (ρ), and on-top density (Π) with an on-top density functional (E_{ot}):</p> $E^{MC-PDFT} = \langle \psi^{MC} \hat{T} \psi^{MC} \rangle + \int \rho(r) v_{Ne}(r) dr + \iint \frac{\rho(r_1)\rho(r_2)}{r_{12}} dr_1 dr_2 + E_{ot}[\rho, \Pi] + V_{NN}$ <p>In this project, we have calculated the barrier heights for the dataset MCGDB86 (206 barrier heights), composed of subdatabases DBH24, CR20, CRBH20, HTBH38, NHTBH38, BHPERI26, WCPT27, and PX13. We have determined the barrier heights for all the subsets except PX13 by using each of nine on-top density functionals (tPBE, ftPBE, tBLYP, ftBLYP, tOPBE, ftOPBE, tOreLyp, ftOreLyp and tPBE0). The active space for the MCSCF calculations was selected based on the CPO (Correlated Participating Orbital) scheme. For most reactions, the reactants, transition state, and products were optimized by using the same active space, mainly nom-CPO. All the calculations were performed in <i>OpenMolcas</i> and using the ma-TZVP basis set.</p> |
| 39. | <p>Riley Kazukiewicz <i>New Phenolate-Based Ligands for Low-Valent Titanium Chemistry</i> Advisor: Ian Tonks Sponsoring Program: UMN Chemistry- Lando Home Institution: St. Olaf College Abstract: Titanium's low toxicity and high Earth abundance make it an attractive metal for use in sustainable catalysis. Previous research in the Tonks group has shown Ti imidos' ability to catalytically produce nitrogen heterocycles as well as other nitrogenous adducts via a Ti^{IV}/Ti^{III} redox cycle; however, Ti^{III}-based catalysis is less chemically accessible. A potential solution to this problem is to ligate a Ti^{IV} center with a redox non-innocent ligand to "mask" a Ti^{III} center as a formal Ti^{IV}. This project focuses on the synthesis and purification of a novel phenolate-based ligand which is capable of ligating Ti substrates to produce a variety of titanium pre-catalysts. Once metallated, recrystallization of the Ti adducts was attempted. Further, the ability of the pre-catalysts to form titanium imido complexes as well as masked Ti^{III} species was investigated.</p> |
| 40. | <p>Cameron Khan <i>Ice nucleation dynamics via a seeding technique</i> Advisor: Sapna Sarupria Sponsoring Program: UMN Chemistry - CTC Home Institution: Princeton University Abstract: The freezing of water, despite its ubiquity, remains a poorly understood process at the molecular level. A robust theoretical framework to accurately predict nucleation rates does not exist, and simulations and experiments routinely produce contradictory results. In this project, I provide a derivation of the Fokker-Planck equation (master equation) and steady-state rate expressions of the classical nucleation theory (CNT), a long-standing picture of homogeneous nucleation. I then demonstrate the seeding method, a molecular dynamics procedure to extract the thermodynamic and kinetic parameters outlined by CNT. I estimate the critical temperature for a seed crystal of 600 TIP4P hexagonal (Ih) ice molecules by observing patterns of growth or decay at varying supercooling temperatures. Then, the molecular attachment rate can also be recovered by analyzing diffusion along the nucleus size coordinate. Growth rates of trajectories far from the critical temperature can be used to describe the drift behavior, permitting a direct comparison to the CNT model.</p> |

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| 41. | <p>Mason Kozody <i>Exploration of Homo-block-Core-shell Bottlebrush Polymer Morphology</i> Advisor: Mahesh Mahanthappa Sponsoring Program: MRSEC Home Institution: Clarkson University Abstract: Block copolymers exhibit a wide range of morphologies formed by thermodynamically-driven self-assembly. These morphologies offer a route for sub-12 nm nanolithographic patterning. This project aims to create unique morphologies that are not intrinsic to linear block copolymers through the use of a block bottlebrush polymers. These bottlebrushes consist of a core-shell brush architecture segment covalently bonded to a homopolymer brush segment. Core-shell macromonomers from sequential ring-opening transesterification polymerization (ROTEP) of ϵ-decalactone and D,L-lactide initiated from exo-5-norbornene-2-methanol. The homopolymer macromonomer structure uses the same norbornyl alcohol initiator for ROTEP of D,L-lactide. These macromonomers are grafted-through using sequential ring-opening metathesis polymerization (ROMP) of the diblock macromonomer followed by lactide macromonomer to form the desired bottlebrush. Characterization of these polymers has been achieved through ^1H NMR and size-exclusion chromatography (SEC) to determine side chain and backbone degrees of polymerization and dispersities. Small-angle X-ray scattering (SAXS) patterns reveal a lamellar phase with a domain spacing range of 14-23 nm, which has been attributed to the lamellar spacing of the core-shell brush block. Extremely small-angle X-ray scattering (ESAXS) was used to investigate a potential superstructure that contains the observed lamellae. Future analysis includes microscopy imaging to visually identify and confirm SAXS microphases.</p> |
| 42. | <p>Jonathan Landeros <i>A Scientific Instrument that Analyzes Metal Acetylacetonate (acac) Precursors for SSMOMBE</i> Advisor: Jalan Bharat Sponsoring Program: MRSEC Home Institution: University of Texas El paso Abstract: Establishing entire stoichiometric control over complex materials within Molecular Beam Epitaxy (MBE) is possible by using solid organic compound precursors. This method synthesizes ultra-low vapor pressure materials and oxidizes them with the supply of complex oxides through an effusion at low temperatures. The purpose of this project is to run an assembled scientific instrument that will allow for metal acetylacetonate precursors or organic sources to be analyzed by quantifying the evaporation/sublimation (vapor pressures) of the compounds and their impurities. This test chamber was initially created and assembled using a CAD software called Solidworks. Once the instrument is properly run, Yttrium acetylacetonate $[\text{Co}(\text{acac})_3]$ will be compared to Ruthenium acetylacetonate $[\text{Ru}(\text{acac})_3]$. Ruthenium acetylacetonate $[\text{Ru}(\text{acac})_3]$ has successfully opened the growth window in previous experiments, allowing for pure perovskite structured epitaxial films to be made. The hypothesis surrounding the comparison of these two metal organic sources is that $\text{Co}(\text{acac})_3$ will contain similar characteristics as $\text{Ru}(\text{acac})_3$ by creating a stoichiometric ratio with the complex compound being mobilized and open the growth window allowing for controlled self-growth to occur. This will allow for a complete doping of the complex compound, resulting to an atomic precise quantum structure, aka a perovskite epitaxial film.</p> |
| 43. | <p>Anne Lashbrook <i>Study of the Two Lepton Channel Sensitivity in Low-p_Tmiss Top Squark Searches</i> Advisor: Nadja Strobbe Sponsoring Program: Physics REU Home Institution: Saint Louis University Abstract: Supersymmetry is a mathematical symmetry that makes identical the equations for force and matter, presenting a relation between fermions and bosons. There exist many new physical models that incorporate supersymmetry and also characterize it with R-parity violation. R-parity is a property of subatomic particles in which all known particles have positive R-parity and supersymmetric particles negative. R-parity violating (RPV) supersymmetric models envision proton-proton collisions resulting in low missing transverse momentum and a spray of jets consisting of quarks and gluons. This research analyzes data from CERN's CMS experiment for signs of new physics. This is accomplished using reconstructed collision events with at least six jets and two leptons at $\sqrt{s} = 13 \text{ TeV}$. Dominant backgrounds are identified and analyzed for additional data selections to further minimize events of interest. RPV signals are analyzed at 300 GeV and 800 GeV. The two lepton channel sensitivity is refined for future analyses.</p> |

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| 44. | <p>Sang Le <i>Controlling DNA Demethylation Machinery with Substrate-Mimetic Ten-Eleven Translocation Dioxygenases Inhibitors</i> Advisor: Natalia Tretyakova Sponsoring Program: UMN Chemistry- Heisig Gleysteen Home Institution: University of Minnesota - Twin Cities Abstract: DNA methylation is a chemical modification that occurs on the nucleobases of DNA. Methylation status regulates gene expression, and the placement of methyl marks across the genome is controlled by various writer and eraser enzymes. Specifically, the enzymes primarily responsible for removing DNA methyl marks are a family of ten-eleven translocation dioxygenases (TET1-3). Aberrant TET enzymatic activity is hypothesized to play a role in many pathologies, ranging from various cancers to neurodegeneration. To investigate the contribution of dysregulated TET enzymes in disease, we sought to develop a series of small molecules that inhibit TET-mediated demethylation <i>via</i> structure-based design. We utilized computational molecular docking to design potential binders to TET, followed by the synthesis of 15 initial candidate TET inhibitors. Preliminary liquid chromatography/mass spectrometry (LCMS)-based biochemical assays showed that the most potent molecule in our series had an IC₅₀ value of ~1 μM <i>in vitro</i> and affected DNA methylation levels in human embryonic kidney (HEK) cells. This work represents a critical first step in developing potent and selective TET inhibitors to serve as chemical tools that can elucidate the role of DNA methylation in human disease.</p> |
| 45. | <p>Hyunmuk Lee <i>Applications of automated collective variable discovery via autoencoder neural network</i> Advisor: Sapna Sarupria Sponsoring Program: UMN Chemistry- Lando Home Institution: St. John's University Abstract: Biased molecular dynamic simulations allow for the exploration of free energy surfaces beyond potential barriers too high to overcome in a reasonable time scale. However, the choice of appropriate collective variables (CVs) that can best describe the behavior of a molecule is a nontrivial problem, often requiring chemical insights into the system beforehand. Ferguson et al. suggests the usage of an autoencoder neural network. This method named MESA (Molecular Enhanced Sampling with Autoencoders), takes a novel approach of automated CV discovery, through iterated improvements on the hypothetical CVs using a neural network followed by biased simulations to test its effectiveness. In this study, the performance MESA has been applied on various systems involving a simple protein Trp-cage, an engineered peptide known to be one of the smallest systems with highly stable folded states. Trp-cage in various solutions, and its interaction with a graphene surface has been studied by umbrella sampling simulations to explore metastable states past high energy barriers and explore the effects on its free energy surface using MESA.</p> |
| 46. | <p>William Leija <i>Measurement of Leak Properties of Mu2e/Mu2e-II Tensioned Straws</i> Advisor: Dr. Ken Heller Sponsoring Program: Physics REU Home Institution: Texas State University Abstract: The Muon to Electron (Mu2E) project represents the search for physics beyond the "Standard Model". We prepared Mylar straws which will be used to make up the trackers. These straws are comprised of aluminum and gold layers and will receive beams of muons. The composition of the straws will facilitate the muon to electron conversion. As of now the next generation of Mu2E: Mu2E-II is being designed and for my experiment I focused on the next generation of straws which may be used for Mu2E-II. The difference with my straws is that the gold layer inside the straw was removed and the aluminum layer was left. This makes the straws more sensitive to the muon beam since less material can interfere with the muon. Unfortunately, this also predicts that the straws will be more delicate which can affect the straws integrity when under tension. My experiment was to test how the leak rates will increase under tension by figuring out how to keep the straws under a constant tension and test how the leak rates changed when going from 0 tension to 800 grams of tension. This provides insight in how these straws would perform if used for the trackers.</p> |

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| 47. | <p>Zoe Lelas <i>Binary mixture vapor-liquid equilibrium: toward sustainable acrylic acid synthesis and commercial production.</i> Advisor: Paul Dauenhauer Sponsoring Program: Center for Sustainable Polymers Home Institution: University of Wisconsin-Madison Abstract: To provide alternatives to high-volume petrochemical intermediates for producing acrylic acid, Paul Dauenhauer and Chris Nicolas' company Låkril Technologies has been developing bio-based technology for using renewable feedstock instead. The company's goal is to provide alternatives that will help decrease the world's CO₂ emissions through their catalyst technology for catalytic dehydration of α-hydroxy acids, such as lactic acid, allowing the supply of sustainable acrylic acid derivatives as drop-in replacements. Mass production of this product involves fractional distillation, a stepwise condensation of vapor to liquid, allowing better separation to be achieved. Designing the distillation column requires phase diagrams to understand the composition of the solution at any temperature throughout the process. To develop these diagrams, understanding how to use the Fischer VLE machine and validating the system were needed to ensure it would be conducive to the solutions that apply to the project. The ethanol-water binary system was used as there have been extensive reports on this system to check my values with those in literature. The results concluded that this system could be used to develop reliable phase diagrams for future research.</p> |
| 48. | <p>Julia Lies <i>Synthesis of P4MCL-PLLA Triblock Copolymers for Degradation Studies</i> Advisor: Marc Hillmyer Sponsoring Program: Center for Sustainable Polymers Home Institution: University of Illinois at Urbana-Champaign Abstract: With less than 10% of plastic recycled worldwide, developing degradable plastics is essential. Most elastomers are thermosets with chemical crosslinking limiting recyclability. Thermoplastic elastomers, however, are composed of ABA block copolymers. ABA block copolymers have a rubbery midblock with glassy endblocks. These copolymers utilize physical crosslinks, offering a more sustainable option. A Poly(4-methyl-ϵ-caprolactone) midblock with Poly(L-Lactide) end blocks were synthesized to analyze the degradation of these triblock copolymers. Poly(4-methyl-ϵ-caprolactone), or P4MCL, was chosen as the rubber midblock due to its amorphous structure which is suited for tough elastomers. Poly(L-Lactide), or PLLA, was chosen for the glassy arms of this triblock due to its semi crystallinity which increases the strength and toughness of elastomers. The triblock with the P4MCL midblock and PLLA arms is expected to have high stresses and elongation at break. The triblock acts like a thermoplastic elastomer at low lactide fractions and more of a hard plastic at high lactide fractions. Triblocks with three ratios of P4MCL to PLLA were targeted: 1:1, 1:7, and 3:1. Changing the lactide fraction alters the block polymer morphology. This project aims to observe how the morphology alters degradation rate.</p> |
| 49. | <p>Andrea Ligoeki <i>Dye loading of and release from swelling polymers for agric</i> Advisor: Christy Haynes Sponsoring Program: UMN Chemistry- Heisig Gleysteen Home Institution: University of Minnesota - Twin Cities Abstract: The world's population is expected to hit 9.7 billion by 2050; therefore, we must increase our food production to accommodate this rapid population growth. Nanoparticles are increasingly being used to improve agricultural crop production because they can promote nutrient absorption, lower soil and water contamination, and increase the plant's resilience in non-ideal environments. Polymeric nanoparticles like poly-2-(diethylamino)ethyl methacrylate (pDEAEMA) have extensively been used for drug delivery in medical applications. However, this work aims to use pDEAEMA to deliver beneficial cargo to plants. pDEAEMA is a pH-responsive polymer that reversibly swells in acidic media and is synthesized via a free-radical polymerization. Dynamic light scattering and zeta potential measurements were used to determine the polymer nanoparticle size and surface charge, respectively, as well as the polymer's swelling behavior. Herein, we present the optimization of pDEAEMA loading using 1-pyrene butyric acid NHS ester as model fluorescent cargo by taking advantage of the polymer's swelling and deswelling mechanism. Fluorometry was used to determine the fluorescence spectra of the dye-loaded pDEAEMA system. Preliminary results show that the polymer takes up the dye of interest although further optimization and characterization need to be conducted to further confirm uptake followed by controlled release.</p> |

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| 50. | <p>Sheharyar Malik <i>3D Printing Microfluidics for Plasma Treatment of Biofilms</i> Advisor: Michael McAlpine Sponsoring Program: ME Home Institution: The University of Tulsa</p> <p>Abstract: Biofilms consist of large groups of bacterial cells that arrange into layers and adhere to surfaces such as drinking water pipelines and medical catheters. Plasma treatment is a promising method to reduce or eliminate biofilms. One way this can be achieved is by using Plasma Activated Water (PAW) containing reactive oxygen and nitrogen species (RONS) which are antimicrobial agents. Microfluidic devices can be utilized to study the effect of plasma treatment on biofilms since these devices enable precise control over fluid flow on a microscopic scale using channels, valves, and gradient generators. The current gold standard for creating microfluidics is soft lithography, which involves time-consuming procedures such as PDMS molding and requires a cleanroom for fabrication. Direct Ink Writing (DIW) 3D printing is an alternative method to create microfluidics that allows for rapid prototyping of complex geometry while maintaining the flexibility of the devices for performing traditional microfluidic experiments. Therefore, this technique can be employed to fabricate a Lab-on-a-Chip (LOC) device to study the effect of different concentrations of PAW on biofilms. This study focuses on DIW 3D printing and an analysis of microchannels as well as a gradient generator that will be incorporated into the LOC.</p> |
| 51. | <p>Joi Malone <i>Model Predictions of Ice Nucleation and Growth during Cooling and Rewarming Cycles</i> Advisor: Chris Hogan Sponsoring Program: ATP-Bio Home Institution: Spelman College</p> <p>Abstract: One of the main issues experienced with cryopreservation is ice formation as the material is being cooled and upon rewarming, while the material is still below the freezing point water. Therefore, it is crucial to understand the rate at which water should be cooled and rewarmed to prevent ice formation. This study utilized the traditional Avrami equation, which describes the growth rate of ice from liquid water under isothermal conditions, to develop a model of ice nucleation and growth when cooling, and rewarming, at constant rates. The model incorporates regression equations for the nucleation and growth rate of ice in water from Kangas et al (2021). We find that cooling to 135 K at rates below 5×10^5 K/s will result in complete ice formation. However, a small percentage of ice formation is predicted for higher cooling rates with a power law relationship between the maximum fraction of ice and the cooling rate with a scaling exponent of -3.732. This developed model enables estimation of ice formation during cooling and rewarming cycles, and using nucleation and growth rate inputs, can be used to examine ice formation with cryopreservative agents. Future work will incorporate of spatial heat transfer effects on ice formation.</p> |
| 52. | <p>Armina Mayya <i>Synthesis, Functionalization, and Polymerization of CO₂-Derived Lactone Monomers</i> Advisor: Ian Tonks Sponsoring Program: Center for Sustainable Polymers Home Institution: University of California, Berkeley</p> <p>Abstract: Biodegradable polymers derived from waste feedstocks like CO₂ could help mitigate waste plastic buildup. Unfortunately, CO₂ cannot be directly integrated into polymers with alkenes due to both thermodynamic and kinetic factors. It is therefore useful to synthesize CO₂- and alkene-based intermediate lactone monomers. One such intermediary, 3-ethylidene-6-vinyltetrahydro-2H-pyran-2-one (EVP), is synthesized via the telomerization of butadiene and CO₂, and is 28.9% CO₂ by weight. In attempted polymerizations, however, EVP undergoes 1,4-conjugate additions on its α,β-unsaturated alkene. To avoid this, the pendant alkene chains on EVP can be partially hydrogenated to 3-ethyl-6-vinyltetrahydro-2H-pyran-2-one (EtVP) or fully hydrogenated to 3,6-diethyltetrahydro-2H-pyran-2-one (DEP). EtVP synthesis was previously catalyzed by hexamethylphosphoramide (HMPA), which is carcinogenic. For a safer synthesis, triphenylphosphine oxide was successfully employed in place of HMPA. Additionally, although DEP can be synthesized from EtVP, a direct procedure from EVP is preferable. One was developed using catalytic amounts of Pd and H₂ gas, though purification is still ongoing. Lastly, 1,4-conjugate additions of nucleophiles to the α,β-unsaturated alkene on EVP can modulate the properties of resultant polymers. The addition of nitromethane to EVP was performed to create crystalline polyesters; however, no catalysts thus far have polymerized this monomer, likely due to steric bulk on the α position.</p> |

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| 53. | <p>Chelsea Mikal <i>Magnetic Processing of Block Copolymers</i> Advisor: Michelle Calabrese Sponsoring Program: MRSEC Home Institution: University of Maryland Baltimore County (UMBC) Abstract: Block copolymers (BCPs) are compounds formulated by combining blocks of chemically distinct monomers to create a polymer chain. In particular, poloxamers are triblock copolymers that exhibit hydrophobic and hydrophilic properties with a linear arrangement of polyethylene oxide (PEO), polypropylene oxide (PPO), and PEO. Poloxamers are important for drug delivery purposes, the creation of adhesives, and the creation of batteries for energy production. In this project, we examined how magnetic fields affect the directed assembly of poloxamers to improve their processing and enable new applications. Magnetic fields cause poloxamers to transition from a disordered to an ordered state—thus magnetic fields have the potential to be used to process highly ordered poloxamer geometries for various industrial applications. A poloxamer-water system was studied in this work; the poloxamer was dissolved in deionized water and observed by magneto-rheological experiments. Conditions used for the rheology experiments such as strain, frequency, and magnetic field were varied to explore different processing conditions to establish design parameters for poloxamer hydrogels. Consequently, rheology experiments indicate that there are predictable relationships between these processing conditions and the plateau moduli of the poloxamer-water system. These experiments demonstrate that the magnetic processing of BCPs has the potential to improve their tunability.</p> |
| 54. | <p>Jared Nash <i>The Anti-reflective Properties of Subwavelength Structures on Lenses</i> Advisor: Shaul Hanany Sponsoring Program: Physics REU Home Institution: Albion College Abstract: The Cosmic Microwave Background (CMB) radiation is the oldest detectable light in our universe, imprinted on the sky when the Universe was just 380,000 years old. Produced during the creation of the universe, a fraction of this radiation is slightly polarized – vibrating in preferred directions. The study of this polarization gives physicists an insight into the distribution of energy and matter in the early universe. To study this polarization with precision, astronomers need sensitive equipment which allow the maximum amount of light to be collected during observation. As a result, numerous anti-reflective coating techniques have been developed, including laser ablated subwavelength structures (SWS). This poster will include the process for simulating and modeling the transmission of light through subwavelength structures on alumina lenses.</p> |
| 55. | <p>Sydney Nelson <i>Low-temperature Plasma Discharge at Extreme Pressures</i> Advisor: Sayan Biswas Sponsoring Program: UROP/URS Home Institution: University of Minnesota - Twin Cities Abstract: The nation's sustainable energy initiative has deterred industries from fossil fuels and seeks combustion alternatives. Electro fuels (e-fuels) are one solution to this energy crisis. Current combustion processes are inefficient for the complete combustion of e-fuels. Unlike traditional spark plugs, plasma exerts higher energy onto the fuel. The chemi-ionization process propagates a wave of combustion throughout the fuel. Plasma ignition of e-fuels provides a sustainable solution to conventional combustion engines.</p> |

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| 56. | <p>Timmy Nguyen <i>Optimizing Substrate Design of Surface-enhanced Raman Spectroscopy for Virus Detection</i> Advisor: Christy Haynes Sponsoring Program: UMN Chemistry- Lando Home Institution: California State Polytechnic University, Pomona Abstract: Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical technique used in the field of biosensing for the detection of single molecules or entities, such as viruses. SERS is dependent on the exploitation of the electromagnetic enhancement induced by excitation of the localized surface plasmon resonance (LSPR). We explored the synthesis of alternative LSPR-supporting substrate platforms to develop an optimal SERS detection scheme for viruses. Metal film over nanospheres (FON) substrates and nanoparticle colloids were synthesized as potential SERS substrates to be used with the polymer affinity agent, poly(2-hydroxyethyl methacrylate) (pHEMA). Each substrate's viability was evaluated based on its LSPR, nanoscale surface roughness, and pHEMA SERS signals. To achieve maximum enhancement, we tuned the substrates' LSPR by altering the method and thickness of the gold deposition. When comparing the FONs substrates, those coated using an electron beam deposition produced a more red-shifted LSPR, higher nanoroughness, and stronger polymer Raman peak intensity than the substrates coated with a sputter deposition. Gold nanosphere and nanostar colloids were also synthesized as potential SERS substrates, but both overall performed less well than the FONs. We will continue optimizing the LSPR and conduct virus detection studies with the best performing SERS substrates.</p> |
| 57. | <p>Uyen Nguyen Thanh <i>Interaction of Iron Oxides, Natural Organic Matter and Microplastic</i> Advisor: R. Lee Penn Sponsoring Program: UMN Chemistry- Lando Home Institution: Hollins University Abstract: Organic matter is widely present in the environment and has a significant impact on how groundwater pollutants and microplastic interact with mineral surfaces. For instance, organic matter adsorbs to certain mineral surfaces, and the degree of adsorption is greatly influenced by the conditions in an aqueous solution (e.g. pH, ionic strength). Iron oxides and oxyhydroxides are naturally occurring minerals of interest due to their widespread environmental presence and the facilitation of the Fe(II) reductive rates toward a variety of common, highly oxidized groundwater pollutants. Microplastics are minuscule particles produced during the breakdown of bigger plastics used in commercial product development and interact with mineral surfaces to form plastic-mineral agglomerates. Here, we present results tracking the adsorption of different portions of natural organic matter onto synthetic hematite using excitation emission matrix spectroscopy, total organic carbon analyzer and high-performance size exclusion chromatography. Additional results highlighting the interaction between microplastic with iron oxides in the presence and absence of organic matter are also presented using results from high pressure size exclusion chromatography, powder X-ray diffraction, and Fourier transform infrared spectroscopy. Results will improve our understanding of organic matter and iron oxide mineral surfaces, which can dictate reactivity in environmental systems.</p> |
| 58. | <p>Abbie Nistler <i>Emulsion synthesis of biomass microbeads for consumer products</i> Advisor: Michelle Calabrese Sponsoring Program: Center for Sustainable Polymers Home Institution: University of Utah Abstract: Plastic microbeads are commonly used in consumer beauty products and personal care products to aid in exfoliation and as rheological modifiers. However, billions of microbeads enter the environment daily in the US alone, where they persist as environmental hazards to aquatic life. Replacing these with biodegradable microbeads would reduce plastic pollution in the environment. These biomass microbeads could also absorb toxins and clean up the environment in the process. These beads were synthesized using an emulsion process using Kraft lignin and microcrystalline cellulose, as well as a representative waste biomass, corn leaves. By using low-value products like lignin and waste biomass, bead production is a value-added process. The size and texture of the microbeads can be altered by altering amount of lignin and heating the beads. This allows the beads to be tunable to replace microplastic beads used in consumer beauty products, which range from 150-800 micrometers in diameter. This process can be scaled up to allow for industrial use and mass production of microbeads. The biodegradable microbead can then replace plastic microbeads in consumer personal care products.</p> |

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| 59. | <p>Stride Okorie <i>Developing a Postural Sway Measurement System for Pre-clinical Studies</i> Advisor: Matthew Johnson Sponsoring Program: BME Pathways Home Institution: Morgan State University Abstract: Background: Postural Stability is the ability to control body position in space for the purpose of movement and balance.</p> <p>Goal: Investigate postural stability using Tekscan pressure pad and develop a new system</p> <p>Methods: Building a 16x16 pressure pad with 32x32 sensor arrays in order to detect motion to better understand postural sway.</p> <p>Results: Developing new code in order to read in raw data and take that data to find the center of pressure.</p> <p>Significance: Better understanding of postural sway helps to eliminate many concerns that face this area of study. Seeing how especially the elderly face this problem, this research serves as a means to help combat this problem.</p> |
| 60. | <p>Oluwatobiloba Olayemi <i>The effect of Potassium Chloride on mouse uterine tissue to better understand pregnancy complications</i> Advisor: Kyoko Yoshida Sponsoring Program: BME Pathways Home Institution: Morgan State University Abstract: Preterm labor is typically caused by abnormal uterine contractions, and can lead to health complications including breathing difficulties and underdeveloped organs. Researchers study the factors that can affect contractions using both human and animal models to better understand the factors associated with these contractions. This aids in the development of drugs that can address such complications. In this study, we used a mouse model to examine various conditions that affect uterine smooth muscle contraction such as potassium chloride concentrations and tissue direction. Tissues were extracted from non-pregnant mice, dissected into longitudinal strips and circumferential rings, and mounted in chambers at 37 °C in an organ bath containing phosphate buffered saline. The samples were allowed to equilibrate for 2 to 3 hours. 40-60mM of KCl was then introduced to stimulate contraction. We discovered that there is no significant difference in the contraction force of non-pregnant tissue before and after the addition of KCl. In the future, we intend to explore additional factors such as pregnancy status, with a focus on gestation day of the pregnant mice. Understanding uterine contractions can aid in the development of methods and drugs to reduce problems like preterm birth.</p> |
| 61. | <p>Dina Orozco <i>Investigations of Bismuth Catalysts as Safe, Non-toxic Catalysts for Polymerizations</i> Advisor: Jane Wissinger Sponsoring Program: Center for Sustainable Polymers Home Institution: The University of Texas at Austin Abstract: Teaching experiments play an important role in introducing students to green chemistry. The goal of this project was to replace tin (II) 2-ethylhexanoate, a common catalyst used for ring opening transesterification reactions, with a non-toxic bismuth catalyst. The end goal of this project is to modify current teaching lab experiments involving lactone-based sustainable polymers. Bismuth triflate was explored as a possible replacement, but it was found to be incompatible due to decomposing at temperatures above 100 °C. Bismuth acetate was also explored as an alternative to tin catalysts and yielded better results. As a result, bismuth acetate was employed in two different teaching experiments: The first, a triblock copolymer synthesis, and the second, a polylactide based vitrimer synthesis. Bismuth acetate is capable of catalyzing the formation of the triblock copolymer, but does not yield optimal results. This could be due to interference with diphenyl phosphoric acid, the catalyst used in the first step of the synthesis. Therefore, better results can be obtained using bismuth acetate in the polylactide based vitrimer synthesis, where bismuth acetate is used in both steps of the reactions.</p> |

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| 62. | <p>Santi Parra-Vargas <i>Developing a Sensor to Monitor Ocean Waves (Wave Energy)</i> Advisor: Perry Li Sponsoring Program: ME Home Institution: Rice University Abstract: In the search for a reliable and powerful renewable energy source, many have looked to wave energy due to its abundance and its potential to generate great amounts of power. However, waves are unpredictable as they are dependent on climate, and are therefore difficult to monitor properly, limiting our ability to extract the most power. Work is being done to create methods that would allow us to monitor waves and reliably acquire information, and through that, be able to adjust the necessary procedures to capture the most amount of energy from the waves. The goal of this project is to develop and prototype a sensor buoy that would be able to relay information about the wave's height and direction to an external device in order to accordingly adjust a wave energy converter. The buoy prototype utilizes a color detection program using OpenCV through a Raspberry Pi to detect a set of LEDs that would be placed on land. The fixed LEDs would provide information about the camera's orientation relative to the buoy, and would in turn be translated into information about the wave through a Python algorithm.</p> |
| 63. | <p>Yaren L. Peña Señeriz <i>Understanding nanomaterial toxicity and the potential for resistance evolution in bacteria</i> Advisor: Erin Carlson Sponsoring Program: Center for Sustainable Nanotechnology Home Institution: University of Puerto Rico at Cayey Abstract: Nanomaterials are incorporated into new technologies with increasing frequency, and currently lack proper disposal protocols, so it is critical to understand how these materials affect biological systems. Specifically, we are interested in understanding the molecular-level mechanisms that govern the interactions between various bacterial species and a complex metal oxide nanomaterial, lithium nickel manganese cobalt oxide (NMC) used in electric cars batteries. Recent studies have demonstrated that metal ions dissociated from the NMC nanomaterial drive toxicity to the bacterium <i>Shewanella oneidensis</i>. However, with chronic exposure, <i>S. oneidensis</i> rapidly develops resistance to NMC. The goal of this work is to evaluate the toxicity of NMC to additional bacterial species, <i>Bacillus subtilis</i> and <i>Escherichia coli</i>, and the ability of these species to develop resistance to nanomaterials. To evaluate toxicity, we used a minimum inhibitory concentration (MIC) assay to determine the concentration of NMC that inhibits growth of our model bacteria. We then chronically exposed these bacteria to NMC to evaluate the ability of our model organisms to evolve NMC resistance. Research is just beginning to investigate microbial resistance to nanomaterials and this work is fundamental in understanding the scope of threat that nanomaterial resistance may pose in environmental and clinical settings.</p> |
| 64. | <p>Mario Perez <i>Developing a more representative model chromatographic pore</i> Advisor: Ilja Siepmann Sponsoring Program: UMN Chemistry - CTC Home Institution: University of Texas at Rio Grande Valley. Abstract: Reliable pore characterization of chromatographic bead is important for stationary phase development, and gas adsorption has been widely used to characterize porous materials. However, extracting information, such as surface area and pore size distribution, from an adsorption isotherm relies on the underlying models. Particularly, the pore shape can have a huge effect on the adsorption behavior. Therefore, it is important to examine whether the customary statistical models for pore characterization can yield reasonable results with model chromatographic pores. Our previous work has shown that the model slit pores gave different adsorption behaviors as compared to the real chromatographic beads. Also, it was elusive for a commercially available model to obtain a reasonable pore size distribution. In this work, we aimed to build a more representative pore model. The comparison between the adsorption isotherms of the slit pore and the new model pore can help investigate the effect of pore shape on the adsorption behavior and the reliability of the pore characterization technique.</p> |

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| 65. | <p>Ulises Perez <i>Measuring Quinine-Based Monomer DNA Interactions Through Raman Spectroscopy for use in Polymer Gene Delivery</i> Advisor: Renee Frontiera Sponsoring Program: UMN Chemistry- Heisig Gleysteen Home Institution: University of Minnesota - Twin Cities Abstract: Current gene therapies utilize virus vectors for treatment of disease, but they are expensive and have a limited shelf life. Polymer mediated gene therapies are a suitable alternative because they address these issues. Our group has previously used Raman spectroscopy to investigate quinine-based polymers to further understand the transfection mechanism of DNA. My project is investigating how quinine-based monomers intercalate with DNA to elucidate the effect different monomers will have on the transfection efficiency. Raman spectroscopy can monitor the local environment changes that occur when the polymer interacts with the DNA. We monitor the quinoline ring vibrational mode and its shift as a function of DNA concentration, for different quinine-based monomers. By comparing the trend of frequency shifts for each monomer with their respective transfection efficiency, we can understand the effect quinine-DNA interactions have on the overall efficiency of polymer gene delivery. These results will be used to further the development of new and efficient quinine-based polymers for gene delivery.</p> |
| 66. | <p>Daniel Pert <i>Data-driven autoencoders for accelerated sampling of adsorbed polypeptide configurational space</i> Advisor: Sapna Sarupria Sponsoring Program: Center for Sustainable Polymers Home Institution: University of Michigan Abstract: Polypeptides on surfaces have numerous applications, including biosensors, biofuel cells, peptide self-assembly, and biodegradable plastics. Development of such applications requires detailed knowledge of peptide-surface interactions. However, understanding binding mechanisms and identifying free energy minima relies on efficient exploration of configurational space, which is limited by high free energy barriers. Collective variable (CV) biasing techniques such as metadynamics and umbrella sampling can artificially drive the system across these free energy barriers but rely on preexisting knowledge of CVs that describe large-scale motions and require that CVs are explicit and differentiable functions of atomic coordinates. Recent work has demonstrated the use of auto-associative neural networks ("autoencoders") that can learn data-driven CVs from simulation data, which enables iterative CV discovery and enhanced sampling along discovered CVs. This process can be combined with the weighted histogram analysis method (WHAM) to predict free energy surfaces. In this study, we extend this methodology to study peptide-surface interactions, namely Trp-cage on a graphene sheet. Such work could be extended to study the binding of enzymes such as glucose oxidase and laccase to carbon nanotubes for biofuel cells, develop algorithms to predict the adsorbed structure of a peptide from its sequence, and engineer enzymes for polymer degradation.</p> |
| 67. | <p>Gabriel Phelan <i>Evaluating the Role of CCS in Myelodysplastic Syndromes</i> Advisor: Hai Dang Nguyen Sponsoring Program: UROP/URS Home Institution: University of Minnesota, Twin Cities Abstract: Myelodysplastic Syndrome (MDS) is a bone marrow disorder where improperly functioning blood cells are produced. This causes low blood cell counts among different cell types depending on the exact cause. Approximately a third of MDS patients develop secondary acute leukemia. 50% of MDS patients have mutations in splicing factor genes (U2AF1, SF3B1, SRSF2, ZRSR2) leading to misspliced mRNA. These mutations are mutually exclusive and heterozygous and therefore a target for therapy. A CRISPR-Cas9 synthetic lethality screen by Olivieri et al. identified CCS as a gene that is essential for RPE-1 cell survival when treated with Pladienolide B (Plad B), an inhibitor for SF3B1. In this project I knocked out CCS in HeLa cells and measured differences in cell sensitivity to Plad B. I determined that CCS KO in HeLa cells leads to slight resistance to Plad B when compared to nontargeted (NT) HeLa cells. In the future, I will delete CCS gene in various cell lines to validate Plad B sensitivity due to CCS gene deletion.</p> |

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| 68. | <p>Leigh Preimesberger <i>Estimating the Energy of Neutral Current Neutrino Interactions in the NOvA Detector</i> Advisor: Gregory Pawloski Sponsoring Program: Physics REU Home Institution: The University of Texas at Dallas Abstract: We reconstruct the energy of neutral current (NC) neutrino interactions in the NOvA Far Detector (FD). We loop over Prod5 FD Monte Carlo CAF files, select NC events, and extract caloE and trueE values, where caloE is the energy that is visible in the FD and trueE is the true energy of the incident neutrino. We present two different mappings of caloE to trueE, both of which are based on the average trueE for a given caloE value. We display the relative error between recoE (our estimate of the incident neutrino's energy) and trueE in resolution plots. In the first mapping, the neutrino energy spectrum at the FD is sharply peaked around 2 GeV. We find that some of the distributions of trueE for slices of caloE have a bimodal shape and that the resolution plot is asymmetric about the vertical axis. In the second mapping, we reweight the NC events so that the neutrino energy spectrum at the FD is flat. We find that the distributions of trueE for slices of caloE are now unimodal and that the resolution plot is symmetric about the vertical axis. Our mappings can be used to benchmark machine learning neural networks against.</p> |
| 69. | <p>Luke Omodt <i>Interplay of Ferromagnetism and Weyl Semimetal Behavior in Shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ Single Crystals</i> Advisor: Jeff Walter Sponsoring Program: MRSEC Home Institution: Augsburg University Abstract: Weyl semimetals have recently garnered interest in both condensed matter physics and materials science. Shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ is a ferromagnetic Weyl semimetal, making it a particularly interesting platform to study the interplay of magnetism and band topology. We have grown > 100 Shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ single crystals using chemical vapor transport methods. Through magnetometry we have confirmed our crystals are ferromagnetic with a Curie temperature of 175K. Further, we have found very square hysteresis loops along the c-axis with the remnant magnetization equal to the saturation magnetization, while magnetic fields applied in the a-b plane result in zero remnance and only ~30% saturation in 70 kOe. Together, this demonstrates a <i>giant</i> magnetocrystalline anisotropy of interest for further work. Using electron transport we have measured an anomalous Hall conductivity of 1400 S/cm, which is > 10 times larger than other ferromagnets of similar conductivity, supporting previous literature statements of a giant anomalous Hall effect in this material as a consequence of the interplay between ferromagnetism and Weyl semimetal behavior. Future work will explore whether these magnetic and electronic properties can be tuned by chemical substitutions as well as electrolyte gating.</p> |
| 70. | <p>Daniel Retic <i>Shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ Single Crystal Growth & Characterization</i> Advisor: Jeff Walter Sponsoring Program: MRSEC Home Institution: Augsburg University Abstract: We aim to create electronics that are low cost and made of environmentally responsible and abundant materials. Sulfur fitting these categories, we plan to combine it with transition metals to achieve unique magnetic properties. In this work our goal is to develop and optimize single crystal growth of shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ using a technique called chemical vapor transport. This technique is used by placing a reagent of Co, Sn, and S into an evacuated quartz tube, then placing it into a furnace which is split into a cold and hot zone allowing the reagent to vaporize and condense in the cold zone creating single crystals. We have synthesized over 100 single crystals that are typically shiny, ~10-100 um thick flakes ranging from 0.1 - 5 mm in lateral scale. Using an energy-dispersive x-ray spectroscopy (EDS) as well as x-ray diffraction (XRD), we characterize the stoichiometry and crystal structure, respectively. XRD confirms our crystals are indeed the shandite crystal structure with hexagonal lattice parameters of $a = 5.35739$ and $c = 13.17928$, which are consistent with previous reports. We have identified a calibration issue with our EDS measurements, preventing rigorous confirmation of stoichiometry, though XRD results strongly indicate high quality, stoichiometric crystals.</p> |

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| 71. | <p>Fabian Rodriguez <i>Role of solvent composition during processing of stimuli-responsive PNIPAM copolymers</i> Advisor: Michelle Calabrese Sponsoring Program: MRSEC Home Institution: University of Texas Rio Grande Valley Abstract: With a greater need for energy efficiency, responsive polymer coatings are promising candidates for their scalability. Specifically, poly(N-isopropylacrylamide-co-3(trimethoxysilyl)propyl methacrylate (PNIPAM-co-TMA) has been studied for responsive glass coatings due to optical properties stemming from thermally reversible phase changes. These phase changes result from the abrupt coil-to-globule transition where aqueous solutions shift from clear to opaque with increasing temperature. The coil-to-globule behavior of PNIPAM outlined above is favorable for sprayable smart window coatings. However, the presence of TMA, which allows PNIPAM coatings to bind to glass substrates, can lead to irrecoverable opacity. Cloud point testing will be used to characterize the cyclical phase behavior of PNIPAM-co-TMA. The co-nonsolvency displayed by these systems provide access to the collapsed, opaque, state using solvent mixtures instead of temperature. This may be advantageous for coating processes. The mixtures will be subsequently processed via spin coating onto substrates with different solvent systems where contact angles will be analyzed. The contact angles as a function of temperature will display hydrophobic/hydrophilic shifts in the coating surface properties. Understanding the limitations of PNIPAM-co-TMA and the surface properties associated with the copolymer coating will allow this research to potentially impact the use of polymer responsive coatings to improve energy efficiency.</p> |
| 72. | <p>Carissa Rowan <i>Superparamagnetic Nanoparticles in Energy Research</i> Advisor: Sayan Biswas Sponsoring Program: ME Home Institution: Embry Riddle Aeronautical University Abstract: Superparamagnetic nanoparticles are a special class of nanoparticle that exhibit hyperthermic effects when placed under an alternating magnetic field. The applications of these particles have been limited to biomedical fields as an alternative cancer treatment, targeted drug delivery system, and enhanced MRI contrast. The potential for use in energy and propulsion applications has been less explored, despite the vast promise these particles provide. The magnetic hyperthermia that results from superparamagnetism could benefit an engine's efficiency by preheating the fuel, thus reducing the energy required to perform combustion. Two types of nanoparticles, $Cu_{0.1}Ni_{0.9}Mn_2O_4$ and magnetite (Fe_3O_4), were synthesized via the coprecipitation method and coated with oleic acid to promote dispersion. These particles were then characterized using x-ray diffraction (XRD), transmission electron microscopy (TEM), and vibrating sample magnetometry (VSM). The heating properties were investigated using an externally applied alternating magnetic field (AMF) and measuring the corresponding temperature rise over time. This exploratory research shows great promise for the potential application of these nanoparticles as a fuel additive to enhance engine performance and suggests further research in this matter should be conducted.</p> |
| 73. | <p>Jamie Rowland <i>Temperature effect on properties of polymer blends</i> Advisor: Christopher Ellison Sponsoring Program: Center for Sustainable Polymers Home Institution: The City College of New York, CUNY Abstract: The recycling rate of thermoplastics is limited by the sorting needed to prevent making polymer blends. Blends are often more brittle than their individual components because the dispersed phase may act as an additional source of defects. Compatibilization aims to decrease the impact of these defects. In reactive compatibilization, reactions between one or more phases and an additive form a block copolymer that weaves through the components' interface. This can improve phase adhesion and thus improve properties of a blend.</p> <p>Previous work successfully compatibilized PET/LLDPE using HO-PE-OH. Blends with only a small amount of the additive had properties near the majority phase polymer. To better understand this additive and how the process is affected by temperature, we mixed blends of PETG (an amorphous analogue of PET) and LLDPE at different temperatures. For 270C, the blend made with the additive had a strain of break a factor of 4 higher. Blends mixed at 150C had only a .2% difference in strain of break and were significantly more brittle than the 270C blends. We intend to use microscopy to view the microstructure from processing and testing to understand these differences in mechanical properties. We will also prepare blends at 210C.</p> |

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| 74. | <p>Megan Schoenzeit <i>Experimental Studies of Temporal Evolution of Chain Formation in Magnetorheological Fluids</i> Advisor: Dan Dahlberg Sponsoring Program: UROP/URS Home Institution: University of Minnesota, Twin Cities Abstract: The formation of chains in a magnetorheological (MR) fluid was investigated. The MR samples consisted of 150 μm iron particles suspended in corn syrup, and the volume fraction of particles was 0.5%. The samples were placed at the center of a pair of Helmholtz coils. Several applied magnetic field strengths were explored in the range from 10 to 100 Gauss. Time-lapse images of the temporal evolution of the MR sample in a magnetic field were obtained using a microscope camera analyzed with image processing of individual frames. Analysis of the results is in progress.</p> |
| 75. | <p>Jennifer Scoggin <i>Switchable System between Cationic and Anionic Polymerization</i> Advisor: Jessica Lamb Sponsoring Program: MRSEC Home Institution: The University of Texas Rio Grande Valley Abstract: Switchable polymerization utilizes a universal chain transfer agent that is directed between different polymerizations with select monomers. Current techniques include separate methods between cationic/radical and anionic/radical polymerizations. The ongoing focus is to combine the cationic and anionic polymerization. Cationic polymerization can be completed by creating a photocatalyst that will undergo a catalytic cycle that can switch the polymerization on and off, while remaining stable with components of the anionic system. The first goal of this research project is to develop a new photocatalyst that will be less susceptible to nucleophilic degradation and will have the proper redox potentials. Ultimately, the cationic polymerization will be switchable with an anionic polymerization, which has limited research with thiirane monomers. Therefore, the second goal of this research is to create a wide library of thiirane monomers that can be used for anionic polymerization. In the future, this switchable polymerization will allow for the development of techniques to control polymerization mechanisms.</p> |
| 76. | <p>Aniruddha Seal <i>Enhanced Sampling guided design of Peptide-Surface Complexes</i> Advisor: Sapna Sarupria Sponsoring Program: UMN Chemistry - CTC Home Institution: National Institute of Science Education and Research (NISER Bhubaneswar) Abstract: Rational engineering of peptide assembly at surfaces is crucial for developing numerous applications, such as functionalization of nanomaterials, biosensing, and drug delivery. While the ability of experiments to provide high-resolution structural information in interfacial systems is limited, molecular simulations are well-suited for elucidating the structure of adsorbed peptide species giving a quantitative understanding of their structure-function relationships. Many of these materials-binding peptides are thought to be intrinsically disordered, adopting a spectrum of configurations at the interface. Therefore exhaustive conformational sampling is a necessary tool to rule out spurious structure-function relationships. However, the complexity of the conformational space of intrinsically disordered systems impedes efficient sampling of configurational space using standard brute-force molecular dynamics simulation. We implement a machine learning-based enhanced sampling approach involving rounds of CV discovery and biased sampling interleaved in an iterative framework for studying peptides (biomolecular systems in general) on surfaces by demonstrating the approach for Trp-cage adsorption on graphene. We explore the adsorbed conformations of Trp-cage and their relative stability on graphene. The knowledge of the conformational landscape thus obtained can be used to develop design rules for a target orientation and structure of a peptide in the adsorbed state.</p> |

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| 77. | <p>Tiago Sereno <i>Lie Algebras and Gauge Symmetries of the Standard Model</i> Advisor: Zhen Liu Sponsoring Program: Physics REU Home Institution: Binghamton University Abstract: Our current understanding of the Standard Model of physics involves three quark and lepton families which interact with each other through gauge bosons—the mediators of the strong, weak, and electromagnetic forces. Although there are incredibly important details in the field theoretical approach to the Standard Model, this project focuses on understanding the more profound nature lying in its symmetries. Group theory has historically been a crucial driver of new discoveries in particle physics, which we explore in some detail. Our focus was primarily on Lie algebras as they directly determine how the gauge bosons of $SU(3)_C$, $SU(2)_L$, and $U(1)_Y$ interact with themselves and the quark-lepton families, and have the power to unify all known non-gravitational interactions under a single symmetry group. We begin with an introduction to finite groups and slowly build Lie theory with some physical examples, culminating in a description of the gauge groups that make up the standard model, and a discussion of their grand-unification.</p> |
| 78. | <p>Natalie Steibel <i>Identification of Lyotropic Bicontinuous Network Phases formed by a Plant-Based Surfactant</i> Advisor: Mahesh Mahanthappa Sponsoring Program: MRSEC Home Institution: University of Pittsburgh Abstract: Amphiphilic surfactant molecules, with hydrophobic and hydrophilic portions, self-assemble into lyotropic liquid crystals (LLCs) upon addition of water. This process is driven by minimization of interfacial surface area, maximization of cohesive electrostatic interactions, and molecular packing at a constant density. LLC structure varies with amphiphile properties and water content. Structures of great interest are bicontinuous networks: LLCs with alternating, interpenetrating channels of hydrophobic and hydrophilic domains. Previous studies of inverse bicontinuous LLCs established the ability of these structures to encapsulate siRNA for therapeutic applications. The goal of this project was to synthesize a cationic surfactant derived from isophytol, a plant-based compound, and to understand its self-assembly behavior. This involved first identifying potential synthesis pathways and analyzing their feasibility in terms of safety, yield, and purity. Next, small-scale reactions were performed to produce the target surfactant, and the resulting chemical structure was verified with NMR and elemental analysis. Finally, the surfactant was combined with various amounts of water to form LLCs. These LLCs were analyzed with small angle X-ray scattering (SAXS) to characterize their structures and identify favorable conditions for self-assembling bicontinuous network phases.</p> |
| 79. | <p>Guthrie Stroh <i>Discovery of Virulence-Disarming Inhibitors for Two-Component Systems in Bacteria</i> Advisor: Erin Carlson Sponsoring Program: UMN Chemistry- Lando Home Institution: Truman State University Abstract: Antimicrobial resistance is a growing threat to public health, and presents an especially pressing challenge in the wake of research progress lost during the COVID-19 pandemic. Novel therapeutic approaches are required to combat high rates of evolutionary antibiotic resistance. Widely-conserved bacterial signaling proteins such as Histidine Kinase (HK) have been identified in Two-Component Systems (TCSs), which are involved in regulation of bacterial pathogenicity. By inactivating the catalytic (CA) domain of HKs with a previously-identified suite of benzothiazole-based inhibitors, virulence factors can be prevented from damaging host organisms. Therefore, our approach seeks to discover more potent inhibitors of TCSs using rational drug design. Gel-based activity assays in HK853, one of our model proteins, employ the displacement of an BODIPY-FL-ATPγS fluorophore from the active site to determine IC₅₀ values for various chemical substituents of the benzothiazole pharmacophore and expand our knowledge of the structure-activity relationship between our inhibitors and HK functionality. Additionally, co-crystallization of a PhoQ CA domain construct (part of another HK) in the presence of promising inhibitors will give important insights into the specific binding interactions at active site residues. These data will contribute to the development of highly specific virulence-disarming compounds able to decrease the pathogenicity of bacterial infections.</p> |

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| 80. | <p>Jonathan Te <i>Kinetics of Thermal Injury to Peripheral Nerves: Application in Renal Denervation for Hypertension Treatment</i> Advisor: John Bischof Sponsoring Program: ATP-Bio Home Institution: University of California, Irvine Abstract: Hypertension is a major cause of cardiovascular disease and premature death, affecting over 1.28 billion individuals worldwide. Treatment for hypertension typically consists of lifestyle changes and/or medication. In the case of resistant hypertension, where antihypertensive drugs fail to reduce blood pressure, renal denervation (RDN) techniques such as radiofrequency ablation can be employed. However, technical limitations of conventional RDN methods can prevent sufficient treatment. To circumvent these limitations, we propose a novel RDN technique utilizing nanoparticles to heat the nerves. First, an Arrhenius model parameterizing nerve injury in response to hyperthermia needs to be developed to create benchmarks for nanoparticle heating. Initial methods were to collect and clean nerve samples, heat the nerves on a cryostage for designated temperatures and times, and measure nerve responsiveness before heating, immediately after heating, and every hour after the heating process up to 3 hours. Nerve response at 50°C and 55°C for exposure times varying from 1 to 7 minutes were quantified, however, more testing is needed to fit the Arrhenius model. An alternative method of heating using a water bath is also being explored to verify if nerves behave differently depending on the heating method.</p> |
| 81. | <p>William Isaac Thronson <i>Investigating Shape Degeneracies in Multiple Image Gravitational Lenses</i> Advisor: Liliya Williams Sponsoring Program: Physics REU Home Institution: Grinnell College Abstract: Since the late twentieth century, the astrophysics community has seen a significant increase in efforts to properly assess galactic mass density profiles via investigation into gravitational lensing observables. Computational methods allow us to construct elliptic mass density profiles of galactic scales; varying the angular position of a background source enables the retrieval of several multiple-image solutions for a particular mass configuration. This research focuses on solutions that produce four unique images. Applying the projected Einasto profile we introduce dark matter (DM) haloes, which perturb the elliptic mass configuration. We designate possible dark matter configurations by optimizing – via the Nelder-Mead method – the difference between the arrival time surface of the unperturbed mass density profile and that of the mass density profile which incorporates (N=20) DM haloes. We probe degenerate mass configurations of a given multiple-image lens system by computing the RMS projected mass density; additionally, we seek possible constraints on the viability of degenerate solutions by considering arrival time and magnification ratios.</p> |
| 82. | <p>Nhi Tran <i>Kinetic Effects of the Modification of Glassy Carbon Electrode Surface with Nanocarbon</i> Advisor: Philippe Buhlmann Sponsoring Program: UMN Chemistry- Lando Home Institution: Franklin College Abstract: Ion-selective electrodes (ISEs) have been miniaturized for different research applications, especially wearable devices, where a planar design ISE is desired. The design contains a deposited nanocarbon layer attached underneath the membrane to create a solid contact layer. In this work, I confirm the attachment by investigating kinetic effects of the modification and attachment of the solid-contact. Glassy carbon electrodes (GCE) were used and allowed us to directly compare the results to phenomena happening at the electrode's surface. Under three different conditions of bare, initiated, and modified electrodes, the peak separation generated from cyclic voltammetry was observed. Results showed that the photo-initiated and modified GCE resulted respectively in a triple and double peak separation (ΔE_p) compared to the bare electrode. An increase in ΔE_p as the surface was modified demonstrated a slower electron transfer on the modified surface electrode. Moreover, the same powerful technique was used to monitor the change in the average capacitance across the conditions. The nanocarbon when attached is expected to lead to a higher capacitance due to its higher surface area compared to the GCE. The results confirmed a higher capacitance for the modified electrode, demonstrating the success of the attachment of nano-graphite through UV irradiation.</p> |

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| 83. | <p>An Trinh <i>Characterization and Confirmation of Furan Metabolites in Hepatocytes</i> Advisor: Lisa Peterson Sponsoring Program: UMN Chemistry- Heisig Gleysteen Home Institution: University of Minnesota - Twin Cities Abstract: Furan is anticipated to be a human carcinogen because it can cause liver tumors in rodents and humans are frequently exposed to it. In the liver, furan is activated by cytochrome P450 2E1 to form cis-2-butene-1,4-dial (BDA), which can react with glutathione (GSH) to form a GSH-BDA intermediate. This intermediate can form a pyrrole crosslink with cellular amines like lysine, ornithine, and spermidine. The purpose of this project is to characterize additional unidentified metabolites detected in rat hepatocytes. We anticipate that taurine, glutamic acid (Glu), glycerolphosphatidylethanolamine (GPE), and citrulline (Cit) are potential targets of BDA and GSH-BDA. Synthetic GSH-BDA-amine products are characterized using various NMR and MS spectra and confirmed to be the biological metabolites using LC-MS/MS.</p> |
| 84. | <p>Quin Villwock <i>Energy Efficient and Connected Vehicles</i> Advisor: Songxuan Sun Sponsoring Program: ME Home Institution: Rochester Institute of Technology Abstract: Connected and automated vehicles (CAVs) are becoming more advantageous for transportation, as their ability to communicate with both other vehicles and infrastructure around them has the possibility to make passenger cars safer and more energy efficient than the status quo. Energy efficiency can be optimized by solving a mathematical equation that is made possible by the connectivity between other objects on the road. However, the challenge with studying CAVs is that it is very difficult to predict short-term traffic patterns, especially in a scenario with both connected and unconnected vehicles. The main part of this project is to help collect short-term traffic data by running simulations of 8 different routes using simulation of urban mobility (SUMO) on a section of MN 55. Also, in each simulation, one factor is changed in the environment, such as the speed, acceleration, deceleration, etc. From these simulations, the traffic data can be analyzed to determine the speed and density of certain sections of MN 55, which can then be used on a CAV using a HIL testbed and a living lab.</p> |
| 85. | <p>Lily Watkins <i>Dynamics of waste proteins in brain tissue: numerical insights into Alzheimer's risk factors</i> Advisor: Jeff Tithof Sponsoring Program: ME Home Institution: University of Minnesota Abstract: Over the last few decades, the build-up of waste proteins, like amyloid-β ($A\beta$), in the brain has been linked to neurodegenerative diseases, such as Alzheimer's, but the details of how such proteins are removed from the brain is actively debated due to the complexity of the protein dynamics. We have developed a computational model to investigate the production, build-up, and clearance of $A\beta$ in the brain. Our model captures 50 different species of $A\beta$, ranging from small molecules that are naturally produced to large aggregates called plaques. We quantify the importance of varying conditions in the brain to determine what promotes or inhibits clearance for all 50 species. Our preliminary results provide novel insight into several known risk factors for Alzheimer's disease and cognitive decline, such as poor sleep and heart disease.</p> |
| 86. | <p>Gabriella White <i>The Effect of Chiral Solvents on Enantioselectivity</i> Advisor: Steve Kass Sponsoring Program: UMN Chemistry- Lando Home Institution: University of Oxford Abstract: A series of chiral thioureas were synthesised, and used to catalyse asymmetric reactions in both racemic and enantiopure samples of chiral ether solvents. The e.e. of each reaction was measured, and used to ascertain the potential for chiral solvents to enhance enantioselectivity.</p> |

**Teacher Poster Presentations
Listed Alphabetically by Presenting Author**

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| 87. | <p>Olivia DeSutter <i>Synthesis and Applications of Iron Magnetic Nanoparticles in the High School Chemistry Classroom</i> Advisor: Jane Wissinger Sponsoring Program: MRSEC Home Institution: FAIR School Downtown, Minneapolis, MN Abstract: Iron magnetic nanoparticles (Fe MNPs) were synthesized utilizing a novel procedure that can be performed in a high school chemistry lab. Iron (II) sulfate heptahydrate served as the source of Fe, and plant-derived starches were used as both a stabilizing and reducing agent. Three different starches, potato, corn, and tapioca, were utilized. The physical properties of the Fe MNPs, including color and magnetic strength, were then analyzed. The type of starch used did not affect the color or magnetic strength. However, the time the wet Fe MNPs were exposed to air did affect the color and magnetic strength of the nanoparticles. Finally, in order to explore real-world applications of Fe MNPs, the Fe MNPs were used to degrade rhodamine b and methylene blue dyes. Connections to the high school chemistry curriculum, considerations for the high school lab, and potential extensions were explored throughout the experiment.</p> |
| 88. | <p>Michael Hamann <i>Optical Properties of Mechanically Altered LSCs</i> Advisor: Vivian Ferry Sponsoring Program: MRSEC Home Institution: Waconia High School Abstract: Luminescent Solar Concentrators (LSCs) are a large area light harvesting device. These LSCs send this concentrated light into a thin strip of photovoltaic cells to generate electricity. The surface of LSCs can be damaged when placed outside in the elements over a period of time. We explored how mechanical alteration affected the transmission and attenuation of the LSCs under various wavelengths of light. We utilized transparent acrylic slides that are integrated with inorganic florescent dyes for our LSCs. We then applied various amounts of mechanical alteration to the backside of the acrylic LSC using sandpaper. We found that mechanically altering the back surface does not significantly reduce the concentrated photoluminescence while it drastically reduces the intensity of transmitted light. High School students will be asked to create an experiment that is based upon our research. They will be altering the surface of their LSCs so that they may measure the optical properties under various light sources using the light sensor on their smartphones. This is an engaging project that fits well within new Minnesota education science standards that introduces students to the concepts of light, optics, and green energy through the use of LSCs.</p> |
| 89. | <p>Amanda Sheehan <i>An Example of Phenomenon-Based Learning Through the Exploration of Protein Prenylation in Algae</i> Advisor: Mark Distefano Sponsoring Program: MRSEC Home Institution: Edison High School, Minneapolis Public Schools Abstract: The 2019 Minnesota State Science Standards are shifting focus from content-driven learning to the use of scientific practices to explore and understand new phenomena. This project will use protein prenylation in algae as an anchoring phenomenon in both biology and chemistry courses to support a collaborative multi-year project. Students in chemistry will learn the synthesis of a fluorescent prenylation probe through a click reaction. Students in biology will use a synthesized probe to prenylate proteins in algal cells and visualize the resulting product using gel electrophoresis and staining.</p> |