



Materials Research Science and Engineering Center

UNIVERSITY OF MINNESOTA

Driven to DiscoverSM

Summer Undergraduate Research Expo

August 10, 2017

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

1. **Emily Abdo**

Chemically Recyclable Polyurethane Foams from Sustainable Polymer

Advisor: Marc Hillmyer

Sponsoring Program: Center for Sustainable Polymers

Home Institution: Princeton University

Abstract: Polyurethanes (PUs), a versatile class of polymers, commonly appear as rigid or flexible foams for widespread applications in transportation, automotive, and consumer industries. The attributes that make PU foams desirable, namely their low density and durability, pose inherent issues in their end-of-life processing. In order to mitigate the widespread practice of incinerating or landfilling these thermoset foams, we present the synthesis of a sustainable PU foam that can be chemically recycled. Poly(γ -methyl- ϵ -caprolactone)-based foams can undergo a straightforward depolymerization process to afford the starting monomer in high purity and yield. We also demonstrate that these foams can be synthesized to exhibit a range of mechanical properties. By adjusting the isocyanate index and surfactants in the formulations, we create an array of foams with different compressive strengths, cell morphologies, and densities. PU foams from poly(γ -methyl- ϵ -caprolactone) thus present a robust and sustainable alternative to traditional petroleum-based PUs.

2. **Milton Acosta**

Design of new dinuclear-metal catalysts for the Copolymerization of CO₂ and Epoxides

Advisor: Christopher Cramer

Sponsoring Program: Center for Sustainable Polymers

Home Institution: Carthage College

Abstract: Building off previous studies the design of new dinuclear-metal catalysts for the copolymerization of carbon dioxide and epoxides were explored. The bridging metals of these catalyst contribute a crucial part in the electronic properties of the Co-Co distance where the homopolymerization of epoxides and copolymerization of epoxide and carbon dioxide were found to take place. The R groups in the bipyridine ligand were also tuned in attempts to make the copolymerization more favorable than the homopolymerization.

3. **Demetra Adrahtas**

Fabrication of Larger-Sized Transistors Using Self-Aligned Capillary-Assisted Lithography for Electronics

Advisor: C. Daniel Frisbie

Sponsoring Program: MRSEC

Home Institution: Loyola University Chicago

Abstract: Printed electronics show promise for cost savings in large-area applications such as televisions and solar panels because printing is an additive process. Expensive materials are only printed where they are needed in the device unlike traditional photolithographic methods where material is coated over the entirety of the device and then removed where it is not needed. A drawback of printed electronics is the poor resolution, limiting practical feature sizes to the order of 20 micrometers. To improve upon this limit, a novel technique has been developed called self-aligned capillarity-assisted lithography for electronics (SCALE). The SCALE process utilizes imprint lithography to mold a series of reservoirs linked to capillary channels into a UV curable polymer. Electronic inks are easily printed into relatively larger (10's-100's of μm) reservoirs where they flow along the capillary channel to their feature. Channels are engineered at different levels in order to properly inkjet-print the necessary materials into a multilayered device. Feature sizes on the micron and sub-micron scale have already been successfully produced; however, I will be using the SCALE process to engineer large millimeter sized features for transistors that serve as a demonstration to high school students. This technique allows for easy device fabrication with which students can recognize all the components of a transistor and how they work to power the device. Understanding the device's functionality will be done through monitoring changes in resistivity and semiconductor color.

4. **Oluwakayode Akinjo**

Analysis of Facial Characteristics for Volitional and Spontaneous Smiles

Advisor: Stephen Guy

Sponsoring Program: Computer Science

Home Institution: University of Minnesota - Twin Cities

Abstract: Smiles are a basic attribute of human facial expression. By studying how people smile, this work aims to better understand how facial features differ and change over time between genuine and compelled smiles. Our approach leverages a large dataset captured at the 2015 Minnesota state fair where subjects were first prompted to smile, and later, smiled spontaneously in response to a humorous video. For each, key facial characteristics, such as oral commissure, dental show, and malar eminence, were annotated by hand under the guidance of facial surgeon across thousands of millisecond time frames. Features measured included positions and extents (distances) of key facial landmarks, and durations of phases within each type of smile. By analyzing this data, we seek to quantitatively differentiate key aspects of volitional and spontaneous smiles. This research, once applied, could not only be used to create smiles in games and animations with greater realism, but also re-create more genuine looking smiles amongst the facially impaired through reconstructive surgery. Going forward, we are preparing to train neural networks to automate the annotation process and help draw more determinative differences between the two types of smiles.

5. **Fiona Armstrong-Pavlik**

Development of Siderophore-Based Antimicrobials

Advisor: Valerie Pierre

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota, Twin Cities

Abstract: Iron is essential for the survival of most bacterial species. In order to sequester iron from their environments, bacteria produce small molecules called siderophores, which are regarded as a virulence factor. Many species of bacteria are also capable of taking up siderophores produced by other species. This makes the targeting of bacterial iron acquisition systems a viable option of developing new antibiotics. For this project, functionalized analogues of enterobactin, a siderophore produced by *E. coli*, have been synthesized and complexed with gallium, a metal which does not aid bacterial growth. Using an attachment point on the synthetic siderophores, antibiotic and cytotoxic agents have been conjugated to the molecule in a way that does not impede recognition of the molecule by the iron-uptake transmembrane protein of the bacteria. This will enable the antibiotic or cytotoxic agent to enter bacterial cells using a "Trojan horse" strategy, potentially enabling the treatment of antibiotic-resistant bacteria.

6. **Shelby Auger**

Utilizing Protein Prenylation to modify EpCAM targeting DARPins

Advisor: Mark Distefano, Yi Zhang

Sponsoring Program: UMN Chemistry- Lando

Home Institution: St. Catherine University

Abstract: Protein prenylation is the enzymatic addition of isoprenoid substrates to the C- terminus of a "CAAX" peptide sequence, where "C" represents cysteine, "A" represents an aliphatic amino acid and "X" is a variable amino acid. This CAAX motif, in the form of CVIA, was added to design ankyrin repeat proteins (DARPins) which are engineered to bind to specific target. This motif allows the DARPins to undergo protein prenylation with the enzymes protein farnesyltransferase (PFTase) which naturally catalyze the transfer of farnesyl. PFTase has promiscuous substrate specificity and can accept modification of the farnesyl diphosphate substrate. Shown here is the synthesis of a farnesyl analog functionalized with a terminal azide. By using this synthetic farnesyl analogs to modify the DARPins, subsequent labeling with a fluorophore becomes possible. These fluorescently modified DARPins will target epithelial cell adhesion molecules (EpCAM) in cancer cells allowing for their visualization.

7. **Katherine Avery**, Vaibhav Sharma
Multiclass Classification for Sentiment Analysis using Matthews Correlation Coefficient
Advisor: Daniel Boley
Sponsoring Program: Computer Science
Home Institution: University of Oklahoma
Abstract: Sentiment analysis for short pieces of text, such as blog entries, is relatively accurate for binary emotion classification using standard machine learning methods. However, multiclass classification, in which a piece of text has one of several classifications, is much less accurate, which calls for more sophisticated methods. We propose a new algorithm for multiclass classification using the Matthews Correlation Coefficient (MCC), a performance evaluation parameter, for supervised feature selection. Called the MCC Supervised Text Classifier, the method provides better test accuracy than standard methods and, more importantly, it is computationally more efficient than standard algorithms because it has a linear time complexity. It also avoids the curse of dimensionality and performs well on datasets with unequal class sizes compared to standard algorithms. To evaluate the accuracy of the proposed algorithm, we compare it to deep learning methods, most notably convolutional neural networks (CNNs), by classifying blog entries into six different sentiment categories. The MCC Supervised Text Classifier is again more efficient, while the test accuracy has yet to be compared.
8. **Maria Balderrama**, Louis Corcoran
Breaking Oil—Mapping the Microstructure Morphology Created by Food-Grade Surfactants at an Oil-Water Interface
Advisor: R. Lee Penn, Alon McCormick
Sponsoring Program: Project SEED
Home Institution: Johnson Senior High School, St Paul Public Schools
Abstract: : In April 2010, the Deepwater Horizon drilling rig exploded in the Gulf of Mexico, ultimately releasing 205 million gallons of crude oil into the ocean. In efforts to remediate the impact of the spill, 2.1 million gallons of the marine oil dispersant Corexit 9500 were applied to the spill—the largest dispersant application to an oil spill in history. 1 Despite the widespread use of Corexit, some of the key components of this surfactant blend are known to exhibit some marine toxicity (dioctyl sodium sulfosuccinate), 2 leading to the development of new surfactant systems composed entirely of non-toxic chemicals. Recently, effective dispersant blends containing the food-grade surfactants Lecithin (phosphatidylcholine) and Tween 80 (polyoxyethylenesorbitan monooleate) have shown similar dispersant effectiveness compared to current commercial formulations. However, these new blends have displayed some unexpected properties that are not typical of an effective dispersant. Due to this disparity, we have set out to understand the chemistry that is taking place at the oil-water interface of this novel surfactant system. Specifically, we want to elucidate why this surfactant system is an effective dispersant by characterizing the microstructures that are created at a generic oil-water interface based on changes in the Surfactant:Oil:Water composition.
9. **Ryan Bartz**
Bismuth(III) Subsalicylate as a Replacement Catalyst in Teaching Laboratory Polymer Experiments
Advisor: Jane Wissinger
Sponsoring Program: UMN Chemistry- Heisig Gleysteen
Home Institution: University of Minnesota
Abstract: Widespread use of tin(II) ethyl-hexanoate as a catalyst in published laboratory experiments gives pause to instructors with concerns about the generally toxic qualities of organotin compounds. In response to conversations about the environmental impacts of conventional plastics, demand for polymer experiments that showcase green chemistry principles has increased. Introducing an alternative catalyst commercially available as an over-the-counter stomach relief agent exemplifies how benign reagents can be viable replacements for those currently in use with undesirable characteristics. Previous research indicates that bismuth(III) subsalicylate, the active ingredient in Pepto-Bismol-, is an effective catalyst for the ring opening polymerization of poly-lactic acid and other polyesters. Under less stringent conditions similar to those in a teaching laboratory, increased heating periods or polymerization under vacuum were sufficient adjustments to yield poly-lactic acid with the bismuth catalyst. Following these successes, the same catalyst has been applied and compared to instructional experiments for other degradable polyesters.

10. **Nick Battaglia**

Synthesis of precursor salt and 1,3-bis[(2-pyridyl)methyl]-1H-imidazolylidene and coordination with lanthanum(III) ion

Advisor: Marites Guino-o

Sponsoring Program: University of St Thomas- Chemistry

Home Institution: University of St. Thomas

Abstract: Lanthanides-based materials have numerous applications, including biomedical imaging, optics, and electronic screens. Lanthanide(III) ions are able to weakly emit light because f-f transitions are parity forbidden. Thus, lanthanide(III) ions require both an effective shield to prevent quenching, as well as an efficient chromophore to transfer energy to the ion. In our group, we would like to investigate the possible sensitization of the N-Heterocyclic carbene (NHC) ligand, 1,3-bis[(2-pyridyl)methyl]-1H-imidazolylidene with lanthanide(III) ions. Like many NHCs, precursor salts had to be synthesized in order to create the desired NHC ligands. Herein, we report on the synthesis and characterization of the NHC precursor salt, and the NHC in-situ formation and complexation reaction with lanthanum(III) cations.

11. **Onri Benally**

Fabrication and Analysis of InSb Nanowires for Use in Low Temperature Experiments

Advisor: Vlad Pribyag

Sponsoring Program: MRSEC

Home Institution: Utah State University

Abstract: The future looks very bright for the field of solid state physics because it involves the attempt at understanding the fundamentals of how semiconductors behave in special circumstances at the nanoscale. Thus, we turn to microfabrication processes and lithography, where micro-devices can be put together by means of etching and filling of substrate material over layers upon layers of wafer. We use equipment in the laboratory such as the AFM, Profilometer, and Keyence Digital Microscope to monitor the Reactive Ion Etching Process of an HSQ covered sample. When the processes are determined to be in the right conditions after etching, semiconductor nanowires can then be added to a sample for the planarization step. The planarization of the layer can then allow the nanowires to be contacted with ferromagnetic materials in which are then applicable to nanoscale machines and devices for research. More specifically, the project comprises of devices based on InSb nanowires, Si nanoparticles and InAs-based quantumwells.

12. **Spencer Bingham**

Synthesis of NU-1000 Nanoparticles

Advisor: Lee Penn

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Carthage College

Abstract: Metal-organic frameworks (MOFs) are crystalline, porous materials synthesized from metallic clusters linked by organic ligands with diverse applications in gas separation and storage, sensing, and catalysis, among others. NU-1000 is a Zr-based MOF with tetratopic linkers. It is thermally and hydrolytically stable and contains large mesoporous channels useful for metalation and catalysis. Nano-sized MOF particles have advantageous properties including reduced diffusion time for metalation, increased surface area and reactivity, as well as the potential for drug delivery and other medical use. Further, because of the small particle size, higher chemical mapping resolutions can be achieved. Previously, NU-1000 nanoparticles have been synthesized with the addition of secondary modulators in the formation of the Zr nodes as well as limited growth time. Here, nanoparticles are synthesized without the use of additional modulators and without dependence on time. NU-1000 nanoparticles of 70 - 2000 nm are reported, synthesized using low concentrations of a biphenyl carboxylic acid modulator and basic conditions. Additionally, in syntheses with very low modulator concentrations, NU-1000 sol-gels were formed which were converted into xerogels and aerogels.

13. **Hannah Bossert**
Construction and Verification of an Automated Microcatalytic Reactor's Accuracy Using Solid Acid Catalysts
Advisor: Paul Dauenhauer, Omar Abdelrahman, Katherine Vinter
Sponsoring Program: MRSEC
Home Institution: University of Minnesota Twin Cities
Abstract: Microreactors have made great improvements in reaction engineering research due to their ability to rapidly screen catalysts of interest for any desired chemistry. Evaluating the performance of a catalyst for a given chemical reaction usually requires a well-trained chemical engineer to continuously run and monitor multiple reactions in order to collect enough data to determine a certain reaction's properties. The development of an automated microcatalytic reactor could significantly decrease the amount of manual labor and intensive training required to evaluate new catalysts for reactions, which do not have well known chemistries. The automated microcatalytic reactor was housed within a gas chromatograph (GC), in which the GC inlet contained the reactor and an automated liquid sampler (ALS) was used to deliver the reactant. The reactor is a semi-continuous flow reactor with the ability to reach steady-state, inject the results, and quickly move on to new conditions. Once constructed, the automated microcatalytic reactor's ability to obtain accurate data was tested by running reactions with well-known chemistries, such as alcohol dehydration over solid acid catalysts. This was performed by comparing reaction rates, activation energies, and product selectivity to those in the literature. This validation starts to give the automated microcatalytic reactor the ability to potentially be standardized and be used in more diverse labs.
14. **Brady Bresnahan, Wenyang Zhao, and Andreas Stein**
Increasing Selectivity of Oxozirconium Clusters as Lewis Acid Catalysts
Advisor: Andreas Stein
Sponsoring Program: UMN Chemistry- Lando
Home Institution: Carthage College
Abstract: Metal organic frameworks (MOFs) are an organized, highly concentrated source of catalytically active metallic or oxo-metallic nodes. However, these nodes aggregate upon high temperature treatment and their catalytic activity is lost. To prevent their aggregation, amorphous silica was nanocast inside the pores of the MOF NU-1000 to provide a thermally stable secondary scaffold for the catalytically active nodes. One drawback was that the nanocast amorphous silica provided poor selectivity of the nodes, which we aimed to improve by using zeolitic silicalite-1 as the secondary scaffold. Silicalite-1 has an ordered, porous structure with an average pore size of 0.55 nm, which could provide selective access to the nodes while still acting as a thermally stable secondary scaffold. In this work, we describe attempts to form silicalite-1 inside the pores of NU-1000, a MOF with 3 nm channels and Lewis acidic oxozirconium clusters, as well as to form a layer of silicalite-1 around the silica-nanocast NU-1000 particles. Attempts have also been made to form zirconium-doped silicalite-1 without the use of NU-1000 as the source of zirconium precursors. All the silicalite-1 formation reactions involve the structure directing agent tetrapropylammonium and basic conditions, therefore tetrapropylammonium hydroxide was used in each reaction. The samples were analyzed using X-ray diffraction to check the crystalline structure, scanning electron microscopy and transmission electron microscopy to check morphology, and energy-dispersive spectroscopy for elemental analysis.
15. **Kathryn Breuckman, Kathryn C. Breuckman, Madeline K. Hankard, Kristine H. Wammer, Nicholas C. Pflug, David M. Cwiertny**
Effect of nucleophiles on photolysis, regeneration, and product formation of the steroid trendione
Advisor: Kristine Wammer
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Trenbolone acetate is a synthetic androgenic growth promotor used in cattle and sheep agriculture and is metabolized into trendione (TBO) and two known endocrine-disrupting compounds 17 α - and 17 β -trenbolone. These metabolites enter surface waters via run-off and may pose a threat to aquatic organisms. Trienone steroids such as TBO readily undergo direct photolysis producing photoproducts which may also be biologically active. In the dark, TBO regenerates, photoproducts degrade, and secondary products grow in. Additionally, TBO can react with nucleophiles in the water such as chloride and nitrate, and these nucleophiles can affect regeneration and product formation. The goal of the present study is to better understand the environmental fate of TBO by studying the effect that environmental nucleophiles have on

photolysis rates, extent of regeneration, and product formation. In the absence of a nucleophile, TBO regenerates to 16% of its original concentration, but in the presence of the nucleophile azide, initial experiments appeared to show that TBO initially increased to 7% of its original concentration but quickly degraded. However, control experiments show TBO is stable in the presence of the nucleophile azide, suggesting the initial slight regeneration observed may actually be a reversion to an analog of TBO that is susceptible to nucleophilic attack, unlike TBO which is stable towards nucleophiles. Future work aims to further understand the effects nucleophiles have on product formation and reaction mechanisms.

16. **Eli Broman**

Effects of Crosslinking PB-PLA Diblock Copolymers

Advisor: Frank Bates

Sponsoring Program: MRSEC

Home Institution: University of Wisconsin - Green Bay

Abstract: Diblock copolymers are the covalently linked composition of two different polymers. Studying these is useful to understand structure-property relationships in soft matter. Asymmetric AB diblock copolymers ($f_A \ll 0.5$) easily order into particle-forming structures; the most common is cubic symmetry (BCC lattice). The purpose of this project was to understand the role of chain exchange in model poly(1,2-butadiene)-b-poly((\pm) -lactide) (PB-PLA) diblock copolymers through synthesis and characterization. To do this, PB-PLA diblock copolymers were synthesized using sequential anionic polymerization followed by a ring-opening polymerization technique. ¹H Nuclear Resonance Spectroscopy, Size Exclusion Chromatography, and Differential Scanning Calorimetry were used to quantify the molecular characteristics of the samples. Additionally, the physical characteristics were analyzed via X-ray scattering and rheology. The PB cores were crosslinked by adding a small amount of photo-initiator (< 1 wt%) and activated by UV light. The physical properties were examined during and after crosslinking to note the structural changes in the sample. We hypothesized the crosslinking will eliminate or decrease chain exchange, thus increasing the order-disorder temperature (ODT) and possibly the morphology. This research will provide fundamental information about the physical effects of chain exchange in diblock copolymers, specifically regarding ordered structures and fluctuations in the disordered state.

17. **Rochelle Brooks**

Liquid-Gas Interface Stability of an Inverted Liquid Piston Air Compressor

Advisor: James Van de Ven

Sponsoring Program: CCEFP

Home Institution: University of Minnesota

Abstract: In order for compressed air energy storage (CAES) to be viable as a market solution for incorporating intermittent energy sources in the grid, an improvement in compressor efficiency is necessary. The inverted liquid piston air compressor offers a high power density, low cost, and low environmental impact compressor technology. Here, the piston itself is stationary with a water column resting on it, and the compressor chamber walls and end cap move for compression and expansion. In order to begin assessing the feasibility and exact applications for this technology, the present experimental research explores parameters affecting the liquid-gas interface stability in the inverted liquid piston air compressor. Stability was characterized based on liquid splashing and formation of gas bubbles in the liquid. Testing was first done with only water and air in the compression chamber. A series of behaviors were seen: an initial "parabolic" shape is seen at low frequencies; this becomes unstable, and the surface becomes wavy and begins to splash; at still higher frequencies the surface smooths out and fingers of liquid form along the compression chamber walls; at the highest frequencies tested, these fingers become longer and droplets form on their tips. Compression ratio and crankshaft length were seen to have minimal effect on the interface stability, as these behaviors developed at consistent frequencies for the four compression ratios and two crankshaft lengths tested.

Both interrupted stacked plate and vertical rod porous media were studied. For the interrupted stacked plate media, the length, spacing, and thickness were varied. Spacing and diameter were varied for the vertical rod media. It was found that longer lengths, smaller diameters, and wider spacings provide greater interface stability. Hydrophobic coating was applied to the porous media and was seen to decrease the amount of splashing but increase bubbling.

18. **Nyssa Capman**, Anuj Karpatne
Mapping the dynamics of surface water bodies using Earth-observing satellite data: A comparative study
Advisor: Vipin Kumar
Sponsoring Program: Computer Science
Home Institution: Augsburg College
Abstract: Monitoring the surface extent changes of inland water bodies over time can provide vital signs of human impacts and natural changes on the environment, which informs water management and conservation. This monitoring is accomplished by classifying every location from Earth-observing satellite data as 'water' or 'land' for every time-step. Automated data classification methods can produce such binary labels for global-scale remote sensing data at fine spatial resolutions (every 500m) and at regular time intervals (every 8 days starting from 2000). However, 'water/land' class confusions occasionally arise – for example, at the edges of lakes or in swamp land. To better quantify the situations where these confusions occur, we explored dimensionality reduction techniques to visualize the space of high-dimensional multi-spectral satellite data. A k-means cluster analysis was used to compare the structure of the output from two dimensionality reduction methods. Additionally, the robustness of classification algorithms were examined: Support vector machines (SVM) were applied to training sets of varying sizes to optimize the parameters needed to produce a more accurate classification model.
19. **Sharon Chen**, Zachary L. Robinson, Savanna A. Dautle
Lifetime of Silicon Nanocrystals in Optoelectronics
Advisor: Uwe Kortshagen
Sponsoring Program: MRSEC
Home Institution: Case Western Reserve University
Abstract: Silicon nanocrystals (Si NCs) have the potential to change the field of optoelectronics because of silicon's abundance and non-toxicity as well as our ability to customize the material's photoelectric behavior for its intended applications, such as solar cells and light emitting diodes (LEDs). For example, Si NCs can improve the efficiency of solar cells and LEDs because we can control the way these devices absorb and emit energy by changing the NC particle size. To change the NC size during the plasma reactor synthesis process, we varied the residence time of the NCs in the plasma chamber. We then conducted time resolved photoluminescence tests to measure the lifetime of Si NCs across the emission spectrum and to better understand factors that impact PL lifetime. Some factors we investigated included the oxidation and sintering of Si NCs. Since oxidation reduces particle size, we also examined the size effects of NCs on PL lifetime. We found a direct correlation between the size of the NCs and their lifetime: the lifetime decreased with decreasing Si NC size. On the other hand, sintering the NCs had very little effect on the PL lifetime of the material, possibly resulting from oxidation or negligible facet sizes.
20. **Michelle Chu**
Subthalamic Nuclei Gamma Frequency Deep Brain Stimulation for Parkinsonian Non-Human Primate
Advisor: Greg Molnar
Sponsoring Program: UROP
Home Institution: University of Minnesota Medical School
Abstract: Deep brain stimulation (DBS) has been dramatically effective in the treatment of advanced Parkinson's disease (PD). Traditional DBS delivers continuous, high frequency electrical stimulation to key regions in the basal ganglia thalamocortical (BGTC) 'motor' circuit including STN. For decades, DBS technique hasn't changed much and is accompanied with persistent clinical limitations such as the stimulation-induced, therapy-limiting side effects that might relate to the high frequency delivery of electrical pulses. Limited explorations of novel DBS paradigms in order to reduce stimulated related side effect, increase treatment efficacy, and reduce battery consumption were reported, including some studies that attempted to reduce the stimulation frequency to gamma range (31-100 Hz) while the stimulation could still produce the efficacy the same as, or even superior to tDBS. In the study, gamma frequency DBS will be further explored acutely and compared to tDBS using neurophysiological data and behavioral observation collected from a within-subject design model in a moderate parkinsonian state non-human primate.

21. **Abbie Cotter**

Probing Electronic Properties of Single-Crystal Rubrene

Advisor: James Johns

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Macalester College

Abstract: Rubrene is an organic semiconductor of particular interest due to its high charge carrier mobility. Single-crystal molecular rubrene was grown via physical vapor transport. We attempted to characterize rubrene single crystals with scanning tunneling spectroscopy (STS). STS is useful for not only visualizing molecular surfaces but also probing the electronic structure. The differential conductivity of the tunneling current is indicative of the local density of states. We intended to compare single-crystal molecular rubrene and a fluorinated rubrene derivative to understand how the addition of electron withdrawing groups affected the local density of states. This fluorinated rubrene derivative is understood to share similar characteristics rubrene, such as molecular stacking and charge carrier mobility, but has better stabilization of both the HOMO and the LUMO while maintaining the band gap, which is favorable for electron transport.

22. **James Cox**

Investigating the Effect of Proximal Functionality on the Winstein Rearrangement

Advisor: Joseph Topczewski

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota, Twin Cities

Abstract: The Winstein rearrangement involves the equilibration of allylic azides between branched and linear isomers. This study investigates the effect that proximal functionality has on the Winstein rearrangement. A total of 15 azides, each with different functional groups neighboring the allylic azide group, have been synthesized. These functional groups represent a range of properties and are divided into three classes: oxygen-based, secondary-amine-based, and tertiary-amine-based. After synthesis, each allylic azide was allowed to equilibrate and then analyzed by ¹H NMR. We observe an electronic effect that strongly correlates with the pK_a of the -OR proximal group (oxygen class). We also observe an increase in % branched in the N-H series (secondary-amine class) relative to the N-Bn series (tertiary-amine class), but a lack of solvent effects on the equilibrium position of the rearrangement suggests minimal involvement of an intramolecular hydrogen-bond.

23. **Savanna Dautle, Zachary L. Robinson, Sharon Chen**

Exciton Recombination in Silicon Nanocrystal Films and Solutions

Advisor: Uwe Kortshagen

Sponsoring Program: MRSEC

Home Institution: Rowan University

Abstract: Excitons in nanocrystal semiconductors have become of interest for their industrial applications, ranging from light-emitting diodes (LEDs) to solar panels and photodetectors. This interest has led to the need for better understanding of how excitons are transported in silicon quantum dot (QD) films and solutions. We use Time-Resolved Emission Spectroscopy (TRES) to measure the photoemission from the sample in terms of time and emission energy. This exhibits the radiative decay of the excitons in the sample. Gold nanoparticles, which serve as non-radiative exciton traps, were added to QDs in solution. Exciton diffusion can be studied by observing the changes in photoluminescence (PL) lifetime in film, which was shown to decrease as concentration of gold increases. By adding gold, the volume available for radiative exciton recombination decreases. In addition to looking at excitons in QD films, we also observe the radiative decay of excitons in the QD samples in solution. In contrast with previous studies, a redshift was observed in QD solution samples, of comparable size to the redshift expected and seen in QD film samples. This is hypothesized to be caused by a wide size distribution of non-interacting particles, though further study is needed to support this theory.

24. **Hector De Santiago**, Michael Manno, Eric McCalla, Swati Mohan, Yuanbing Mao, and Chris Leighton
Influence of particle size and stoichiometry on the magneto-electronic properties of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ nanoparticles
Advisor: Chris Leighton
Sponsoring Program: MRSEC
Home Institution: University of Texas Rio Grande Valley
Abstract: Perovskite oxides have been shown to exhibit a plethora of interesting and important materials properties, ranging from high temperature superconductivity, colossal magnetoresistance, and ferroelectricity, to co-incident metal-insulator, structural, and magnetic phase transitions. Perovskite cobaltites doped with alkaline-earth metals, such as $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$, have shown a clear form of magneto-electronic phase separation which is heavily influenced by stoichiometry. In addition to chemical composition effects, magneto-electronic phase separation behavior could also be affected by constraining dimensionality of the material. To study this behavior, nanoparticles of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ are being studied here as a function of composition and particle size. Magnetometry measurements on $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($X_{\text{nom}} = 0, 0.05, 0.1, 0.2, 0.3$) nanoparticles from year-old samples and recently-made samples were first studied and compared to analyses made a year ago. This was done to determine if there was any deterioration in the magnetic properties of the nanoparticles, and to see how particle size affects these properties. Preliminary analysis demonstrates that there is little decay of the magnetic properties with time. Scanning electron microscopy shows that the new samples have slightly smaller particles on average and the size distributions are significantly narrower. Energy dispersive analysis of x-rays (EDAX) proves that both sample batches were strontium deficient while having a high degree of polydispersity of strontium concentration. The old samples also contained chlorine and potassium contamination. Overall, this analysis demonstrates an improvement in the synthesis procedure used to make the nanoparticles. Further work will focus on EDAX mapping to clarify the polydispersity of the nanoparticles. Additionally, x-ray diffraction will be used to confirm the phases of the samples
25. **Derek Delzell**
Application for communication based testing between IoT devices
Advisor: Jon Weissman
Sponsoring Program: Computer Science
Home Institution: Morningside College
Abstract: The Internet of Things (IoT) is opening the door to a multitude of new applications and this program helps test a new form of device communication. Current systems exhibit inefficiencies which stem from applications being isolated and opportunities for sharing and contention resolution ignored. There is no infrastructure for different companies devices to communicate and there these systems have to fight for application resources. Proposed is a new system called Constellation that enables synergies between applications which will lead to IoT systems being more efficient. This project will help to visualize the data involved in Constellation's creation by testing the communication between nodes, while also providing an interface for us to more quickly run tests/experiments. This allows us to gather data on what the nodes are sending and to view the framework of Constellation as it grows.
26. **Anna Folska**
Lipid Membrane Interaction Thermodynamics of Cell-Penetrating Peptides
Advisor: Lisa Prevette
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Cell penetrating peptides (CPPs) efficiently enter cells while transporting proteins, drugs and other cargos. Tat (transactivating transcription factor) peptide is a non-structured, 11-residue CPP with dense positive charge. Tat has been widely used to deliver covalently and noncovalently attached cargo to multiple cell lines and in vivo. It has been shown to enter cells via energy-dependent endocytosis, which is triggered by membrane interactions. Pep-1, a 21-residue amphiphilic CPP, is known for its superior drug delivery rates and low toxicity. Pep-1 is thought to directly penetrate cell membranes instead of using an endocytosis pathway, which could explain its higher internalization rates and the efficiency of its attached drugs. The interaction between these CPPs and lipid membranes is being studied using isothermal titration calorimetry (ITC). Results showed that Tat binds anionic lipid (POPG) vesicles but not zwitterionic (POPC) ones, suggesting an electrostatic mechanism. The contribution of electrostatics to the

binding free energy was determined by altering the ionic strength of the buffer used in the ITC studies. The binding constant ranged from $2.7 \times 10^6 \text{ M}^{-1}$ at 15 mM NaCl to $2.2 \times 10^5 \text{ M}^{-1}$ at 250 mM NaCl, representing a decrease in affinity. 8/10 lipid sites are electrostatically binding to Tat. Pep-1 was shown to bind POPG vesicles with two events, suggesting hydrophobic forces may play a role in addition to electrostatic forces. With these results, the nature of binding between these CPPs and model membranes can be determined, which hopefully sheds light on their different cell uptake mechanisms.

27. Camryn Franke, Xiao Yi

Optimizing Escherichia coli energy usage for chemotaxis and reproduction through experimental evolution

Advisor: Romas Kazlauskas

Sponsoring Program: Project SEED

Home Institution: Washington Technology Magnet High School, SPPS

Abstract: In bacteria, cellular energy is largely consumed by two essential functions: reproduction and chemotaxis, the behavior where single-celled organisms swim up a gradient of nutrients. When both functions are selected simultaneously, the finite energy output of the cell causes a tradeoff between chemotaxis and reproduction. In this research, we implemented a stringent selective scheme forcing E.coli to fully maximize energy usage by selecting both functions continuously and simultaneously. Bacteria reproduced in aqueous medium with limited diffusion; the growing population depleted ambient nutrients, creating a gradient for the cells migrate towards. Hence, the migration speed is a function of both reproduction and chemotaxis. We designed a "treadmill" that constantly and most effectively selects only the bacteria that migrate the fastest. Cells were sampled from the migrating population and their migration speed, rate of reproduction, and average cellular swimming speed were analyzed in standardized test. We used this data to determine how E.coli (re)allocates energy between chemotaxis and reproduction in order to achieve the fastest migration speed and most effective energy usage. These results provide novel insights on how cells adapt to complex environments in the face of fundamental physicochemical constraints of life

28. Nick Fuhr

3D Printing Silicon Nanocrystal Light Emitting Diodes

Advisor: Michael McAlpine

Sponsoring Program: MRSEC

Home Institution: University of St. Thomas

Abstract: Bulk silicon crystals do not typically luminesce because of bulk silicon's intrinsic narrow indirect band gap; this engenders silicon's semiconducting properties. However, as the diameter of silicon crystals approaches the nanoscale, quantum confinement effects take affect—quantum confinement effects occur when a material's diameter approaches the de Broglie wavelength of the electron's wave function. As the diameter of a semiconductor approaches the electron-hole pair radius (also known as the Bohr radius), the orbital overlap of the atoms composing the nanocrystal decreases, which creates discrete energy levels and consequently increases the energy needed for an electron to move to the conduction band from the valence band. By injecting holes and electrons into silicon nanocrystals (SiNCs), exploitation of the expanded band gap may transpire and will result in the emission of light with a wavelength that is dependent on the size of the nanocrystal. The tunability of SiNCs is an advantageous property when considering materials needed to create solid-state lighting devices. Through the utilization of 3D printing, a new avenue is created for fabricating solid-state lighting, like light emitting diodes (LEDs). This approach will expand the range of functional materials that 3D printers are capable of extruding. Examples of the types materials used in this printing process are, but not limited to: (1) liquid and solid metal electrodes, (2) conductive organic polymers, (3) emissive inorganic quantum dots, and (4) silicon based substrates for printing on top of. By fabricating LEDs via 3D printing, novel three dimensional designs incorporating LEDs, that are not typically accessible by microfabrication techniques, become conceivable.

29. **Hannah Ganzel**
Binding Affinity of PAH-Coated Au Nanoparticles to Gram Positive Bacterial Cell Walls
Advisor: Lisa Prevette
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: With their potential in drug delivery, imaging, and sensing, engineered nanoparticles are a fast-growing and beneficial novel technology. Their surfaces are often functionalized for stability and/or enhanced cell interactions, but the effects of these different coatings on the environmental impact of the nanoparticles are largely unknown. Polyallylamine (PAH)-coated Au nanoparticles are known to be toxic to gram-positive bacteria, likely by attaching to the cell wall at one of three locations: the lipid bilayer, the peptidoglycan layer, or the lipoteichoic acids. A study was done in order to determine where on the gram positive cell wall PAH-coated Au nanoparticles (PAH-AuNPs) bind. Due to strong electrostatic interactions between the positively charged PAH polymer and the negatively charged lipoteichoic acids, it was hypothesized that the PAH coating on the nanoparticles would cause them to bind to this site with the highest affinity. To confirm this, binding studies were performed using isothermal titration calorimetry (ITC). The results showed no binding of PAH to model lipid bilayers, though binding was observed to both peptidoglycan and the lipoteichoic acid chains. Unexpectedly, the PAH-AuNPs showed binding to peptidoglycan but no binding to model lipid bilayers or lipoteichoic acids. Zeta potential data indicates the NPs may have been unstable, leading to their charge neutrality. Therefore, synthesis of new PAH-AuNPs must be completed prior to further experimentation to confirm the ITC data collected.
30. **Christina Geiser**
Sensor Calibration on a Power Regenerative Test Platform
Advisor: Kim Stelson
Sponsoring Program: CCEFP
Home Institution: College of Saint Benedict
Abstract: A power regenerative test platform has been built at the University of Minnesota to understand how a hydrostatic transmission operates in a wind turbine. There are many sensors on the test bed to monitor performance. The focus of my project was calibrating the pressure and flow sensors. It is important to calibrate these sensors so that the data given by the sensors can be trusted. The pressure sensors were calibrated by supplying a known amount of pressure using a dead weight tester. The flow sensors were calibrated by supplying a known amount of flow using a CMA valve. For each known amount of pressure or flow, the sensor gives a voltage output. This data is then plotted with a linear best-fit line. The slope and y-intercept of the best-fit line are used to calibrate the sensor.
31. **Beau Gilles**
Development of a Green Suzuki-Miyaura Coupling for the Instructional Laboratory
Advisor: Jane Wissinger
Sponsoring Program: Wissinger Group
Home Institution: University of Minnesota
Abstract: To prepare the next generation of chemists to be conscious of sustainable chemistry, it is necessary to expose students to syntheses which demonstrate the principles of green chemistry, minimize waste and improve safety in the lab. Described herein is a new teaching lab experiment which involves the Suzuki-Miyaura coupling reaction of 5-iodovanillin and 4-methylphenyl boronic acid. The procedure exemplifies green methodologies by using water as a benign reaction solvent, employment of a catalyst, and the use of 5-iodovanillin which was synthesized by students from renewable vanillin. An instructional procedure was adapted from the literature to give students a hands-on experience with the Nobel-prize winning Suzuki coupling. This will replace a low atom economy Grignard reaction in the curriculum. Two versions of the experiment, one using microwave technology and one using standard reflux conditions were trialed in the introductory organic chemistry laboratory course, CHEM-2311, at the University of Minnesota. The results of these trials will be shared-along with student and TA feedback of the experiment.

- 32. Alexander Gomez**
Synthesis of Novel BACE1 Inhibitors
Advisor: Joseph Topczewski
Sponsoring Program: UMN Chemistry- Lando
Home Institution: Lawrence University
Abstract: BACE1 inhibitors have shown promise as therapeutic agents for Alzheimer's disease. Therefore, it is important to expand our ability to synthesize a wide variety of these drugs and assess their biological activity. We are developing a novel and versatile synthetic route to molecules with potential for inhibitory activity. This involves a highly stereoselective azide resolution previously reported by our group. Pharmaceutical researchers have had some difficulty creating molecules that can pass the blood-brain barrier. We hope that the scope of products made possible by our synthesis can help overcome this issue.
- 33. Rebecca Goncalves**
Developing sustainable acrylates for 3D printing
Advisor: Theresa Reineke
Sponsoring Program: Center for Sustainable Polymers
Home Institution: The College of New Jersey
Abstract: 3D printable photopolymers have seen expanding applications in prototyping, medical devices, and particularly, in the advancing field of digital dentistry. Stereolithographic 3D printers are used to print orthodontic devices such as dentures, retainers, and bridges. Dental resins with high precision, good strength and toughness, fast photo-curing, biocompatibility, and antiseptic properties, are growing in demand for greater strides in this direction of additive manufacturing. Our effort aims at developing acrylate monomers and formulations based on sustainable feedstocks, in order to replace bisphenol A (BPA)-based monomers which have significant health concerns. Eugenol, guaiacol, and vanillin, bearing natural aromaticity are synthesized to (meth)acrylates to impart structural rigidity into a free-radical photo-crosslinked network. With the photoinitiator (0.5 wt% TPO), the sustainable monomers were formulated with flexible polyethylene glycol (meth)acrylates and the photo-curing kinetics and dynamic mechanical properties of the formulations were investigated. Photo rheology demonstrated that the gel time is affected by the viscosity and molecular structure of the monomer (meth)acrylates in the formulations. The storage modulus, glass transition and cross-link density measured by dynamic mechanical analysis (DMA) indicate the improved manipulation of those properties by the novel thiol-ene clicked eugenol acrylate monomer. Continuing work on mechanical tests, antibacterial test and further enhancement on curing rate and 3D printability will be performed.
- 34. Joey Gotchnik**
Epitaxial LCO Thin Films and Ion Gels Used for Dual Gated Transistors.
Advisor: Chris Leighton
Sponsoring Program: Independent Research
Home Institution: University of Minnesota
Abstract: Lanthanum Cobalt Oxide (LCO) lies high on the interest list of scientists with its strange ferromagnetic properties that arise when grown into an epitaxial thin film. This substance is also an insulator in bulk to make things more interesting. From growth to characterization of lattice parameters, thickness and surface morphology, pursuit of understanding this strange property continued. Equally, these thin film can exist as a semiconductor in a dual-gated transistor. Within these transistors, an external field is applied and has been proven to alter the magnetism of these LSCO thin films. LSCO means the LCO thin films were doped with strontium. The ion gels in these transistors were optimized for their thickness, uniformity and smoothness. Therefore the next goal is to alter the magnetism of LCO thin films without the doping of strontium.
- 35. Brittany Haas**
Biodegradable Tri-block Copolymer Self-Assembles for Drug Delivery
Advisor: Lisa Prevette
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Polylactide (PLA) was synthesized by ring-opening polymerization of L-lactide using 3-(benzyloxy)-1,2-propanediol as an initiator and stannous octanoate as catalyst. The resulting PLA has two terminal secondary alcohols and a central benzyl ether group, which can be deprotected to yield a primary alcohol. Three molecular weights of PLA were synthesized and

confirmed by ¹H NMR integration and GPC. Conjugation of monofunctionalized dextran to the terminal alcohols of the PLAs by DCC coupling will yield a biocompatible, biodegradable triblock copolymer for drug delivery. Covalent attachment to the deprotected central alcohol of the PLA allows for well-controlled, hydrolysable drug conjugation. Certain mass ratios of dextran to PLA should also self-assemble into polymersomes, which can be used to deliver both hydrophilic and hydrophobic drugs through noncovalent encapsulation. Drug release is expected to be controlled by the degradation of the polymersome due to hydrolysis of the PLA.

36. Hirbod Heidari

Calculation of thermochemical data by a linear scaling method

Advisor: Donald Truhlar

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Sharif University of Technology

Abstract: Most calculations of the molecular partition function utilize the Harmonic Oscillator (HO) approximation, which produces qualitatively inaccurate results for systems exhibiting torsional motion. This failure is partly due to that fact that such systems involve multiple minima (aka conformers) and partly due to the strong intermode coupling of large amplitude motions. Most available methods to address these systems require a complete representation of the torsional potential and are only affordable for small systems. The MS-T method developed by the Truhlar group uses only the minimum energy structures of the conformers (i.e., it does not require explicit optimization of the torsional barriers) to estimate the partition function, and is currently the best available one in terms of both accuracy and computational cost. However, it still needs to find all of the conformers, which is a task that scales exponentially with the number of torsions and consequently it is unaffordable for systems with more than about 8 torsional coordinates. In this project, we are developing and testing linear scaling analogs of the MS-T method that are appropriate for treating larger systems.

37. Shannon Herzog

Transamidation of Activated Polyacrylamide Via Destabilization of Amidic Resonance

Advisor: Marc Hillmyer

Sponsoring Program: MRSEC

Home Institution: Drake University

Abstract: Transamidation is of major interest in organic synthesis. However, this reaction is difficult to perform under mild conditions due to the high stability of the amide bond through amidic resonance. We seek to assess the effect of using tert-butyloxycarbonyl (BOC) groups to weaken the amidic bond stability and thus increase its reactivity in transamidation reactions. This strategy is known in small molecule chemistry, but has yet to be applied to polymer chemistry. First, we synthesized a highly activated monomer from commercially available acrylamide, and polymerized it to form a polymer with weakened amidic resonance. This polymer was then tested in individual transamidation reactions with a variety of amines that range in nucleophilicity. The resulting polymers were characterized by ¹H-NMR, ¹³C-NMR, SEC, TGA, and DSC. Overall, we observed that, because of the weakened amide bond, these reactions successfully produced their respective, transamidated polymer products with full conversion in mild conditions. This method of transamidation provides a more accessible route for generating polymers that would be otherwise difficult or impossible to generate through radical polymerization alone. Thus, this strategy opens the door to the synthesis of unique and novel acrylamide-based polymers with an extensive variety of functional uses, real-world application, and further potential benefits in materials such as copolymers, block polymers, and hydrogels.

38. Abby Hilker

Dyeing to Degrade: A Bioplastics Experiment

Advisor: Jane Wissinger

Sponsoring Program: Center for Sustainable Polymers

Home Institution: Ripon College

Abstract: Polymers are extremely prevalent in society today, however most are made out of non-renewable and non-degradable materials leading to the depletion of natural resources and accumulation of harmful waste. Due to their widespread impact, it is important to bring the concept of polymers into high school and undergraduate chemistry courses. Many students do not have previous knowledge of polymers, so experiments, like the one presented in this work, introduce chemistry students to polymeric structures and properties. Students synthesize and then study the degradation of three different polymer samples made from a combination of citric acid, tapioca starch, and glycerol, all common, plant-based materials. Improvements have

been made over a previous version of this experiment to the composition of the polymers, the method of synthesis, and the use of dye for degradation to optimize material quality and degradation reproducibility. This exercise allows students to learn about the characteristics and lifecycle of polymers as well as other general chemistry principles like reaction order and Beer's Law.

39. Marc Ho

Using Deep-Learning for Fault Detection in Robotic Systems

Advisor: Junaed Sattar

Sponsoring Program: Computer Science

Home Institution: University of Minnesota - Twin Cities

Abstract: Autonomous robotic systems are susceptible to malfunction due to component failure, leaving the robot in operable condition but producing flawed behavior. Such failure modes are difficult to detect and can lead to more severe, costlier malfunctions and breakages. This project investigates the detection of such problems by learning to differentiate between nominal and problematic behaviors using machine learning tools. To that effect, a convolutional neural network (CNN) that analyzes a robot's actions in concert with the associated sensory data has been created to allow the robot to detect malfunctions or false readings from its sensors. The network has been trained with data obtained from a ROS (Robot Operating System) Gazebo simulation of a mobile robot performing various tasks, so the network can learn what sensory data accompanies different actions. After training, the CNN is used to aid the robot in detecting failures and preventing it from taking detrimental actions when it detects a malfunction. Ideally the network will accurately detect malfunctions, but it is of equal importance that it does not detect false positives or else it simply becomes another component vulnerable to malfunctions.

40. Yun Hu

Co-culture induced discovery of antibiotic compounds from soil bacteria

Advisor: Erin Carlson

Sponsoring Program: UMN Chemistry- Lando

Home Institution: College of the Holy Cross

Abstract: Since the discovery of the first antibiotics, many pathogenic strains have evolved resistance in large part due to the overuse of these important drugs. New antibiotics are urgently needed, yet the process of discovery is slow and inefficient. Many of the most prolific producers of current antibiotic compounds, soil actinomycetes, possess a wealth of additional biosynthetic genetic potential, but the resulting products remain undiscovered due to the organism's inability to create these molecules under standard culturing conditions. We have developed a platform to elicit production of normally dormant secondary metabolite genes by co-culturing the isolated organisms with competitors. Soil samples obtained from Wisconsin were screened, and from those samples bacteria with actinomycete-like phenotypes or those that inhibited the growth of neighboring species were selected and purified. Amongst 28 isolated bacteria samples, one showed a promising zone of inhibition against *Bacillus subtilis*. Efforts are ongoing to perform comparative mass spectrometry-based analysis on the compounds isolated from this organism to identify the bioactive component.

41. Mitsuo Inukai

High modulus and Conductivity Polymer Electrolyte Membranes

Advisor: Timothy Lodge

Sponsoring Program: MRSEC

Home Institution: University of Texas Rio Grande Valley

Abstract: Polymer electrolyte membranes (PEMs) with mechanical robustness and high ionic conductivity at room temperature are vital components of next-generation lithium-ion batteries. PEMs were produced via polymerization-induced microphase separation (PIMS) facilitating long-range continuous conducting nanochannels, and a cross-linked mechanical phase. The design of PEMs involves the growth of cross-linked polystyrene phase off poly[oligo(ethylene glycol) methy ether acrylate] (POEGA). During the reaction, lithium salt, lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), and succinonitrile (SN), a plasticizer partitions to the POEGA phase to form the conducting domain, while a glassy polystyrene (PS) phase provides the mechanical stability to the PEMs. The addition of SN as a plasticizer increases the ionic conductivity and permits the miscibility of styrene/divinylbenzene monomers with POEGA and lithium salt. The current work will utilize POEGA at various molecular weights, variations concentrations of lithium salt and SN to simultaneously optimize the ionic conductivity and mechanical properties. The resultant PIMS PEMs will be tested and measured for its ion

conductivity at different temperatures using an AC impedance spectroscopy, mechanical properties by a tensile bar loaded to obtain elastic tensile modulus at different temperature ranges, observe morphology by small-angle x-ray scattering(SAXS) imaging & transmission electron microscopy (TEM), and its thermal stability using a thermogravimetric analysis under nitrogen atmosphere. The system developed will help in the understanding and advancement of Lithium-ion batteries.

- 42. Ariya Ishida**, Xin Chen, Philippe Bühlmann
Synthesis of a phenanthroline dicarboxylate ionophore for the development of a zinc (II) ion-selective electrode
Advisor: Philippe Bühlmann
Sponsoring Program: UMN Chemistry- Lando
Home Institution: Hamline University
Abstract: Zinc (II) selective electrodes for the detection of zinc (II) ions in aqueous samples are a promising tool for clinical and soil testing as well as toxicology. Zinc (II) selective electrodes may be used to accurately determine patients' levels of zinc deficiency, which can cause a variety of negative health effects because of zinc's participation in chemical catalysis and its key role in maintaining the structure and stability of proteins.^{1, 2} These electrodes may also be helpful in testing for nutritional deficiencies in soil which can stunt the growth of crops such as wheat.³ To develop a zinc (II) selective electrode, the potential zinc ionophore, dioctyl 1,10-phenanthroline-2,9-dicarboxylate, was synthesized with the intention of incorporating it into an ion-selective membrane within the sensor. A Steglich esterification of 1,10-phenanthroline-2,9-dicarboxylic acid was performed using excess alcohol, followed by a standard work up. To remove excess alcohol and isolate a pure sample of the ionophore, solvent systems including tetrahydrofuran/hexane, methylene chloride, and 1,2-dichloroethane were tested for their ability to isolate the desired diester. In addition, the same reaction was performed using excess acid, with alcohol as the limiting reagent in anhydrous conditions. Proton NMR was used to monitor the progress of the reaction and confirm isolation of the diester. This pure diester product will be incorporated into a sensor to test its selectivity for zinc (II) ions.
- 43. Anaa Jibicho**, Matt Huisenga, John Rosenow
A Diels-Alder Competition Study Utilizing 1-methyl-2-(1-(1-methyl-1H-imidazol-2-yl)viny)-1H-indole and N-phenylmaleimide
Advisor: Wayland Noland
Sponsoring Program: Project SEED
Home Institution: Washington Technology Magnet High School, St Paul Public Schools
Abstract: Diels-Alder adducts from 2-vinylheterocycles are well known in literature. The Diels-Alder reaction is a useful tool for annulated ring formation in organic chemistry. Less is known about Diels-Alder adducts from 2,2'-vinylidiheterocycles, which have conjugated systems where multiple Diels-Alder reaction sites are present, both inter- and intramolecularly. This study involves the synthesis of 1-methyl-2-(1-(1-methyl-1H-imidazol-2-yl)viny)-1H-indole to be used as diene with multiple Diels-Alder reaction sites. The diene will be used in a Diels-Alder reaction with N-phenylmaleimide to determine the favored Diels-Alder adduct. My results will be compared with other 2,2'-vinylidiheterocycles under the same conditions.
- 44. Samuel Johnson**
Growth of Single to Few Layer Black Phosphorus
Advisor: James Johns
Sponsoring Program: MRSEC
Home Institution: Louisiana Tech University
Abstract: Black phosphorous is a Van der Waals material and an allotrope of phosphorous with properties useful for electronics, including a layer dependent band gap, a high charge mobility, and chemical stability. One of the problems with black phosphorous is that all known techniques to manufacture few layer black phosphorus are "top down" approaches, including exfoliation of bulk black phosphorous. The limitations of exfoliation are that the orientation of an exfoliated black phosphorous grain is random, the thickness of the exfoliated film is not consistent or controllable, and the size of the film created is limited. We attempted two methods to grow few layer black phosphorus in a more useful bottom up approach. The first method included sublimating bulk black phosphorous in a physical vapor transport furnace and depositing the vapor downstream. The second method was to raise the temperature of molten tin with black phosphorus, which was inspired by a growth mechanism hypothesis stating that phosphorous and tin form a eutectic alloy at high temperatures, and then, as the mixture cools, black phosphorous precipitates out of this alloy.

45. Zane Joiner

The Importance of Field of View in Increasing the Effectiveness of Augmented Reality

Advisor: Victoria Interrante

Sponsoring Program: Computer Science

Home Institution: Beloit College

Abstract: The Microsoft HoloLens is an augmented reality (AR) head-mounted-display (HMD) with many potential applications in education, entertainment, and medicine. HMDs have several advantages over 2D displays in how they present information and how this information can be used more effectively. For example, during pacemaker surgery key information is placed on monitors that the surgeon may not be able to view easily from every angle. An application was designed to overlay key information onto the HMD to counteract this. However, the limited Field of View (FOV) reduces the effectiveness of this application and the effectiveness of HMDs in general. Part of the benefit of HMDs is the reduced drop-off in awareness of off screen elements compared to traditional 2D displays. A task was designed where a subject would stand in the center of a virtual set of objects arranged at cardinal positions around them, and would be tested on their awareness of objects outside of their FOV. Under one condition the subject would wear the HoloLens with the external world visible, and under another the subject would wear a VR HMD with the FOV restricted to the FOV of the HoloLens, with the real world not visible. Theoretically the real world visible through subject's peripheral vision may overwrite the virtual objects around the person, and they should demonstrate decreased awareness as compared to the VR HMD condition. Our goal is to demonstrate the need for larger FOVs on Mixed Reality HMDs to guide future development.

46. Isobel Jones, Jake Brutman, Sebla Onbulak

Synthesis and Crosslinking of Carboxy-Telechelic Polyolefins

Advisor: Marc Hillmyer,

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota

Abstract: Vitrimers are polymeric networks that present the possibility of replacing thermosets, which have desirable material properties but cannot be reprocessed or recycled without sacrificing their physical integrity. Crosslinks between polymer chains in a vitrimer can undergo exchange reactions at elevated temperatures allowing the material to flow without permanently damaging the material. In this work, a new polyethylene based vitrimer was prepared and its stress relaxation was studied. A carboxy-telechelic polyolefin was synthesized by ring-opening metathesis polymerization of an ethyl-substituted cyclooctene followed by hydrogenation of the olefinic groups in the polymer backbone. The synthesized polymer was then cross-linked with a triglycidic isocyanurate to form an insoluble network. Cross-linked films were able to relax stress, suggesting that dynamic chemical bonds were present between the polyethylene chains and exchange reactions occurred by transesterification between the end groups and the crosslink junctions. Further studies will be carried out to fully understand the mechanical properties of this material and to test its reprocessability. Future work will include mechanical testing on existing materials, preparing films with variable crosslink density, and characterizing reprocessed samples.

47. Elizabeth Juarez Diaz

Synthesis and Characterization of Two-Dimensional SnS Nanoparticles

Advisor: John Dwyer

Sponsoring Program: MRSEC

Home Institution: St. Catherine University

Abstract: Layered metal chalcogenides are emerging as two-dimensional (2D) materials with a wide range of electronic, optical, chemical, mechanical and catalytic properties dependent on thickness. Like graphene, tin sulfide (SnS) may be separated to form single or few layer nanosheets. SnS is promising because of its high theoretical efficiency at converting light into energy of (24%, comparable to silicon), abundance in nature, and non-toxicity. The overall goal for this research was to synthesize high purity single or few layer tin monosulfide via a green hydrothermal synthesis. Specifically, we discuss strategies to control growth of single or few layer nanosheets with large lateral dimensions (> 1 micron). Three different variables were tested when optimizing the synthesis; reaction solvent, reaction time, and sonication conditions for exfoliating many layer SnS. The resulting nanosheets were characterized by XRD, SEM, AFM, TEM, Raman, and UV-visible spectroscopy. Synthesis in water was observed to yield large (several micron) nanoplates with an abundant side product of tin oxide. Synthesis in ethylene glycol as the solvent was observed to create flower-like nanoflowers with very different morphologies than

water, and without any tin oxide side product. The time dependence observation was that the growth of the nanoparticles in both water and ethylene glycol did not affect basic morphologies but rather resulted in a gradual evolution of size. Sonication followed by centrifugation was successful in exfoliating the nanoparticles into large (> 1 micron) single and few layer nanosheets. These findings suggest that these methods may provide a scalable and green means for producing 2-D SnS.

48. Raksha Kandel

A better characterization of the chemistries of gold nanoparticles: a step towards novel antimicrobial agents.

Advisor: Valerie Pierre

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Carleton College

Abstract: Antibiotic-resistant bacteria cause at least 2 million infections which leads to over 23,000 deaths in the United States each year. It is thus imperative that we come up with new antibiotic classes. Siderophore-decorated gold nanoparticles could potentially be used as a novel intravenous systemic antibiotic or laser-mediated thermal ablation. Siderophores are low molecular weight virulence factors produced by bacteria to facilitate iron uptake. Enterobactin, a siderophore which is produced and recognized by most Enterobacteriaceae, can be used to provide specificity to bacteria; however, there are no available sites to attach antimicrobial moieties. Fortunately, the trilactone backbone of enterobactin is not necessary for its recognition by the outer membrane receptor FepA and can be replaced with different molecular scaffolds with attachment sites to conjugate it to gold nanoparticles. One of the current problems with this project is that there is no good way to quantify the number of siderophore mimics attached to gold nanoparticles. The most common method is bulk analysis, which is not very useful in understanding the complete distribution since it only reports an average. My goal over the summer has been to synthesize a similar platform to perform the quantification using single event analysis via mass cytometry. I have been working on the synthesis of lanthanide-chelating siderophore mimics because lanthanides have molecular weight that falls within the analytical range of mass cytometer. After completing the synthesis, I will conjugate them to gold nanoparticles, perform metallation using Terbium and then perform the analysis using mass cytometry.

49. Alexander Kautz

A Cultural Heritage Oriented User Interface for Image-based Relighting

Advisor: Gary Meyer

Sponsoring Program: Computer Science

Home Institution: University of Rochester NY

Abstract: A new user interface is being developed for IBRelight, a tool for graphics research in the area of image-based rendering. In image-based rendering, a collection of photographs of an object are converted into a three-dimensional rendering of the object. IBRelight takes this further, using flash photographs to render the optical properties of the object by creating an unstructured lumigraph. This has applications for cultural heritage, such as archiving items at the Minneapolis Institute of Art. Unfortunately, IBRelight's current interface is research-oriented. As result, it is crowded, complex, and unintuitive for new users. A new interface oriented towards cultural heritage fixes these problems. It allows a user to easily define and save cameras, lights, and environment maps. In addition, projects in IBRelight can be exported into an all-inclusive archive file, allowing the transfer of a full rendering of an object and its configurations. In the future, IBRelight will also allow users to animate both lights and cameras.

50. Alexandra Khlyustova

Collective motion of athermal active ellipses

Advisor: Xiang Cheng

Sponsoring Program: UROP

Home Institution: University of Minnesota-Twin Cities

Abstract: One of the newly developed fields in Physics is Soft Matter Physics that studies colloidal suspensions, polymers and Active Matter. Active Matter includes a large variety of living creatures: birds, fish, bacteria and others. The most studied topic in Active Matter is collective motion and trafficking. The physicists were working on trying to find specific patterns in the motion of living systems and explain it. So far, there were many different explanations to the collective motion. For example, some scientists tried to explain the motion by applying the equation of the state into the collective motion, but the system did not fit into any equation,

which meant the system was out of the equilibrium. Therefore, there is still no certain answer that explains the collective motion. In my research this summer, I tried to model the collective motion of the living systems by designing my own particles that have an elliptical shape and I used "hex bug" robots as a source of motion for them. The reason why I chose ellipses was that they had asymmetrical shape, which was not highly explored, yet. After creating a video of moving particles, I used numerical methods to analyze their motion. Specifically, I focused on studying how their density and orientation changed over time.

51. Katherine Kidder

Optimization of Transition State Geometries using Multiconfiguration Pair-Density Functional Theory

Advisor: Laura Gagliardi

Sponsoring Program: CTC/ICDC Summer Undergraduate Research Fellowship

Home Institution: Franklin & Marshall College

Abstract: The accurate determination of barrier heights for chemical reactions is very important for many areas of chemistry, including catalysis. Quantum computational methods are often used to study these areas of interest, but to obtain good results, one must use methodologies that are able to obtain accurate transition state structures and accurate energies. This is often difficult due to strong electron correlation near the transition state which requires the use of multireference methods. In this work, we examine the performance of multiconfiguration pair-density functional theory (MC-PDFT), a recently developed method which combines multireference wave function theory with a relatively new type of density functional. MC-PDFT has previously been shown to have lower time and memory costs but similar accuracy to complete active space second order perturbation theory (CASPT2). Seven reactions were studied, and the MC-PDFT and CASPT2 results were benchmarked against coupled-cluster results from literature. We also discuss the ongoing implementation of analytic gradients in MC-PDFT which allows for much faster determination of transition state and equilibrium structures.

52. Cecelia Kinane

The Effects of Morphology on the Luminescent Properties of Upconverting Lanthanide Doped Phosphors

Advisor: Dr. J. Thomas Ippoliti, Dr. Brittany Nelson-Cheeseman

Sponsoring Program: University of St Thomas- Chemistry

Home Institution: University of St. Thomas

Abstract: The effects of varying the flux on the luminescent properties of $Y_2O_2S:Yb,Er$, $Y_2O_2S:Yb,Ho$, $Y_2O_2S:Yb,Tm$ materials are being investigated. These materials are upconverting phosphors. When excited with 980 nm near-IR laser, these materials give off either red, green, or blue light depending on the dopant. The goal is to determine how morphology effects upconversion efficiency and emission brightness. The flux used include Na_2SO_4 , Li_2SO_4 , K_3PO_4 , K_2O_3 , Li_2O_3 , Li_3PO_4 , Na_2CO_3 , in a variety of combinations. A total of 81 materials were made by varying the flux and the dopants. It is found that certain flux effect different emission colors more significantly than others. The material will also be characterized by X-Ray Diffraction, particle sizing, fluorescence spectroscopy, and fluorescence lifetime.

53. Kaitlin Landy, Joseph Buchman, Wade Elmer

Synthesis of Mesoporous Silica Nanoparticles used to Increase Growth and Disease-Fighting Ability in Watermelon

Advisor: Christy Haynes

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota

Abstract: Fusarium wilt of watermelon, a disease caused by the fungus *Fusarium oxysporum*, can cause up to 100% losses in fields that do not use resistant cultivars. In this study, mesoporous silica nanoparticles containing ordered cylindrical pore structures were synthesized and characterized to investigate the potential for these nanoparticles to increase growth and ability to fight disease in watermelon plants exposed to *Fusarium oxysporum*. ~42 nm mesoporous silica nanoparticles functionalized with FITC/APTES for imaging were first synthesized and characterized with transmission electron microscopy, dynamic light scattering, zeta potential, and nitrogen adsorption desorption analysis. Two batches of nanoparticles were sent to collaborators at the Connecticut Agricultural Experiment Station for use in plant studies, while two became aggregated as confirmed by higher hydrodynamic diameters observed with dynamic light scattering and could not be used. To investigate the impact of nanoparticle size on uptake in and growth of watermelon plants, mesoporous silica nanoparticles were also synthesized at

diameters of 20, 35, and 50 nm with and without functionalization with FITC/APTES. All six batches were used in watermelon growth experiments where seedlings were treated with the nanoparticles and eventually transplanted into field plots, where half were inoculated with *Fusarium oxysporum*.

54. Gemma Lein-McDonough

Exploring Provisions of Instrumental Support in Online Health Communities

Advisor: Svetlana Yarosh

Sponsoring Program: Computer Science

Home Institution: Simmons College

Abstract: For patients and families grappling with serious medical conditions, online health communities have become a prominent mechanism for exchanging social support. However, these platforms are not well-designed to facilitate offline services or needs, i.e. "instrumental support". Recently, sharing economy platforms such as Uber, Airbnb, and TaskRabbit have emerged to provide users with new means of conveniently providing and receiving services. A wealth of research has begun to explore trust and utilization of these platforms, yet little work has been done to integrate sharing economy functionalities in an online health community context. For this research, we are collaborating with CaringBridge, an established online health community for writing about personal health experiences. We explore how users currently seek and provide instrumental support with inductive coding and machine learning methods. First, we developed a coding scheme for categorizing journal updates by author and for explicit help exchanges. A preliminary analysis of 200 journal update samples has shown discussions of help activities to be a significant theme of the CaringBridge journaling experience; food, transportation, and prayers are examples of some commonly expressed needs. Next, we propose a classifier for identifying journal update authors as patients or caregivers in order to distinguish who is asking for help. Finally, we will use machine learning methods to automatically classify journal updates for explicit help received. These results will be used to provide design implications for implementing sharing economy functionalities in online health communities.

55. Biniam Lemma

Improving Bitcoin Simulator to Better Analyze Future Instability

Advisor: Nicholas Hopper

Sponsoring Program: Computer Science

Home Institution: Century College

Abstract: It is important to provide a mining simulator that can quantitatively be able to test the effects of various attacks on Bitcoin. Bitcoin uses a public ledger called blockchain that records and verifies all Bitcoin transactions. Individuals called miners verify the Bitcoin activity approximately every 10 minutes by creating a block of transactions and performing a computationally expensive task using a hash function to add the block to the ledger. Block reward and transaction fees are rewarded to miners for their contribution. The creator of Bitcoin set the block reward to halve every 210,000 blocks, which is approximately every four years. Transaction fees are paid by the size of the transactions in the block. As the block reward diminishes to zero, it is expected that the transaction fees will increase. Previous work shows that when the transaction fee becomes the vast majority of the mining revenue, miners will start to deviate from the normal behavior. This action of deviation will cause instability to the network. For a purpose of keeping the blockchain secure and advancing warning against the attacks on Bitcoin's future, we modified a Bitcoin mining simulator. The original simulator assumes miners always to have a space to include all available transactions in their block. However, the actual Bitcoin block size is limited. We limited the the number of the transactions that could be included in the block. This way the simulation better aligns to the actual Bitcoin, and we can get better quantitative results on the prediction of the future instability of the Bitcoin.

56. Diana Luc

Integrating Sensors of a Wind Turbine Test Platform to a Data Acquisition System

Advisor: Kim Stelson

Sponsoring Program: CCEFP

Home Institution: Macalester College

Abstract: At the University of Minnesota, a 100 kW power regenerative wind turbine test platform has been built to understand the performance of a hydrostatic transmission in a wind turbine. The test platform contains 27 sensors. These sensors are used for real-time measurements to monitor the performance. Integration of all sensors for the data acquisition (DAQ) system with a breadboard have proven to be difficult. The signals from all the sensors are converted to voltage

signals for the DAQ. During this period, a cleaner circuit has been designed. A handmade printed circuit board has been developed to integrate all sensors. A cleaner, simpler wire layout has been suggested to improve readability and avoid ground loops. The current design is more robust, reliable, organized and easier to troubleshoot if problems arise.

57. Sofia Maltseva

Synthesis of fluorinated amino acids for study of peptides by ^{19}F NMR

Advisor: William Pomerantz

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota, Twin Cities

Abstract: ^{19}F MRI poses a significant advantage over ^1H MRI in the detection and identification of fluorinated species within a biological system where high concentrations of water impede analysis through ^1H MRI. These advantages extend its application into chemical biology and medicinal chemistry, as the presence of fluorine can aid in monitoring a drug's distribution or function within the body where the natural abundance of fluorine is low. However, the method is highly sensitive to the varying environments of each of the fluorine atoms—leading to peak resolution and thus a lower signal to noise ratio. Therefore, in order to detect the presence of fluorine, the concentration of the atoms in similar environments must be high. Here we show that peptides containing alternating residues of trifluorinated amino acids with the positively charged lysine prevents a secondary structure of the amino acid, while retaining its water solubility, leading to a single ^{19}F NMR resonance. We also extend the hypothesis to show the synthesis and incorporation of nonfluorinated cysteine residues into a similar peptide. These results demonstrate the potential for the use of similar peptides for the detection of fluorinated species in target molecules within biological systems through ^{19}F MRI.

58. Cedric Mannie

Optimization of parameters for Zinc Oxide thin film synthesis for semiconductor application

Advisor: Sarah Swisher

Sponsoring Program: MRSEC

Home Institution: Utah State University

Abstract: ZnO thin films has potential as a multifunctional material to applied in PH sensors, surface acoustic wave devices, optical waveguides, solar cells, biosensors, etc. ZnO can be manufactured utilizing low-cost wet processing methods that include electrochemical, chemical bath, and sol-gel spin coating practices. The solution based deposition processes provides a cheap and basic production route for depositing ZnO layers because there is no need for vapor deposition equipment. Although the sol-gel method is a simple technique, many factors affect the quality of the ZnO film such as precursor concentration, pre-heating temperature, sol aging temperature, coating speed, etc. The effects of 'precursor concentration, sol-aging time, and spin speed will be examined for their effects on film quality. Characterizations will include XPS to clarify chemical composition, UV visible transmission spectroscopy to determine film absorption, XRD to examine crystallinity. Due to stabilization of the solution as the sol ages, it is expected to see Zinc oxide increase compared to Zinc Hydroxide. The average thickness of films decreases with increases in spinning speed.

59. Jarrett Mansergh

Recycling Phosphate using Gadolinium Metal Complexes

Advisor: Valerie Pierre

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota-Twin Cities

Abstract: Phosphate is essential to the function and growth of organisms, including plants. For this reason, phosphate rock is universally used in fertilizers and is critical to maintaining the food supply of our world. However, the runoff from this fertilizer causes excess amounts of phosphate nutrients to accumulate in waterways. This results in algal blooms that block the sun from entering the water and decreases the oxygen level available for aquatic life. Additionally, the overabundance of certain algae creates toxins harmful to humans and vertebrates. The environmental cost of phosphate pollution in the US exceeds \$2 billion annually. On the other hand, the world supply of phosphate rock is diminishing rapidly, thus phosphate rock is increasing in price. These problems create the need to find and capture the excess phosphate in waterways in such a way that it can be recycled as fertilizer. With the goal of solving this problem, we are synthesizing and testing a library of lanthanide complexes for a simple recycling process. Through competition and pH studies, the selectivity for phosphate and the capability of releasing the anion at low pH of these metal complexes are evaluated. Beyond creating novel

technology for the environmental remediation of phosphate, our studies are advancing our understanding of lanthanide coordination chemistry and supramolecular recognition of anions.

60. Ahmad Matar Abed

Electronic transport behavior in BaSnO₃ and NdTiO₃ thin films grown using hybrid molecular beam epitaxy

Advisor: Bharat Jalan

Sponsoring Program: MRSEC

Home Institution: University of Puerto Rico-Humacao

Abstract: Complex oxides with perovskite structure are in the focus of research because they exhibit impressive multifunctionality such as high temperature superconductivity, colossal magnetoresistance and multiferroicity. Barium stannate (BaSnO₃) has a cubic perovskite structure with a wide band gap of ~ 3 eV and is optically transparent. Recently, it has been shown to possess high room-temperature electron mobility. This makes it an impressive material for potential room-temperature applications including transparent conductors. My research focused on the growth of epitaxial, single-crystalline BaSnO₃ films grown on various substrates using hybrid molecular beam epitaxy (MBE) approach. Films were characterized using x-ray diffraction (XRD), grazing incidence x-ray reflection (GIXR), and atomic force microscopy (AFM). Electronic properties were measured using physical properties measurement system (PPMS) where I studied the temperature dependence of resistivity. Temperature dependent data was analyzed to study the governing transport mechanisms at different temperatures for stoichiometric as well as non-stoichiometric films. Furthermore, neodymium titanate (NdTiO₃) films were grown using the same hybrid MBE approach. NdTiO₃ has an orthorhombic perovskite structure and is an antiferromagnetic Mott-insulator with a Mott-Hubbard gap of 0.8 eV. Recently, it has been shown that NdTiO₃/ SrTiO₃ forms two-dimensional electron gas (2DEG) at the polar/nonpolar interface. This makes it a promising material for understanding the longstanding issues concerning the true characteristics of the polar discontinuity at oxide heterojunctions. My research focused on exploring the electrostatic gating on NdTiO₃ films. The properties were measured using PPMS.

61. Ben Matz

Synthesizing a Zwitterionic Organocatalyst

Advisor: Steven Kass

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Washington University in St. Louis

Abstract: The Kass group has worked to synthesize a series of organocatalysts based on the observation that the conversion rate of the catalyst correlates with its acidity. To enhance the acidities of these Bronsted acids, positively charged centers have been introduced into these species. One example is the pyridinium ion derived from the alkylation of 3-hydroxypyridine. Although this strategy has enhanced the reactivity of several organocatalysts, one issue is the requirement of a counteranion. Such species shield the positive charge, may influence reaction selectivity, and can hydrogen bond to the acidic site and diminish the catalyst's reactivity. Accordingly, a zwitterionic catalyst in which the counteranion is covalently linked to substrate and is remotely located from the acidic site was targeted. Progress towards its synthesis is reported.

62. Eleanor Mayes

Synthesis of 7-Oxanorbornene Monomers and their Subsequent Polymerizations via ROMP

Advisor: Thomas Hoye

Sponsoring Program: Center for Sustainable Polymers

Home Institution: The University of Chicago

Abstract: Renewable feedstock sources for monomers are crucial in creating sustainable and degradable polymers. Previously 7-oxanorbornene derived monomers had been proposed via a Diels-Alder reaction of itaconic anhydride (as the dienophile) and furfural alcohol (as the diene.) Both compounds are abundant in biomass. Producing furfurylamine derivatives via reductive amination of this biomass-obtained furfural with primary amines results in further functionalization of the monomer. However the Diels-Alder reaction of furfurylamines with itaconic anhydride does not reach completion and intramolecular Diels-Alder does not happen. It was found that maleic anhydride as the dienophile produced a more favorable equilibrium in this reaction; towards that of the Diels-Alder product at room temperature, thus aiding the synthesis of monomers in this experiment. Our goal is to produce polymeric materials from these bio-derived

feedstocks: Diels–Alder reactions with maleic anhydride produced 7-oxanorbornene derivatives that were polymerized through ring opening metathesis polymerization (ROMP), initiated by a Grubbs 3rd generation catalyst. A variety of polymeric and oligomeric materials with high glass transition temperatures were produced based on this reaction; different substitutions of the amine resulted in a range of molecular weights and T_g.

63. Patrick McCauley

Effects of pH on Bentonite-Humic Acid Flocculation

Advisor: Cari Dutcher

Sponsoring Program: MRSEC

Home Institution: University of Michigan

Abstract: Polymer flocculation is commonly utilized to remove colloidal particulates in solution. Flocculation (floc) performance depends on several solution properties such as pH, ionic strength, and natural organic material (NOM) content. Traditional flocculation experiments, known as jar tests, were conducted at pH levels of 3 to 11 and a range of polymer dosages to determine the flocculation efficiency by measuring turbidity. Internal floc structure was characterized using laser confocal microscopy. Fluorescently-tagged polymer flocs were imaged with laser confocal microscopy to determine internal floc structure. Not only does bentonite aggregate morphology change as a function of pH, but also humic acid charge density changes, which impacts the flocculation behavior. Flocculation performance of the bentonite-humic acid system differs strikingly from the bentonite only system. Competitive flocculation of bentonite and humic acid worsens flocculation performance with increasing solution pH.

64. Edgar Mejia, Jon Nath, Brett Neubauer

“Emulating a Plastic Ankle-Foot Orthosis with a Hydraulic Ankle-Foot Orthosis”

Advisor: Will Durfee

Sponsoring Program: CCEFP

Home Institution: University of California, Merced

Abstract: People with cerebral palsy live most of their life using passive ankle-foot orthosis (AFO) to support their ankles since they have weakened muscle coordination. The methods currently used to prescribe passive AFO products to a disabled patient are time consuming, often taking several hours and multiple clinic visits. The purpose of this project is to create a hydraulic AFO that can emulate the stiffness of any passive AFO, thus, allowing the patient to experience a variety of stiffness's within a single apparatus. At the current final stages of this project, the validation and performance testing of the hydraulic AFO was accomplished using a Bi-articular Reciprocating Universal Compliance Estimator (BRUCE). Data acquisition hardware along with National Instruments Data Acquisition (DAQ) software was used to record data, and it was analyzed through another computer software to determine stiffness coefficients. After the first set of tests, due to parts within the HAFO that added elasticity, it was determined that a calibration factor of had to be added to the input stiffness within the Arduino Encoder script. A test consisting of 65 trials with input stiffness ranging from (1-4 Nm/degree) was performed on the hydraulic AFO. After comparing the averaged output stiffness coefficients with the input stiffness coefficients, an overall variation of 2.84% was calculated. A confidence interval of 0.124 was calculated as well, altogether demonstrating that the hydraulic AFO can successfully emulate the stiffness of any passive AFO.

65. Sam Merlus

Nanotoxicity Evaluation Of Doped Silicon Nanocrystals

Advisor: Christy Haynes

Sponsoring Program: MRSEC

Home Institution: Tuskegee University

Abstract: Doped silicon nanocrystals (DSNCs) have demonstrated their biocompatibility and various applications compared to their alternatives quantum dots containing heavy metal content, and have drawn the attention of researchers as a result of its potential application in sensing, bio imaging, and energy conversion. *Shewanella oneidensis* MR-1 (*S. oneidensis* MR-1) is commonly used as the model microorganism in studying the nanomaterial toxicity of silver nanoparticles (Ag NPs), gold nanoparticle (Au NPs), and Li-ion battery materials. We synthesized NCs doped in boron and phosphorus of various concentration attempting to assess the bacterial toxicity in *S. oneidensis* MR-1. The bacterial toxicity was determined using the colony counting assay (drop plate method) which includes a 10-fold serial dilution to assess toxicity using quantitative analysis.

66. **Akshay Naik**, Dr. James Flaten, Garrett Ailts, Jordan Diers, Kate Kwiecinski
Tracking National Eclipse Progression with High Altitude Ballooning
Advisor: James Flaten
Sponsoring Program: NASA MN Space Grant Consortium
Home Institution: University of Minnesota, Twin Cities
Abstract: A total solar eclipse is a rare phenomenon that occurs approximately every 18 months. On August 21st, 2017, a total solar eclipse will be visible from various locations within North America. The Minnesota Space Grant Consortium is conducting a ballooning project that will allow the public to see this rare phenomenon from 100,000 feet up into the air. The first purpose of this project is to live stream the eclipse from high altitude. The second purpose is to provide near-real-time footage of the moon's shadow on Earth and the darkened sun. The balloons that will be sent into the stratosphere will have various payloads attached to collect various sets of data points including temperature, pressure, altitude, and longitude-latitude. In conclusion, this project will be opening doors for possibilities of live streaming other natural phenomena that can be observed at stratospheric altitudes.
67. **Dominic Najjar**, Arnold Groehler IV, Suresh Pujari
Synthesis and Characterization of 1,2,3,4-diepoxybutane and 3,4-Epoxy-1-butene N5-alkyl-Formamidopyrimidine Adducts
Advisor: Natalia Tretyakova
Sponsoring Program: UMN Chemistry- Heisig Gleysteen
Home Institution: University of Minnesota
Abstract: 1,3-butadiene (BD) is a known carcinogen found in cigarette smoke, automobile exhaust, and wood burning fumes. BD is bioactivated by cytochrome p450 monooxygenases in the liver to reactive epoxide metabolites, 1,2,3,4-diepoxybutane (DEB), 3,4-Epoxy-1-butene (EB), and 1,2-dihydroxy-3,4-epoxybutane (EBD). These metabolites are all capable of alkylating nucleophilic positions on DNA. The major adducts form at the N7 position of guanine, which in the presence of base can undergo imidazole ring opening to the corresponding EB-formamidopyrimidine (FAPy) adducts. However, EB-FAPy adducts have not been previously reported. We hypothesized that the C8 position of EB-Guanine (EB-Gua) I and EB-Gua II can be attacked by hydroxide anions at to ultimately generate Fapy-dG adducts. Previously characterized Aflatoxin B1 (AFB1)-FAPy adducts have been proven to be mutagenic. By analogy, it is conceivable that FAPy adducts formed after exposure to BD could yield comparable effects as those previously studied and warrants further investigation. In our study, authentic standards of EB-FAPy were synthesized for structural characterization via mass spectrometry and NMR. We have begun to investigate EB-FAPy in vitro and in formation in cells using mouse embryonic fibroblasts deficient base excision repair enzyme, Neil 1. Additionally, the synthesized standards are currently being used to develop a sensitive liquid chromatography-tandem mass spectrometry assay to detect EB-FAPy adducts in cells and tissues.
68. **Maria Neuzil**
Solid-State Studies of Benzonitrile Oxides and their Dimers: Crystal Structure of a 1,2,4-Oxadiazole
Advisor: William Ojala
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Benzonitrile oxides (Ar-C-N+-O- where Ar = Aryl) are known to be useful in solution-phase reactions, but their solid-state chemistry has been understudied. We are crystallographically examining benzonitrile oxides and their three possible solution-phase dimers to determine whether different polymorphs of a given nitrile oxide yield different solid-state dimers. Our studies of a variety of benzonitrile oxides by infrared spectroscopy demonstrate that we can reliably synthesize reactive benzonitrile oxides and can monitor their solid-state dimerization. While examining selected dimers, we have now determined the crystal structure of a compound that we unexpectedly obtained while attempting to prepare and crystallize one of the dimers of 4-nitrobenzonitrile oxide, the bis(4-nitrophenyl)-1,2,4-oxadiazole-N-oxide, by solution-phase dimerization of the benzonitrile oxide in the presence of a catalytic amount of triethylamine. The compound actually obtained has proved to be simply the bis(4-nitrophenyl)-1,2,4-oxadiazole. Previous workers have determined that this deoxygenated product can form upon reaction of the initially formed oxadiazole N-oxide with the reactant benzonitrile oxide. The crystal structure is disordered, with molecules occupying two positions about crystallographic twofold axes. Our ongoing work will include obtaining a complete set of crystal structures for the parent benzonitrile oxides and their dimers in the 2-nitro-, 3-nitro-, 4-nitro-, and 2-chlorobenzonitrile oxide series.

69. **Mikayla Newby**
Synthesis of precursor salt, 1,3(Bis)-picolyl benzimidazolium bromide, and coordination with lanthanum(III) ion
Advisor: Marites Guino-o
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Lanthanide based luminescent materials have many applications, ranging from medical equipment to anti-counterfeit usages. However, their luminescence are weak because the transition is parity forbidden. To increase luminescence, a ligand is needed for the "antenna effect", in which the ligand acts as an antenna to absorb light and transfer the energy to the lanthanide(III) ion. The ligand also helps prevent quenching. In our group, we aim to explore an N-heterocyclic carbene's (NHC's) ability as an "antenna" to lanthanide(III) ions. Herein we report our preliminary results in the synthesis of the NHC precursor, 1,3(Bis)-picolyl benzimidazolium bromide, and the in-situ formation of NHC and its coordination with the lanthanum(III) ion as tracked by ¹H NMR spectroscopy. Our results reflected that the synthesis of the NHC precursor was successful, as well as the coordination with the lanthanide(III) ion.
70. **Huan (Kyle) Nguyen**
Optimizing the Loading of Perfluorocarbons in Ultraporous Mesostructured Silica Nanoparticles for Oxygen Sensing
Advisor: Christy Haynes
Sponsoring Program: UMN Chemistry- Lando
Home Institution: The College of Wooster
Abstract: Oxygen homeostasis is essential to the functions and vitalities of biological organisms. Thus, in situ oxygen sensing is important for clinical diagnoses. Such measurements, which are necessarily highly sensitive and noninvasive, can be accomplished by ¹⁹F-fluorine magnetic resonance imaging (¹⁹F MRI) that utilizes perfluorocarbons as sensing molecules. Since perfluorocarbons possess strong hydrophobicity and lipophobicity that prevent effective dispersibility in biological systems. Previous work has shown ultraporous mesostructured silica nanoparticles (UMNs) are able to encapsulate perfluorocarbons and disperse in aqueous media for ¹⁹F MRI-based oxygen sensing. However, perfluorocarbon-loaded UMNs (PERFUMNs) currently possess low fluorine concentrations that result in suboptimal detection, which lowers their clinical applicability. Thus, loading of perfluorocarbon needs to utilize all internal space provided by UMNs. The present work attempts to increase the loading efficiency of PERFUMNs by testing four loading parameters: pH of water, sonication time, ratios of UMN mass or volume of water to volume of perfluorocarbons. ¹⁹F nuclear magnetic resonance is used to quantify perfluorocarbons. Preliminary data have not demonstrated statistically significant results to precipitate any conclusions. More holistic results will be acquired for further analysis.
71. **Phong Nguyen**, Ben Greenberg, Jacob Held, Chad Beaudette, Eray Aydil, Uwe Kortshagen, Andre Mkhoyan
Infilling of Nanocrystal Networks Using (Plasma-Enhanced) Atomic Layer Deposition
Advisor: Andre Mkhoyan
Sponsoring Program: MRSEC
Home Institution: University of Missouri
Abstract: Development and implementation of photodetection, photovoltaic, and photocatalysis technologies in the past decades have driven demand for transparent conductive substrates to an all-time high, with indium tin-oxide (ITO) glass being the substrate of choice. Though ITO glass boasts superior conductivity and transparency with respect to alternatives, indium production is dependent on zinc-sulfide ore mining, making production of ITO glass an expensive and environmentally-taxing endeavor. In searching for viable alternatives, we demonstrate the use of atomic layer deposition (ALD) and plasma-enhanced atomic layer deposition (PEALD) in infilling porous nanocrystal networks as an efficient and cost-effective method to synthesize metamaterials with desirable electrical and optical properties. By infilling ZnO with TiN using PEALD, we achieve a conductive, plasmonic material that absorbs strongly in the infrared region of the electromagnetic spectrum, allowing for possible applications in photodetection devices, photocatalysis, and photovoltaic energy conversion. Using ALD, we infill ZnO nanocrystals sequentially with further ZnO, followed by Al₂O₃, creating a robust, highly interconnected nanocrystal network, useful for physics studies of the insulator-metal transition in such networks. By comparing uniformity of elemental distribution throughout the thin films and their capacity to achieve desired properties, we discuss the potential and the limitations of ALD

and PEALD as a nanocrystal network infilling technique.

72. Michael Nitzsche

Testing Platform for a Partial Stroke Piston Pressurization Pump/Motor

Advisor: Thomas Chase

Sponsoring Program: CCEFP

Home Institution: Rutgers University

Abstract: In previous research efforts, a design was realized for a partial stroke piston pressurization hydraulic pump/motor. This design is noteworthy because it can achieve variable displacement by changing the pressurization duty cycle of the pump rather than by varying the angle of its swashplate. Simulations suggest that this novel design represents a significant improvement in efficiency compared to similar variable displacement pump/motors, particularly at low displacement levels. Previous efforts to characterize the performance of a prototype of this pump/motor were only partially successful, as the prototype can achieve higher pressure and torque levels than the existing setup could accommodate. This project involved the development of a new testing platform to characterize the performance of the pump/motor over its entire displacement and power range. The new setup supplements the pressure supply through recirculation, enabling high pressure levels to be reached and sustained without overheating the lab's supply line. Additionally, an array of sensors including thermocouples, flowmeters, pressure transducers and torque and rotation sensors were incorporated into the setup to gather detailed data about the pump/motor's performance. A computer GUI was implemented to enable real time control and parameter visualization for the testbed.

73. Kerry Owusu

The Biosynthesis of N-acetyl-serine for Antifouling Materials

Advisor: Kechun Zhang

Sponsoring Program: Center for Sustainable Polymers

Home Institution: University of Pittsburgh

Abstract: Marine industries as well as healthcare suffer from the effects of biofouling on their products. Currently, there are antifouling products out in the market, however, these products are very expensive and/or ecologically harmful. One promising solution are zwitterionic materials, which is ecologically friendly; however, traditional chemical production is complex and expensive. Our approach is to design an artificial pathway to produce a zwitterionic monomer in *E. coli* by utilizing natural serine biosynthetic modules. We are using the principles of pathway design, metabolic engineering, and protein engineering to promote the production of the acetyl-serine monomer, which is a platform zwitterionic monomer that can be co-polymerized with other monomers like styrene to form a zwitterionic polymer. To achieve this, we will be using engineered *E. coli* as the host cell. We will then obtain plasmids that were genetically engineered to code for mutations that help promote the pathway that produces L-serine. Next, we will engineer proteins to allow L-serine to be a sufficient substrate for downstream reactions.

74. Alan Owusu-Poku

Generation of Complex Morphologies in Diblock, Copolymers via blending using Self Consistent Field Theory (SCFT)

Advisor: Kevin Dorfman, Akash Arora

Sponsoring Program: MRSEC

Home Institution: Iowa State University

Abstract: The combination of polymers to a single material can be done in different ways. These combination can lead to different phase behaviors. In recent years, Self-consistent field theory (SCFT) a powerful tool for the designing and interpretation of experiments on phase behavior of block polymer has been used to study and predict different morphologies of polymer blends. SCFT determines phase behaviors by analyzing how the configuration of a test polymer chain is affected by the presence of other chains and vice versa. In this research a numerical implementation of SCFT known as Polymer Self Consistent Field (PSCF) is used to calculate phase diagrams of block copolymer by comparing free energies of competing ordered phase. The numerical evaluation of the different phases of block copolymer directly influences the physical properties and applications of polymers.

75. **Annika Page**
Reactions of HDDA-derived benzyne with electron-deficient thioamides: Evidence for a novel [3+2] cyclization
Advisor: Thomas Hoye
Sponsoring Program: UMN Chemistry- Heisig Gleysteen
Home Institution: University of Minnesota, Twin Cities
Abstract: o-Benzyne, one of the set of reactive aryne intermediates, is a powerful intermediate in organic chemistry. Valued for their versatility and reactivity, benzyne can be trapped by a variety of organic functional groups. One such class of reactions is the hexadehydro—Diels-Alder reaction, which was developed in 2012 by the Hoye Group. This reaction of a diyne with a diynophile proceeds via a benzyne intermediate and results in substituted fused ring systems. Due to the high energetics of the benzyne intermediate, many substrates can 'trap' across the bond to create new and interesting products. One such moiety is a thioamide, the sulfur-containing analog of an amide. Previous work by the Hoye group found that aromatic thioamides trapped the benzyne to form a 6-membered thiazine ring. Here, reactions of electron-deficient thioamides were studied. We provide evidence for a novel [3+2] concerted cyclization to form a 5-membered thiazole ring. This mechanism is supported by computational studies.
76. **Adam Pancoast**, Evan Beaumier, Hunter Wilson, Jason Goodpaster, Ph.D.
Utilizing Ti Redox Catalysis for the Synthesis of Unsymmetrical Carbodiimides
Advisor: Ian Tonks, Ph.D.
Sponsoring Program: UMN Chemistry- Lando
Home Institution: Augsburg College
Abstract: Traditionally, important reactions in homogeneous catalysis use noble metals such as Pd, Pt, and Ir, among others. However, these metals tend to be very expensive, and often have extremely depleted reserves. Thus, the need for an inexpensive and abundant transition metal catalyst has increased in recent years. Previous work by the Tonks group synthesized poly-substituted pyrroles via a Ti(III)/IV redox catalytic cycle, and there are several other examples in literature of the use of Ti catalysts for C-X bond formation, where X = O or N. However, the early transition metal catalyzed formation of unsymmetrical carbodiimides is extremely limited to a few examples currently present in literature, which generally utilize very restricted conditions. In this work, we propose to synthesize unsymmetrical carbodiimides via a Ti(III)/IV catalytic coupling of p-substituted diazenes and t-butylisocyanide, as well as the catalytic coupling of sterically hindered azides to a variety of isocyanides. We aim to further prove the utility of Ti(III)/IV redox catalysis and to expand the early transition metal catalyzed formation of unsymmetrical carbodiimides.
77. **Karla Paraiso**
Effects of a Realistic Avatar on Perception and Depth in Virtual Reality
Advisor: Victoria Interrante
Sponsoring Program: Computer Science
Home Institution: Arizona State University
Abstract: Human performance in virtual environments differ from the real world, especially when making distance estimations. In past studies errors in perceptual estimations have been found to occur less when the constructed environment is more realistic (Lane Phillips and Victoria Interrante (2011) IEEE Virtual Reality). These indications have provided us inferences on how VR technology can be improved. In this experimental study, we explore the impact of the presence of a realistic avatar in an immersive virtual environment. Instead of a generated 2D image, the avatar was based on a 3D scanned model of a real person and then imported, rendered and animated in the virtual environment. The participant was presented three different, virtually constructed hallways and three different avatar renditions. The participant was then required to walk without vision to a certain array of distances (8,10,12,14 and 16 feet). Blindfolded walking is a common method used in other VR distance estimation research. The participant's recorded distances was then averaged and compared to the original array of distances where their estimation would then be analyzed if the virtual avatar had an effect. Potential applications of this research is intended to provide improvements to distance estimation in virtual environments.

- 78. Mike Patton**
Shape Anisotropy and Filament Orientation Effect on Magnetic Properties of 3D Printed Structures
Advisor: Brittany Nelson-Cheeseman
Sponsoring Program: University of St. Thomas- Materials Science and Engineering
Home Institution: University of St. Thomas
Abstract: A fused deposition modeling process (FDM) is a type of 3D printer that deposits material (typically a thermoplastic polymer) to build a part, layer by layer. Some FDM printers can print with composite filaments to make structures that have magnetic properties. A magnetic filament consisting of PLA and 40 wt.% iron was used in an FDM process to print magnetic samples. Samples of different lengths and widths were printed using two different filament print orientations (printed along the long axis vs along the short axis) and evaluated using a vibrating sample magnetometer (VSM) to determine the anisotropy and filament orientation effect on the magnetic properties. Hysteresis loops were obtained from the VSM for each sample to determine what effects these had on the magnetic response to an applied magnetic field. Each sample was measured in both the longitudinal and transverse directions and the hysteresis loops were used to compare the magnetization, magnetic moment, and susceptibility between the two directions and between each sample. The results show that the shape anisotropy of the sample has a prominent effect on the magnetic properties, whereas the orientation of the printed filament had a subtler effect. Determining the anisotropy and filament orientation effects on the magnetic properties will help better understand how an FDM process can be utilized to make applicable magnetic components.
- 79. Bethany Pertzsch, Erin Birdsall, Songlin Wang**
Preparation and Oriented-Sample Solid-State NMR Study of Sarcolipin, a Calcium ATPase Inhibitor
Advisor: Gianluigi Veglia
Sponsoring Program: UMN Chemistry- Lando
Home Institution: Dordt College
Abstract: Sarcolipin (SLN) is a 31-residue membrane protein, expressed in skeletal and cardiac muscle, that regulates muscle relaxation through inhibition of sarco(endo)plasmic reticulum calcium ATPase (SERCA). Both solution- and solid-state nuclear magnetic resonance (NMR) spectroscopy have been used in efforts to characterize SLN and its interaction with SERCA. Oriented-sample solid-state NMR relies on magnetically-aligned lipid bicelles as a membrane mimic, and thus may be used to characterize the topology of SLN. Associated with such experiments, however, are challenges regarding sample preparation and reproducibility. The requisite isotopically-labeled SLN is obtained through a multi-step process of expression, purification, and lyophilization before packing into bicelles. Recent work has succeeded in improving purification yields, quantifying protein concentration in NMR samples, and shortening experimental time. Such protocol refinement provides the foundation for future investigation of the mechanisms by which SLN and other membrane proteins regulate SERCA.
- 80. Phan Phu**
Examining the Reactivity of Mononuclear Copper (II) Superoxide Complexes Supported by Pyridinedicarboxamide Ligands as Mimics for Monooxygenase Enzymes.
Advisor: William Tolman
Sponsoring Program: UMN Chemistry- Lando
Home Institution: California State Polytechnic University, Pomona
Abstract: Copper-oxygen species are proposed to be key intermediates in oxidative transformations carried out by single copper monooxygenase systems such as peptidylglycine α -hydroxylating monooxygenase (PHM), dopamine β -monooxygenase (D β M), tyramine β -monooxygenase (T β M), and lytic polysaccharide monooxygenases (LPMOs). LPMOs garner particular interest as they activate recalcitrant C-H bonds of polysaccharides and degrade the biopolymer via an oxidative pathway. As such, understanding the mechanism and active speciation of LPMO could lead to new catalysts and a sustainable biofuel source through polysaccharide cleavage. Currently, the active Cu-oxygen species in LPMO is unknown, however many researchers have proposed that a Cu(II)-superoxide could play a pivotal role. We have synthesized a handful of Cu(II)-superoxide model complexes supported by hindered pyridinedicarboxamide ligands and characterized these small molecule mimics by UV-vis and EPR. The reactivity of these Cu-superoxide complexes was evaluated using C-H and O-H organic substrates. It was found that the superoxide species were not oxidizing enough to cleave stronger C-H

bonds, but did react with weaker O-H bonds of TEMPOH and some phenols. The reaction kinetics are presented as well. Overall, the low reactivity of the superoxide core would suggest that it is not the active oxidant in LPMO, but cannot be ruled out as a reaction intermediate.

81. Jack Queenan

Pancreatic Polymersomes: acid-sensitive nanoparticles for glucose-responsive insulin

Advisor: Lisa Prevette

Sponsoring Program: University of St Thomas- Chemistry

Home Institution: University of St. Thomas

Abstract: Diabetes Mellitus is a group of metabolic diseases wherein blood glucose levels become elevated due to a defect in the glucose-insulin response. Even with current treatment strategies, this disease is not easily controlled leading to adverse health effects and costly treatment. Thus, a "closed loop" system to treat diabetes has been the focus of recent research. This project describes the design and characterization of one such closed loop system. Amphiphilic diblock copolymers were synthesized from RAFT polymerization of 2-(((5-methyl-2-(2,4,6-trimethoxy-phenyl)-1,3-dioxan-5-yl)methoxy)carbonyl)amino)ethyl methacrylate (TTAMA) monomer with a polyethylene glycol chain transfer agent and. These polymers (PEG-b-PTTAMA) self-assemble in solution to form nanoparticles called polymersomes. Several such polymersomes were formed from PEG-b-PTTAMA copolymers of different hydrophobic block molecular weight, resulting in varied nanoparticle morphology and size. Hydrolysis of the acid-labile cyclic benzylidene acetals of the TTAMA repeat unit was monitored by spectrophotometry and resultant polymersome disassembly by dynamic light scattering. The optimized polymersomes will be loaded with insulin and the enzyme glucose oxidase, which converts available glucose to gluconic acid, to create a glucose-responsive insulin delivery system.

82. Anirudh Raghavendran

Gel Relaxation of Asymmetric Block Copolymer Micelles

Advisor: Timothy Lodge

Sponsoring Program: UROP

Home Institution: University of Minnesota

Abstract: The UROP project examines the material properties of gels of Asymmetric Block Copolymer. Rheology is used to study the relaxation of these gels on heating. Various factors that contribute to and affect relaxation time are examined.

83. Maria De La Luz Rico Mendoza

Progress towards probing BPTF binding interactions via photocrosslinking

Advisor: William Pomerantz

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Augsburg College

Abstract: High levels of the BPTF (bromodomain PHD finger transcription factor) protein are implicated in cancers such as melanoma, leukemia, colorectal and bladder cancer. Selective inhibition of bromodomains has shown potential as a therapeutic strategy to treat these diseases¹. In this study, photocrosslinking is used to probe BPTF's bromodomain interactions with a small molecule inhibitor ligand (AU1). Photocrosslinking applied in a discovery-oriented mode allows for the identification and mapping of protein-ligand interactions through mass spectroscopy analysis. Here, we report the synthesis of a BPTF specific photocrosslinker probe and our findings of BPTF's site specific interactions with the ligand.

84. Kathleen Riley

Immobilization of Earth Abundant Metals Coordinated in Heterobimetallic Ligand Scaffolds on Metal Organic Frameworks (MOFs)

Advisor: Connie Lu

Sponsoring Program: UMN Chemistry- Lando

Home Institution: Mississippi State University

Abstract: Earth abundant metals such as Co, Fe, and Mn are critical to the sustainable catalysts. Herein, we report the synthesis of bioinspired heterobimetallic FeMn and CoMn complexes, which feature metal-metal interactions. These bimetallic complexes were previously shown to undergo metal scrambling, making them poor catalysts. To make these bimetallics more robust, we have covalently attached these complexes onto a metal organic framework (MOF), and thereby making them heterogeneous. The hybrid M-Mn/MOF materials (where M = Fe or Co) were further characterized to demonstrate the successful incorporation of 1 M-Mn unit per node, a repeating unit of a MOF. Furthermore, these materials were tested for their ability to perform

heterogenous catalysis such as olefin epoxidation and oxidative dehydrogenation of N-heterocycles.

85. Nicolas Rothbacher

Mixing Lead Free Tin and Strontium Halide Perovskites for Solar Cells

Advisor: Russ Holmes

Sponsoring Program: MRSEC

Home Institution: University of Puget Sound

Abstract: The term "perovskite" denotes a broad class of materials that have the stoichiometry ABX_3 where A and B are cations (with A being larger than B) and X is an anion. Halide perovskite solar cells are one of the most exciting new technologies in the field of photovoltaics (PVs). Solar cells using these materials have improved in efficiency rapidly in the decade since their emergence and are approaching efficiency parity with more mature technologies like silicon PVs. They are also relatively simple to synthesize using a wide variety of techniques and some have properties that make them ideal as active PV materials, like excellent absorption properties, direct bandgaps and long carrier lifetimes. The main issues facing this promising new technology are rapid degradation in ambient conditions and a reliance on lead as the B cation in the most successful materials studied, such as the archetypal methylammonium lead iodide ($CH_3NH_3PbI_3$). Lead perovskites are sensitive to light, heat and moisture, and can release toxic lead compounds during degradation, making industrial implementation a difficult prospect. To reduce problems with toxicity, several groups have replaced lead with tin. Unfortunately, tin perovskites appear to have worse stability than their lead counterparts. The work of this project will be to attempt to improve the stability of tin perovskites by partially replacing tin with another cation such as Sr. In lead perovskites, both experimental results and density functional theory calculations indicate that partial Sr replacement of Pb leads to improved stability. In addition, $MAPbI_3$ showed a marked improvement in several factors important to photovoltaic use with just 2% strontium, making this method promising for continued study. This project seeks to optimize thin film synthesis methods and to identify the optical and degradation properties of tin halide perovskites with partial strontium replacement. This will shed more light on the ability of substituting strontium to improve stability and reduce the toxicity of perovskite materials for PVs, and thereby enhance the prospects of the commercial viability of perovskite solar cells.

86. Ramitha Rupasinghe, Sahil Arora

Investigation of the hexadecahydro-Diels-Alder (HDDA)-derived benzyne with diaziridines

Advisor: Thomas Hoye

Sponsoring Program: UMN Chemistry- Lando

Home Institution: University of Minnesota - Morris

Abstract: The extent to which benzyne, one of the most versatile reactive intermediates in organic chemistry, can react with different trapping agents is an important question in synthetic chemistry. The HDDA-reaction allows the generation of benzyne via thermal activation, without using any external reagents, which then can be efficiently trapped to synthesize compounds which have biological and materialistic applications. This exciting HDDA-chemistry has inspired us to look for new trapping reagents and re-examine those previously studied. Reactions of HDDA-derived benzyne with different trapping agents such as silyl ethers, azides, pyrroles, thioamides and multifunctional natural products have been investigated by our group. In this project, reactions of HDDA-derived benzyne with nucleophilic 1,3-dialkyl diaziridines were explored. It was observed that diaziridines usually react with in situ generated benzyne to give hydrazones, i.e. products in which the diaziridine ring is no longer intact. These hydrazones are well-known precursors for the synthesis of indoles via the Fischer indole synthesis. In this research, synthesis and characterization of various 1,3-dialkyl diaziridines along with their corresponding trapping reactions with different HDDA-derived benzyne were investigated. Synthesized hydrazones were later reacted to form functionalized-indoles, which are biologically relevant molecules that play an important role in pharmacological drug discovery and analysis.

87. Andrew Schmitz

Characterization of Heavy Atom Effect on Metal Carbonyl Complexes using Pump Probe and 2DIR Spectroscopy

Advisor: Aaron Massari

Sponsoring Program: UMN Chemistry- Heisig Gleysteen

Home Institution: University of Minnesota

Abstract: The heavy atom effect refers to the impact of a central heavy atom on the vibrational dynamics of molecular vibrations within the molecule. This has a wide potential for application in

photo chemistry and specific group shielding. The vibrational dynamics of cyclopentadienyl iron (II) dicarbonyl dimer (Fp2) were analyzed using pump probe and 2DIR spectroscopic methods. These findings will be compared to a congruent analysis of Bis(cyclopentadienylruthenium dicarbonyl) dimer. The vibrational lifetime as well as the linewidth broadening will demonstrate the impact of a heavy atom on the dynamics of the molecular vibrations, and will be used to create a model of this interaction.

88. Mary Solomon, Joshua Wissbroecker, Deana Bui, and Hao Fei Cheng

Chatbot Mediated Group Decision Making

Advisor: Haiyi Zhu, Max Harper

Sponsoring Program: Computer Science

Home Institution: Bowling Green State University

Abstract: Increasing numbers of individuals are turning to intelligent agents to help them complete tasks efficiently. However, few exist to assist groups of users in discussion or decision making. Designing intelligent agents for group decision making is difficult due to complex communication in discussion such as expression of preference and negotiation. We introduce MLBot, an interactive chatbot that aids group decisions for movies by interacting with users in a chatroom, providing movie recommendations, and assisting the decision making process. MLBot is based on MovieLens, a collaborative filtering recommender system that curates recommendations through user ratings. Our objective for MLBot is to understand and analyze factors of intelligent agents that impact group decision making. We hypothesize a chatbot that actively interacts with users will facilitate the group decision making process. Therefore, an active bot could lead to higher satisfaction and a faster group decision making process. To test this hypothesis, we are conducting a Wizard of Oz study in which the bot will appear to be an intelligent agent to the participant, but is operated by a researcher. We are using a 2x2 factorial design comparing interventions of enforcing structure and giving opinion. We are comparing the impact of each factor to study which of the bot behaviors can benefit group decision making the most. In the future, this study can inform researchers on chatbot designs that can streamline the flow of the discussion and help groups make better decisions.

89. Luis Sosa

Chemical Composition Analysis of Ligands bound to CdSe Quantum Dots before and after Ligand Exchange

Advisor: Eray Aydil

Sponsoring Program: MRSEC

Home Institution: University of Texas - Rio Grande Valley

Abstract: Quantum Dots (QDs) have drawn attention due to their variety of potential applications. QDs are remarkably unique in that they feature the ability to efficiently convert energy into light of nearly any color in the visible spectrum by tuning the QD diameter. To further understand the particular behavior of QD, Cadmium Selenide (CdSe) nanocrystals will be synthesized by reacting a mixture of precursors via Schlenk line, resulting in QD nucleation and growth. When the desired size of nanoparticles is reached, the reaction is quickly terminated by quenching the temperature. The resulting QDs are stabilized in solution by trioctylphosphine oxide (TOPO), trioctylphosphine (TOP), and octadecylphosphonic acid (ODPA), which serve as ligands on the QD surface. To demonstrate the effect that reaction time of TOPSe in the solution has on QD size, a series of syntheses will be performed where the reaction time will be altered. To test the effect of ligands on QD stability in solution, the ratio of ligand chemicals (TOPO, ODPA, and TOP) will be adjusted. In addition, ligand exchange, or the replacement of some TOPO ligands for Polyethylene Glycol (PEG), will be assessed to disperse the nanocrystals in more polar solvents, such as chloroform. Furthermore, QDs were analyzed via Ultraviolet-visible spectroscopy (UV-Vis) to determine their respective absorption peaks and size distributions. Dynamic Light Scattering (DLS) was used to determine aggregation of nanoparticles in various solvents and observe changes upon ligand exchange. Fourier Transform Infrared Spectroscopy (FTIR) was used to determine the ligand coverage on the QDs before and after ligand exchange.

90. Molly Srour, Wei Zhang, Raphael Petegrosso

Remote Homology Detection through Semi-Supervised Learning on Massive Biological Networks

Advisor: Rui Kuang

Sponsoring Program: Computer Science

Home Institution: Saint Olaf College

Abstract: Bioinformatics research accumulates and analyzes large collections of genomic and proteomic data into massive databases used for a variety of analyses, including the creation of

networks linking related sequences. Most existing programs such as PSI-Blast and HMMer utilize these databases to compare protein sequences to find similarities in sequence alignment. These search engine programs allow for user-friendly searches where users enter a query sequence and receive a list of sequences that most closely match the query. The results of these programs merely encompass pairwise sequence similarity, but lack the evolutionary information necessary to produce a network of proteins based on homology (similarities in either structure, function, or sequence alignment). In this case, we propose two label propagation algorithms where semi-supervised learning with a nearest-neighbors technique classifies unlabeled data. One approach utilizes sparse matrices and the other approach incorporates a low-rank algorithm with the Kernel Nystrom Approximation. The sparse method utilizes Rankprop, a classic label propagation algorithm that leads to the creation of homology networks. However, Rankprop cannot handle massive databases at an efficient rate, which often leads to a failure to detect more nuanced remote homology between proteins across species. Our label propagation algorithms incorporate the mostly unlabeled 500,000 sequences in the Uniprot database into the classic benchmark database SCOP-40. This larger network enables more comprehensive remote homology detection so more subtle relationships between proteins can be determined. Multiple parameters were tested to hone the algorithm's efficacy, confirming that the sparse algorithm gives more accurate and comprehensive results with larger networks. Additionally, both algorithms proved most accurate when looking at proteins in smaller superfamilies (classification groups). While the low-rank algorithm sometimes provided more accurate results, both label propagation algorithm techniques outperform Rankprop the majority of the time.

91. Matthew Stiller

Characterization of Thin-Film β -Ga₂O₃ Using Raman Spectroscopy

Advisor: Steven Koester

Sponsoring Program: MRSEC

Home Institution: Saint John's University

Abstract: Thin-layered semiconductors are of importance since they exhibit useful properties which are absent in their bulk counterparts such as photoluminescence, tunable band gap, or increased electron mobility. These properties can provide enhancements to current electronic and optoelectronic devices such as transistors and photodetectors. Their two-dimensional size provides an avenue for smaller functioning devices and greater energy efficiency. Gallium oxide is a semiconductor which has a monoclinic structure and can be separated along its (100) cleavage plane. It also possesses a high energy band gap of 4.9 eV. These properties allow it to be implemented in thinner and higher power electronic devices. We attempted to create monolayer Gallium oxide through mechanical exfoliation techniques and observed the corresponding Raman spectra. Monolayer thicknesses have been successfully identified in Transition metal dichalcogenide (TMDC) semiconductors by observing frequency shifts in their Raman spectra. Therefore, the spectra of two TMDC semiconductors, Molybdenum disulfide and Tungsten ditelluride, were gathered for comparison with Gallium oxide.

92. Michael Stodolka

Solid-State Studies of Halogenated Benzonitrile Oxides and their Dimers

Advisor: William Ojala

Sponsoring Program: University of St Thomas- Chemistry

Home Institution: University of St. Thomas

Abstract: Benzonitrile oxides (Ar-C-N⁺-O⁻, where Ar = Aryl) dimerize in solution, forming a furoxan (in the absence of catalyst), a dioxadiazine (in the presence of added pyridine), or a 1,2,4-oxadiazole N-oxide (in the presence of added triethylamine). We are investigating the crystal chemistry of halogenated benzonitrile oxides, motivated by the published observation that the solid-state stability of these compounds is strongly dependent on the ring substitution pattern; 2-chlorobenzonitrile oxide and 4-chlorobenzonitrile oxide possess reported stabilities of 3-6 days and 10 days, respectively, while the reported stability of 3-chlorobenzonitrile oxide is only 50-60 minutes. We have now determined the crystal structure of the bis(3-chlorophenyl)furoxan obtained from solution and found it to be isomorphous with our previously examined bis(3-bromophenyl)furoxan. Unlike the crystal structures of many other symmetrically substituted furoxans, this structure shows little evidence of twofold disorder about the approximate molecular twofold axis. No chlorine...chlorine approaches closer than the sum of the van der Waals radii are observed in our structure. We are also examining the bis(4-bromophenyl)furoxan to determine whether it is isomorphous with our previously investigated bis(4-chlorophenyl)furoxan or bis(4-methylphenyl)furoxan; we intend to determine whether the solid-state phase transition we observe in the chloro and methyl derivatives also occurs in the bromo

derivative.

- 93. Cameron Swenson**, Anatoli Purchel, Monica Ohnsorg
One-Pot Synthesis of a Block Copolymer Using RAFT Chain Transfer Agent (CTA) Specificity
Advisor: Theresa Reineke
Sponsoring Program: UMN Chemistry- Heisig Gleysteen
Home Institution: University of Minnesota
Abstract: Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization is a controlled free radical polymerization technique frequently used in research settings to achieve polymer samples with low dispersity under mild conditions. The control of the polymerization kinetics is afforded by using a thiocarbonylthio moiety containing chain transfer agent (CTA), which stabilizes growing chains by producing dormant radical species. These dormant species greatly reduce the amount of available free radicals in solution, causing radical initiation to significantly outpace chain growth such that all chains start to grow at approximately the same rate. CTAs can be tuned to have inherent specificity towards certain classes of monomers by controlling the radical-stabilizing group. By tailoring this specificity, a block copolymer was synthesized in a single step composed of tert-butyl acrylate block vinyl acetate. The di-functional CTA was composed of 2-methyl-2-(propylthiocarbonothioylthio)propanoic acid and 2-methyl-2-(methyl(phenyl)carbamothioylthio)propanoic acid linked by an ethylene glycol core. The resulting polymer was analyzed by NMR spectroscopy, size-exclusion chromatography (SEC), and differential scanning calorimetry (DSC) to determine monomer incorporation, molecular weight, and dispersity. These techniques confirmed the formation of a low dispersity polymer with two blocks of differing composition.
- 94. Pa Thao**, Kiall Suzao
Probing levels of protein prenylation: synthesis of an Azide-modified isoprenoid analogue
Advisor: Mark DiStefano
Sponsoring Program: Project SEED
Home Institution: 2017 Graduate, Harding High School, St Paul Public Schools
Abstract: Protein prenylation is an essential post-translational modification of proteins where isoprenoids farnesyl (C15) and geranylgeranyl (C20) are attached to their C-terminal from farnesyl (FPP) and geranylgeranyl (GGPP) diphosphates. While this pathway has been extensively studied using chemical probes, in vivo investigations (e.g. in live cells) such as quantification of levels of prenylated proteins has not been widely explored. Such approach is desirable in probing the prenylation status in disease systems where this pathway is dysregulated. This research project describes the synthesis of an analogue of the isoprenoids, C15-Az-OPP, which can be used to tag prenylated proteins via strain-promoted azide-alkyne cycloaddition (SPAAC) reaction with a fluorophore reporter. Farnesol was first protected with tetrahydropyran (THP) followed by selective allylic oxidation to form an alcohol. Subsequent alcohol azidation, followed by deprotection and phosphorylation afforded the desired chemical probe in a reasonable yield. All of the compound in each steps of the synthesis was characterized by using mass spectrometry and nuclear magnetic resonance (NMR) spectroscopy. This successfully synthesized C15-Az-OPP is currently under evaluation for its efficiency in quantifying levels of prenylated proteins in live cells.
- 95. BaoNhia Thao**, Qian Tang
Development of a Method to Identify of IAA Amino Acid Conjugates in Arabidopsis
Advisor: Jery Cohen
Sponsoring Program: Project SEED
Home Institution: 2017 Graduate, Harding High School, St Paul Public Schools
Abstract: Indole-3 Acetic Acid (IAA) is a vital auxin class plant hormone in plants that regulates growth and development. It was the first plant hormone to be identified and is the major auxin in plants. IAA can be conjugated into amino acids and they are a form of metabolite which can be biosynthesized to other conjugates. IAA Aspartate and IAA Glutamate are conjugates with the least amount of conversion back to free IAA and will be the focus of this study. Even with today's high technology for analyzing the biochemistry within plants, it remains challenging to detect IAA Aspartate and IAA Glutamate. This investigation will employ the use of Ultra High-Performance Liquid Chromatography (UHPLC) and Q Exactive High Resolution Accurate Mass Spectrometry (MS) in identifying the IAA conjugates in Arabidopsis seedlings.

96. **Xee Thao**, Molly Kresire, Michael Burns
Determining if Methyl IAA is Present in Arabidopsis thaliana
Advisor: Jerry Cohen
Sponsoring Program: Project SEED
Home Institution: Washington Technology Magnet School, St Paul Public Schools
Abstract: The most common and naturally occurring hormone found in plants is Indole-3-Acetic-Acid (IAA). Auxins have many conjugates and Methyl Indole-3-Acetic-Acid (Me-IAA) is one of them. Me-IAA was recently thought to be naturally found in plants. In experiments looking for unconjugated IAA, labs will use chemical substances such as methanol to see if IAA is present in plants. When a chemical like methanol is used to find IAA, the result is the methyl-ester of IAA. In this experiment acetonitrile was substituted for methanol, which allowed for auxin to be extracted without forming methyl conjugates. For this experiment, *Arabidopsis thaliana* was grown on Murashige and Skoog media and after extraction, the samples were stored at -80 degrees Celsius. To extract auxin, the samples were homogenized in acetonitrile, and run through an HPLC-MS to look for the presence of Me-IAA. After the samples were run through the HPLC-MS, the chromatograms showed no peak at the time corresponding to the Me-IAA standard.
97. **Kamala Varma**
Assessing the Relevance of Eye Gaze Patterns During Collision Avoidance in Virtual Reality
Advisor: Victoria Interrante
Sponsoring Program: Computer Science
Home Institution: Vanderbilt University
Abstract: Developers of virtual reality environments strive to create immersive experiences that feel realistic to the user, which requires careful consideration of the subtleties in human behavior. In the case of collision avoidance, one often overlooked detail is eye animation. Prior research has found that head orientation can cue directional intention, but little attention has been given to eye movement; thus most simulations use avatars with painted-on eyes. A recent study has shown that humans infer other people's trajectories by their gaze directions and plan their own movement accordingly, but the tests were done with participants seated in front of a 2D screen. The current study will extend this finding into an immersive 3D virtual environment, providing a more realistic simulation that allows the participant to make actual avoidance movements as they avoid colliding with an approaching avatar. To determine whether eye movement aids, distracts, or is irrelevant to the directional cues coming from the head, the import of eye gaze will also be assessed in conjunction with head orientation through scenarios where the eyes and head act in either agreement or contrast. The participant's eye gaze will be monitored in terms of the visual cues they focus on, for how long, and how these coincide with their path of avoidance. A better understanding of the extent to which people infer a virtual human's locomotor trajectory from his gaze direction will inform future efforts to populate virtual environments with crowds of autonomous intelligent agents who use non-verbal cues to negotiate collision avoidance.
98. **Noah Vineberg**
Verification of an Automatic Microcatalytic Reactor's Accuracy Using Solid Acid Catalysts
Advisor: Paul Dauenhauer, Omar Abdelrahman, Katherine Vinter
Sponsoring Program: MRSEC
Home Institution: University of Delaware
Abstract: While industrial laboratories own expensive equipment to test catalyst activities over a wide range of conditions, catalyst screening in academic environments can be a tedious process that takes ample time and effort using traditional flow reactors. To solve this problem, a new reactor has been designed for rapid catalyst screening, solely within a gas chromatograph (GC). The new reactor is contained within a gas chromatograph quartz liner and is a semi-continuous flow reactor. It can quickly achieve steady state, where a sample is taken and then a new condition can be set. The validity of the reactor was tested by studying alcohol dehydrations, a common and well documented reaction, and the results were compared with known experimental data. Alcohol dehydration involves the reaction of an alcohol to form either an alkene or ether and water. The catalysts of interest are solid acid catalysts, which include industrial zeolite catalysts such as ZSM-5 and H-BEA. The results were analyzed using gas chromatography and mass spectroscopy, and then compared to data found from scientific

literature. More data needs to be collected, but we anticipate that the reactor will be successful, and that it will revolutionize the way data is collected from catalysis, making it a more affordable and efficient process.

99. **Ydana Virgen**, Mitra Ganewatta, PhD, Will Boyle
Synthesis of Poly(N-(2-(diethylamino) ethyl) acrylamide) for Cell Transfection.
Advisor: Theresa Reineke
Sponsoring Program: MRSEC
Home Institution: The University of Texas Rio Grande Valley
Abstract: Poly(N-(2-(diethylamino) ethyl) acrylamide) is a novel water-soluble cationic polymer which exhibits thermo-responsive properties. We hypothesize that this polymer can form polyplexes with DNA that can be used to transfect cells. If the polymer crosses its LCST during transfection, the resulting destabilization of polyplexes may lead to efficient in vitro gene delivery. The monomer N-(2-(diethylamino) ethyl) acrylamide (DEAEAM) was synthesized according to a literature protocol. Solvent extraction and column chromatography was used to purify it. ¹H and ¹³C NMR as well as IR spectra validated the successful synthesis. Subsequently, polymerization of the monomer was performed using RAFT (Reversible Addition Fragmentation chain Transfer) polymerization to finally obtain three polymers (A, B, and C) with different molecular weights. The final product was dialyzed and freeze dried to obtain the pure material. Several characterization techniques such as Gel Permeation Chromatography (GPC) and ¹H NMR were performed to determine the molecular weights of the polymers. Lower Critical Solution Temperature (LCST) which, as its name states, determine the critical temperature at which the material is miscible, was determined as well. The pKa values were measure by potentiometric titrations and found to be 9.25 for the monomer and 8.47 for the polymer, indicating therefore that these two are highly charged at physiological pH. The polymer's ability to form complexes with DNA was analyzed using Dynamic Light Scattering (DLS), and a gel electrophoresis retention assay, which indicated that starting at N/P ratio of 2.0, binding between polymer and DNA was effective. Finally, the transfection efficiency of the polymer in HeLa cells was analyzed using a green fluorescent protein (GFP) reporter assay analyzed by flow cytometry. Toxicity of the polyplexes was assessed by propidium iodide staining quantified by flow cytometry. The acrylamide polymer based polyplexes showed efficient cellular internalization and low toxicity at low N/Ps. However, efficient delivery of the DNA to the nucleus require further optimizations.
100. **Quentoria Walton**
Synthesis of Perfectly Alternating Poly(lactic acid-co-3-hydroxypropionic acid) From a Renewable Cyclic Diester Monomer
Advisor: Marc Hillmyer
Sponsoring Program: Center for Sustainable Polymers
Home Institution: Tuskegee University
Abstract: The synthesis of perfectly alternating poly(lactic acid-co-3-hydroxypropionic acid) from a renewable cyclic diester monomer is projected. In this study, a linear precursor to the desired 3-methyl-1,4-dioxepane-2,5-dione has been obtained from the methyl ester of LA and ethyl ester of 3-HP via a sequence of simple, organic transformations requiring very little purification and producing intermediates in good to excellent yields.. The synthesis of the copolymer of LA and 3HP cannot be made by other methods. Through lactic acid isomers (L,D,DL), the stereochemistry of the monomer can be changed; hence, allowing the monomer to display various properties. The goal is to yield pure monomer in high yield and polymerize to possibly give a semicrystalline polymer. NMR spectrum data gives evidence that precursor to monomer was successfully synthesized. Current research focusses on probing cyclization methods of the monomer and polymerization through ring opening polymerization (ROP).
101. **Kathleen Wang**
Kinetic study of novel silane-mediated phosphine oxide reductions
Advisor: Courtney Aldrich
Sponsoring Program: UMN Chemistry- Heisig Gleysteen
Home Institution: University of Minnesota Twin Cities
Abstract: Kinetic studies were performed to identify reaction rates of phosphine oxide substrates, and the effects of electron-withdrawing and electron-donating substituents on the reaction rates were determined. A Hammett Plot was constructed, and the resulting reaction constant has implications in the mechanistic underpinnings of the reduction.

- 102. Qining Wang**, Manuel A. Ortuño, Lauren Mitchell, Megan Fieser, William B. Tolman, Christopher J. Cramer
Role of Directing Groups for Catalytic Decarbonylation of Fatty Acids
Advisor: Christopher Cramer
Sponsoring Program: UMN Chemistry- Lando
Home Institution: University of Minnesota
Abstract: Linear alpha-olefins (LAOs) are of great importance in the polymer industry. LAOs are traditionally generated from petroleum, a nonrenewable and depleting resource, thus a sustainable way of producing them is quite appealing. Herein we propose a decarbonylative dehydration of fatty acids, which are inexpensive and renewable raw materials. However, carboxylic acids are hardly reactive per se, and transition metal catalysts and activator groups are usually required. In this study we use a Ni-phosphine catalyst and various alcohol directing groups to promote the decarbonylative dehydration of 4-phenylbutanoic acid as test substrate. We employ density functional theory (DFT) to gather mechanistic information at the atomic level of detail. We explored several reaction pathways and, interestingly, we found that the chelating nature of the directing group does not have a strong impact on kinetics; instead it drives the thermodynamics of the process.
- 103. Zane Weltman**
Comprehensive Model of a Free Piston Engine
Advisor: Zongxuan Sun
Sponsoring Program: CCEFP
Home Institution: University of Minnesota
Abstract: The free piston engine (FPE), as an alternative of the conventional internal combustion engine, could significantly impact the energy consumption and emissions of both on-highway and off-highway vehicles. In this engine, there is no crankshaft, so piston motion is dependent on the combustion chamber gas dynamics and the loading dynamics in real time. Since combustion is rapid and highly unpredictable, the greatest barrier to widespread FPE use is precise piston motion control. In this poster, I present a simulation of the operation of a hydraulic FPE with an opposed-piston opposed-cylinder design. My specific contribution to this research was to integrate MATLAB code designed to simulate in-cylinder combustion forces into a Simulink model of overall engine operation in order to create the most comprehensive possible model of engine operation. The MATLAB code predicts both the chemical kinetics and the thermodynamics of the gases inside each combustion chamber, while the Simulink model combines this code's combustion force with forces generated from the engine's hydraulic control system and from friction to generate an overall picture of piston dynamics during operation. Preliminary results of this updated model are presented in the poster. Though this code represented the majority of my work this summer, I also installed a surveillance camera system in the test cell in order to better monitor engine operation. Photos of this work are included as well.
- 104. Luke Westawker**
Manipulating Microparticles in Active Matter using Phototrophic Agents
Advisor: Xiang Cheng
Sponsoring Program: Independent Research
Home Institution: Carleton College
Abstract: Many microscopic particles are difficult to control while in dilute solutions. This project investigated how to isolate and move microparticles, ranging from cell samples to impurities. This was found to be possible by placing microparticles in active matter, a type of solution composed of moving objects called agents. *Chlamydomonas reinhardtii* and *Euglena gracilis* were two types of agents used as they are phototrophic algae, meaning the organisms move toward light. When a solution of the algae was exposed to a beam of light, most of the agents moved to occupy the well-lit region, leaving fewer agents to move around in the darker regions. When these agents moved, they exerted what is called swim pressure on their surroundings, like the pressure created by moving atoms. It was hypothesized that a pressure differential would be created between the region of higher algae concentration in the light beam and the region of lower concentration outside of the light beam. This was tested using 1 micrometer polystyrene microparticles. The results confirmed that microparticles were forced out of the higher pressured regions and into the lower pressured region. This showed that microparticles could be isolated

and then moved by using phototrophic agents to impose pressure differentials in active matter.

- 105. Quinn Whiting**, Joe Herrli, Kris Wammer, and Stephanie Berg
Investigation of indirect photolysis on select pesticides and pharmaceuticals along the St. Louis River
Advisor: Kris Wammer
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: The use of many pesticides and pharmaceuticals contribute to the contamination of natural water systems, where these anthropogenic compounds persist. One pathway of degradation for some of these contaminants is photolysis. Due to their chemical structures atorvastatin, carbamazepine, DEET, and venlafaxine absorb sunlight poorly. Consequently, these compounds undergo indirect photodegradation with reactive intermediates (RIs) produced by dissolved organic matter (DOM). These RIs are formed through the absorption of sunlight by DOM and include singlet oxygen (1O_2), triplet DOM (3DOM*), and hydroxyl radicals (OH). To investigate the kinetics of each compound under environmental conditions, samples were collected at various sites along the St. Louis River and used to make 10 M solutions of each compound. They were then photolyzed in a Suntest CPS+ solar simulator for up to four hours. Before and during photolysis, samples were analyzed on an Agilent 1100 Series HPLC to quantify the first-order rate constant of each compound. Total organic carbon (TOC) was measured for each sample site and used to calculate the rate per unit carbon (rate/hr/mgC). Observed rate differences between sites could be due to differences in RIs between sites. To investigate the individual effects of each RI on the overall rate constants of each compound, we added a quenching molecule at a concentration of 3mM to each of the 10M solutions. Furfuryl alcohol (FFA) is used to quench 1O_2 , IPA is used to quench OH, and potassium sorbate is used to quench 3DOM*.
- 106. Emily Whitwam**
Electromagnetic Interference Shielding by Fused Deposition Modeling
Advisor: Brittany Nelson-Cheeseman
Sponsoring Program: University of St. Thomas- Material Science and Engineering
Home Institution: University of St. Thomas
Abstract: The possibility of using fused deposition modeling to produce electromagnetic interference (EMI) shields may reduce drawbacks of current EMI shields made from sheet metal. In order to do this, the electrical properties of polymer-matrix composites will be tested in order to assess their shielding effectiveness. Physical vapor deposition will be used to adhere thin films of titanium and gold to the fused deposition modeled composite samples. The electrical conductivity of the samples will then be assessed using a four-point probe test. A conclusion will then be made as to which composite displays the highest shielding effectiveness. A comparison will also be done of the shielding effectiveness between the fused deposition modeled samples, injection modeled samples, and current sheet metal shields.
- 107. Thomas Wieser**
Acetylated and Phosphoryl Cholinated G5 Poly(amidoamine) Dendrimers for Gene Delivery: Balancing Toxicity and DNA Packaging Efficiency
Advisor: Lisa Prevette
Sponsoring Program: University of St Thomas- Chemistry
Home Institution: University of St. Thomas
Abstract: Gene therapy has become a growing area of interest as it allows for the treatment of various diseases ranging from arthritis to cancer, but it requires delivery of nucleic acids to cells. Polycations are popular delivery agents as they bind nucleic acids via electrostatic interactions with their phosphate backbones. G5 poly(amidoamine) dendrimer (PAMAM), a spherical, branching polymer with 128 terminal amines, is an effective gene delivery agent. Unmodified G5 PAMAM, however, is cytotoxic. Previous studies show that the cytotoxicity of G5 PAMAM can be reduced by conjugating neutral acetyl (Ac) groups or zwitterionic phosphoryl choline (PC) groups to the terminal amines. Here, G5 PAMAM was conjugated with Ac and PC groups in varying end group ratios to study their effect on DNA binding. Acetylated PAMAM (Ac-P) and phosphoryl cholinated PAMAM (PC-P) products were characterized by NMR spectroscopy. Electrophoretic mobility shift assays and isothermal titration calorimetry were used to study the structural effects on DNA binding. It was found that increasing the degree of conjugation in both Ac-P and PC-P leads to higher DNA binding stoichiometry.

108. **Emily Wilborn**
Using Directing Groups to Facilitate the Decarbonylation of FAMES
Advisor: William Tolman
Sponsoring Program: Center for Sustainable Polymers
Home Institution: Cal Poly San Luis Obispo
Abstract: Currently, the chemical industry derives most polymers from olefins produced in petroleum refining. Therefore, the price and availability of common chemicals is dependent on oil, a finite resource. For this reason, there has been interest in using more abundant biological resources for the development of commodity chemicals. Past research efforts have identified pathways where carboxylic acids could be used as precursors to produce polymers. However, biodiesel is already produced to scale in industry and contains fatty acid methyl esters that could be decarbonylated to allow a more direct route from bio-feedstocks to useful olefins. Currently, there are no reports of homogeneous catalysts available for this process. In addition, the carbon-oxygen single bond within the ester is difficult to activate causing decarbonylation to be unfavorable. For these reasons, a dual-catalytic strategy was designed to incorporate a directing group into the substrate to facilitate the reaction by activating the C-O bond. Reported herein are efforts to optimize the transesterification step used to incorporate the directing group. In addition, there has been work to synthesize fatty acid methyl esters and esters with the directing group for use in control reactions and for catalyst testing.
109. **Nyla Worker**
Exploration of Different Distributed Machine Learning Architectures
Advisor: Abhishek Chandra
Sponsoring Program: Computer Science
Home Institution: Carleton College
Abstract: Machine learning is widely used in various big data applications such as natural language and image processing. Neural networks are a key machine learning tool. However, with ever growing datasets, they are too intensive computationally. Hence, it becomes unfeasible to perform such tasks in one GPU or one CPU. We explore different architectures of distributed machine learning systems and test their speed and accuracy. For our experiments we focus on image processing using the Cifar-10 dataset, which consists of 60 thousand images and ten categories. As a base, we recreate past successful algorithms trained with this dataset, such as AlexNet [1]. These algorithms consist on a combination of convolutional, pooling, dropout and fully connected layers. We distribute these architectures among various workers, in this case CPUs, and connect them to a parameter server, where the parameters get updated with the information of each of the workers. These architectures increase the speed at which they train, but they lose their accuracy in general. However, we found that dividing a convolutional neural network speeds computation, decreasing efficiency marginally by one percent. We do this asynchronously by updating the parameter server every time an epoch is finished. We hope to find an architecture following this initial scheme that will be scalable to bigger datasets and with increased efficiency.
110. **Ka Lia Xiong, Evan L. Anderson**
Determining The Solubility of Ag⁺ Containing Salts In Room-Temperature Ionic Liquids
Advisor: Philippe Bühlmann
Sponsoring Program: Project SEED
Home Institution: 2017 Graduate, Washington Technology Magnet High School, St Paul Public Schools
Abstract: Ideally, reference electrodes allow for the reproducible measurement of potentials when measured against other electrodes. Of the many types of reference electrodes reported, ionic liquid (IL) reference electrodes have been shown to provide stable potentials when in contact with aqueous solutions of varying composition. In a newly developed IL reference electrode, a Ag/AgCl-coated wire is used as an electron-to-ion transducer to contact a AgCl saturated IL. The concentration of Ag⁺ at this interface determines the potential between the AgCl-coated Ag wire and IL and determines overall potential reproducibility of the electrode. To better understand this interface, we seek to determine the solubility limit of AgCl in a variety of ILs as this data is presently unknown. Stripping voltammetry was first implemented to determine the free concentration of Ag⁺. The limit of detection was found to be too high to measure AgCl solubilities in IL. Potentiometry was then used with a highly soluble Ag⁺ salt to generate a calibration curve of Ag⁺ in IL. Based on the Nernst equation, this calibration curve was used to determine the concentration of Ag⁺ in salts of lower solubility by extrapolation. This solubility data now provides fundamental data for further development of IL reference electrodes.

111. **Diana Zhang**
Investigating the Micellar Liquid Crystal Phases of Hydrated Nonionic Surfactants
Advisor: Mahesh Mahanthappa
Sponsoring Program: MRSEC
Home Institution: The University of Texas at Austin
Abstract: Surfactants – amphiphilic molecules consisting of a hydrophilic headgroup and hydrophobic tail – form lyotropic liquid crystal phases upon the addition of water. In their liquid crystalline state, these materials have the potential to serve as water desalination membranes, polymer electrolytes in Li-ion batteries, and drug delivery vehicles. However, to effectively design these soft materials for technologically important applications, we must better understand how various factors govern the phase behavior in these systems. Micellar phases have been reported in detail for both polymer and ionic surfactant systems, but studies on nonionic surfactants are largely outdated with general or tentative phase assignments. Thus, using Polarized Light Microscopy and modern Small Angle X-Ray Scattering techniques, we investigated the micellar phases upon hydration of two nonionic surfactants: Brij 58 and C₁₂E₁₀. In Brij 58, we report the formation of BCC, FCC, and the Frank-Kasper phase A15. When heated and cooled back down, the phases seem to evolve in curious ways. In C₁₂E₁₀, we report the formation of a less common HCP phase as well as some interesting, more complex phases upon cooling to near 0 °C temperatures. Our findings suggest that there may be additional Frank-Kasper or more complex phases lurking in our systems, setting the stage for further studies on how and why such phases form.
112. **Weifeng Zhang**
Rainbow trapping elastic waves in tunable metamaterial
Advisor: Stefano Gonella
Sponsoring Program: Civil Engineering
Home Institution: University of Minnesota, Twin Cities
Abstract: One of the most daunting limitations of phononic crystals and acoustic/elastic metamaterials is their passivity: a given configuration can only display its phononic properties in specific, pre-determined operating conditions. In the past decade, this shortcoming has inspired the design of phononic media with tunable wave characteristics using piezoelectric elements shunted to passive electric circuits. One of the most popular shunting circuits is the resistor-inductor, which allows the shunt system to behave as an electromechanical resonator. A common motif among the works employing shunted piezos for phononic control is periodicity: the patches are typically periodically placed in the domain, and the circuits are identically tuned. The objective of this work is to demonstrate that the wave attenuation performance of structures with shunted piezoelectric patches can be improved by leveraging notions of organized disorder. Based on the idea of rainbow trapping--broadband wave attenuation obtained by tuning an array of resonators at distinct neighboring frequencies--we design and test an electromechanical waveguide capable of attenuating waves over broad frequency ranges without relying on the constraint of periodicity in the placement of patches. In an attempt to demonstrate tunability, we take advantage of the reconfigurability of the circuits to show how a single waveguide can attenuate both waves and vibrations over a wide range of frequencies.
113. **Aristotelis Zografos**, Seamus Jones, Dr. Michael Maher.
Using Graft Architecture to Toughen Poly(lactide)
Advisor: Frank Bates
Sponsoring Program: Center for Sustainable Polymers
Home Institution: University of Maryland, College Park
Abstract: Poly(lactide) (PLA) is a compostable, biodegradable thermoplastic with potential to replace various petroleum-derived, non-degradable plastics. However, due to its brittle nature, the use of PLA is currently limited to applications where toughness is not essential. Herein we investigate the use of graft copolymer architectures to toughen PLA. Alternating copolymers of styrene and maleimides were synthesized via reversible addition fragmentation chain transfer polymerization (RAFT) to form macroinitiators. From these macroinitiators, block copolymers of 4-methylcaprolactone (P4MCL) and PLA were grafted via ring opening transesterification polymerization (ROTEP). For the PLA block, both crystalline and amorphous stereoisomers were studied. Furthermore, different degrees of crystallinity were used in order to investigate the corresponding effects on toughness. As a control, samples of neat poly(L-lactide) (PLLA) and PLA-P4MCL-PLA triblock copolymers were compared. Using a graft copolymer architecture, the toughness of PLLA was increased by a factor of 17, with elongations at break increasing from 6%

to over 100%. Furthermore, this improved toughness was achieved while maintaining elastic moduli comparable to that of PLLA. The graft architecture was also shown to be as much as 5.5 times tougher than the triblock copolymers, while maintaining larger elastic moduli.

Teacher Poster Presentations Listed Alphabetically by Presenting Author

- 114. Natalie Strauss**
Teaching About Enzymes in High School Chemistry
Advisor: Ben Hackel
Sponsoring Program: MRSEC
Home Institution: Saint Paul Public Schools
Abstract: Enzymes are a topic covered in the biochemistry unit of most higher level (AP, IB, Advanced) and some general level high school chemistry classes. It is typical to have students complete lab work look at how enzymes interact with proteins specifically how enzymes work to degrade proteins. However, enzymes also interact with lipids and carbohydrates. Because enzymes only interact with specific substrates, one enzyme will not interact with proteins, lipids and carbohydrates. This lab can be used to teach students about the selectivity of enzymes for different substrates and has the possibility to teach about kinetics using colorimetry.
- 115. Michael Maudal**
Dystopian Literature Enhancing Student Engagement in Chemistry
Advisor: Christy Haynes, Natalie Hudson-Smith
Sponsoring Program: MRSEC
Home Institution: Red Wing High School
Abstract: Cross-curricular teaching has been suggested as a potential solution to increase student engagement across several disciplines. Cross-curriculum teaching is an approach to teaching that requires a conscious effort to apply knowledge and principles to more than one academic discipline simultaneously. According to the Minnesota Department of Education, 21.3% of students did not meet reading standards and 18.8% only partially met reading standards in 2016. Despite this, there are still limited efforts to combat these statistics in high school science classrooms. One way to combat this is by introducing dystopian literature into the classroom, which offers students an opportunity to develop their English and language arts skills, while simultaneously learning chemistry concepts. Reading dystopian literature is also a popular teen leisure activity that can help students better connect with the cross-curricular lessons and better retain chemistry content. These lessons focused on the dystopian literature *Divergent* and were developed for the 2017-2018 academic year for general chemistry high school students. These lessons introduced students to microfluidics and were intended to promote critical reasoning skills, engineering and designing, reading comprehension, and application of chemistry concepts to dystopian literature. These lessons were designed to challenge students to see chemistry in activities outside of academia, such as movies and literature.
- 116. Cassandra Knutson**
Sustainable Chemistry for High School Classrooms
Advisor: Jane Wissinger
Sponsoring Program: MRSEC
Home Institution: White Bear Lake High School
Abstract: In chemistry classrooms around the world, some educators have re-designed their labs and demonstrations to be greener and safer. They are training tomorrow's chemists using the principles of green chemistry. In order to extend these approaches we offered a three day workshop on green and sustainable chemistry for high school teachers. Nineteen participating teachers from Minnesota received instruction on the principles of green chemistry, industrial applications, and potential impacts to human health and the environment. Participants gained hands-on experience with safer, cost-effective labs that minimize waste and are drop-in replacements for traditional secondary chemistry labs. Topics such as bioplastics, polymeric medical sutures and biomimicry were explored demonstrating relevance to societal needs. Following the workshop, an experiment that explores the synthesis of bioplastics and the rates of their degradation was developed for a high school audience to address the need for green chemistry curricula that align with standards and support inquiry based-learning.

