



# Materials Research Science and Engineering Center

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UNIVERSITY OF MINNESOTA

**Driven to Discover**<sup>SM</sup>

## Summer Undergraduate Research Expo

August 11, 2016

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 odd numbered posters

5:00 - 6:00 even numbered posters

1. **Andrew Ajaluwa**

*Improving the Extraction of the Facet Capsular Ligament*

**Advisor:** Victor Barocas

**Sponsoring Program:** MSROP

**Home Institution:** University of Minnesota- Twin Cities

**Abstract:** As the weight-bearing segment of the spine, the lumbar region experiences the stresses which lead to lower back pain. As a resistor to these loads to aid in spinal stabilization, the facet capsular ligament flanking each vertebrae and disc has now been identified as central cog in lower back pain and a checkpoint for disc degeneration. In the majority of studies dealing with the study of the Lumbar Facet Capsular Ligament (FCL), methods for removing the ligament from the joint are subjective and suggestive, in terms of dissection. The device design smooths the delicate dissection process while addressing the need for stability, elevation and support while making decisive cuts. The detachable device is expected to elevate the lumbar segment, provide stability through its opposite processes and allow the ligaments to be accessible and intact. Though the dimensions and model were successful as expected, the 3D plastic filament failed in its weight-bearing area. With the only improvement of the device being the switch from plastic to a metal, the design was a success and can be implemented not only for spine separation, but also for a range of specimen sizes in the upcoming future.

2. **Tamirat Ali**

*Sorption of Methane by Fungi: Study to detect methane capture by biofilter fungi*

**Advisor:** Jonathan Schilling

**Sponsoring Program:** Northstar STEM Alliance

**Home Institution:** Minneapolis community and technical college

**Abstract:** Emission of methane (CH<sub>4</sub>), a hydrophobic volatile organic compound, to the atmosphere has a significant contribution to climate change. As it had always been, human activities are to blame for destroying the environment. Of the human activities that result methane emission is livestock operation. Approximately, a third of the total U.S anthropogenic methane emission comes from livestock operations. To control the methane emission, biofiltration, a technique that uses microorganisms to degrade and capture malodorous volatile compounds such as CH<sub>4</sub>, are used. This method is believed to have the potential to reduce greenhouse gas emissions. Research have shown that biofilters with higher fungal biomass improve the capture of hydrophobic gases, thus improving performance. This is due to the unique nature of fungi, and I hypothesize that fungi can improve capture of CH<sub>4</sub> and enhance the biofiltration process, but that varies among strains. To test this, different isolates of fungi were tested using a gas-capture microcosm set-up to detect if there was any methane capture by the different strains of fungi. Results didn't show methane capture by the fungi. Given the Special physiology of fungi and the evidences that showed methane capture by fungi, I would suggest further investigation and with an optimized system.

3. **Kimberly Alley**

*Synthesis of a Fluorescent Enterobactin Derivative as a Diagnostic Tool for the Detection of Gram-Negative Bacteria*

**Advisor:** Valerie Pierre

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Connecticut College

**Abstract:** Acute cystitis (UTI) is one of the most common diseases that requires antibiotic therapy. The gram-negative E. Coli accounts for up to 75-95 % of normal genitourinary tract infections. Current diagnostic tests – urine dip sticks and cultures – are not useful due to either poor sensitivity or testing delays (~48 hr turnaround time), respectively. The bacteria responsible for acute cystitis obtain Fe (III) from the environment via the regulated production of low molecular weight compounds called siderophores. Enterobactin, a type of siderophore primarily produced by these enterobacteriaceae, captures Fe (III) via coordination chemistry, and is recognized by the gram-negative bacteria using the receptor FepA. Enterobactin derivatives can be recognized by gram-negative bacteria via the same mechanism as their analogue. This poster presents preliminary results of the synthesis of an enterobactin derivative that could act as a diagnostic tool with comparable accuracy to urine culture but with reduced wait time. In future studies, the derivative will be equipped with a fluorescent moiety, and will be tested against several gram-negative enterobacteriaceae.

4. **Oluwatosin Alliyu**

*GroupStart: Incorporating Group Projects into Moocs*

**Advisor:** Haiyi Zhu

**Sponsoring Program:** Computer Science

**Home Institution:** Haverford College

**Abstract:** GroupStart: Incorporating Group Projects into MOOCs

Massive Open Online Courses (MOOCs) give students free access to high quality, educational content on a global scale. They provide an online learning environment where diverse groups of students can satisfy their academic interests. However, most MOOCs rely on individual activities, which means collaborative activities such as group projects are difficult to implement. Many challenges exist in designing a MOOC group project such as establishing group accountability, accounting for high attrition rates, and allowing for the vast diversity of MOOC students. While many effective group communication and task management systems currently exist, few software platforms focus on online group projects. We introduce GroupStart; an experimental web application that seeks to facilitate the formation of groups as well as the establishment of familiarity among group members in a MOOC group project. We implement different group formation algorithms to test levels of homogeneity and heterogeneity within groups based on different attributes. In an effort to establish familiarity among group members, we provide a platform for students to create a shared document to establish their group purpose, goals, and communication methods. We will use GroupStart to test different mechanisms for establishing group accountability in the early stages of online group work.

5. **Bret Andersen**

*Synthesis of Several Tetrazine Products for their use as Trapping Substrates in the HDDA Reaction*

**Advisor:** Thomas Hoye

**Sponsoring Program:** UROP

**Home Institution:** University of Minnesota

**Abstract:** In this project, sponsored by the University of Minnesota's UROP program, we synthesize three substituted tetrazine molecules for use as "trapping" substrates in the Hexadehydro-Diels-Alder (HDDA) reaction. Tetrazines are molecules which resemble benzene molecules in that they contain an aromatic 6-membered ring moiety; the key difference being that the carbon atoms in the 1,2,4, and 5 positions in benzene are instead nitrogen atoms in tetrazine molecules. In this project, three tetrazine molecules are synthesized in a two-step reaction wherein, in the first step, two (in some cases substituted) benzonitrile molecules are joined together in a reaction with hydrazine. The product of this reaction is then oxidized using sodium nitrite to yield the desired tetrazine product with aromaticity across three rings (two benzene rings and a central tetrazine ring). These tetrazine products are of interest because they can be used to "trap" reactive benzyne intermediates generated in the HDDA reaction. The products of these benzyne trapping reactions are of further interest because, in highly aromatic instances, they often have intense fluorescent activity under ultraviolet light, making them potentially attractive for use in organic LED (OLED) devices. Such tetrazines, then, make interesting "trapping" substrates since they both represent novel chemistry in and of themselves, and because they have the potential to add large aromatic moieties to HDDA products, perhaps resulting in new, highly-fluorescent compounds.

6. **Fiona Armstrong-Pavlik**

*Detection of Bacteria through Siderophore Uptake and Fluorescence*

**Advisor:** Valérie Pierre

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota - Twin Cities

**Abstract:** Urinary tract infections (UTI) are among the most commonly occurring bacterial infections in people (3). If it is not detected and treated at an early stage, a UTI can spread to the kidneys and the rest of the body, causing sepsis; therefore, a rapid and accurate method for diagnosis of UTI is needed (2). Bacteria including *E. coli*, a common cause of UTI, secrete a type of small molecule called a siderophore to take up iron, a mineral essential to their survival (1). The goal of this project has been to test the efficacy of a UTI detection agent that is structurally similar to enterobactin, one of the siderophores produced by *E. coli* (4). The detection agent contains a fluorescent dye and is in complex with gallium, a metal that shares similar properties with iron but is inactive in bacterial metabolic pathways. Due to the addition of a fluorescent probe attached to the siderophore backbone, the detection agent will be able to be used to diagnose an infection after a short incubation time (around 20 minutes) using a fluorimeter, which will be significantly faster than waiting at least 48 hours for a bacterial culture, the current most accurate diagnostic tool (3).

7. **Gregory Aronson**

*Incorporating Quorum Consistency in the Tiera/Wiera Framework*

**Advisor:** Abhishek Chandra

**Sponsoring Program:** Computer Science

**Home Institution:** George Mason University

**Abstract:** Data distributed across the cloud can offer efficiencies in storage, retrieval, and analysis, as well as redundancy to prevent data loss. To fully capitalize on the benefits of distributed data, policies for storage and retrieval must be individually tailored to the needs of the user, such as fast retrieval, parallel processing in the cloud, or redundancy. To manage data across multiple large-scale cloud storage systems, such as Amazon's S3 and Microsoft's Azure, the middleware Tiera/Wiera was created here at UMN, which enables the provision of multi-tiered cloud storage instances that are easy to specify, flexible, and enable a rich array of storage policies. Depending on the purpose for storage, several different protocols exist that allow these storage systems to replicate data across multiple data centers. Consistency policies dictate how data is propagated amongst different storage centers and each have tradeoffs. For example, the Strong Consistency Policy emphasizes accuracy at the cost of efficiency. Conversely, the Eventual Consistency Policy underscores efficient data propagation with the concession of reliability. Thus it is important that systems offer a diverse set of consistency models to accommodate the varying needs of storage replication and fault tolerance management. To extend the set of policies available to users in the current Tiera system, we are implementing the Quorum consistency policy to create a middle ground between Eventual and Strong consistency models. The Quorum Policy is a flexible Consistency Policy that guarantees Strong or Eventual consistency in an efficient manner by maintaining a set of constraints. Moreover, these parameters can be altered to customize efficiency based on user specifications. My focus is the implementation of the Quorum policy to ensure data integrity efficiently and create an interface where the user can change the parameters mentioned above.

8. **Jesus Au**  
*High modulus and Conductivity Polymer Electrolyte Membranes*  
**Advisor:** Timothy Lodge  
**Sponsoring Program:** MRSEC  
**Home Institution:** New Mexico State University  
**Abstract:** Solid polymer electrolyte membranes offer many advantages over traditionally used liquid electrolytes, such as the capability of storing higher energy densities while addressing hazard concerns associated with liquid electrolytes. So far, lithium ion batteries have allowed us to store more energy, yielding smaller, more powerful and reliable devices, but still, fail to reach their full potential due to problems associated with the use of a liquid electrolyte. Liquid electrolytes allow the unobstructed formation of dendrites capable of spanning the electrolyte reducing performance and ultimately causing failure of the batteries. The liquid is composed of volatile and flammable species which raise hazard concerns especially during short-circuiting of the battery. A solid state electrolyte exhibiting orthogonal mechanical robustness and high ionic conductivity allows the possibility of achieving higher energy density storage devices without compromising reliability and safety in rechargeable electronics. We propose using a solid polymer electrolyte exhibiting simultaneous high modulus, high ionic conductivity achieved via polymerization induced microphase separation (PIMS) to suppress dendrite formation on the electrolyte. To improve on previous work is done we proposed the addition of succinonitrile into the PIMS system, which has allowed a remarkable increase in the orthogonal properties of similar prior systems.
9. **Taysir Bader**  
*Structural and Functional Characterization of Arrhythmogenic Q136P Calmodulin Mutant*  
**Advisor:** Gianluigi Veglia  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** Minnesota State University Moorhead  
**Abstract:** Calmodulin (CaM) is a calcium-binding regulatory protein that influences many key processes in eukaryotic cells. One such process is modulating calcium release from the sarcoplasmic reticulum of cardiac muscle cells by regulating the calcium channel RyR. This in turns regulates the relaxation rate of ventricular cardiomyocytes. Mutations in CaM can lead to several chronic heart diseases such as ventricular arrhythmias. One such mutation is Q136P where a glutamine residue in one of CaM's calcium binding sites is replaced with a proline residue. In this study the calcium dependent dynamics and thermo-stability of the Q136P mutant were characterized using solution state nuclear magnetic resonance (NMR) and circular dichroism.
10. **Paola A. Baldaguez, Mammad Nasiri, Derek Saxon**  
*Isosorbide Based Triblock Copolymer for Thermoplastic Elastomers*  
**Advisor:** Theresa Reineke  
**Sponsoring Program:** Center for Sustainable Polymers  
**Home Institution:** University of Puerto Rico at Mayagüez  
**Abstract:** Novel environmentally friendly materials that are produced from sustainable and functional polymers have recently drawn great attention to improve the quality of our lives without further contamination of our environment. Isosorbide is a sugar derivative that is being studied for incorporation into block copolymers. Exo-acetyl isosorbide (AI) was synthesized and purified via column chromatography on silica gel. AI was then acrylated to afford endo-acryl-exo-acetyl-isosorbide (AAI), which was subsequently used, as the hard segment, to produce ABA-type triblock copolymers as thermoplastic elastomers, utilizing n-butyl acrylate (nBA) as the soft segment. Poly(n-butyl acrylate) (PnBA) was synthesized using Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization to be able to controllably target the desired molecular weights. An outgrowing bifunctional chain transfer agent (CTA) was employed and PnBA macro-CTAs in a range of 71–87 kDa were synthesized. Subsequently, PnBA was chain-extended with AAI via RAFT polymerization to afford PAAI-PnBA-PAAI triblock copolymers. Triblock copolymers containing  $\geq 30\%$  of the isosorbide-based monomer were prepared and characterized Nuclear Magnetic Resonance (NMR) spectroscopy, Gel Permeation Chromatography (GPC), Thermal Gravimetric Analysis (TGA), and Differential Scanning Calorimetry (DSC).

11. **Francisco Balderrama**, Paul Fiesel, Jerry D. Cohen  
*Hydrogen Deuterium exchange at various pH and acidic solutions using gas chromatography–mass spectrometry*  
**Advisor:** Jerry Cohen  
**Sponsoring Program:** Project SEED  
**Home Institution:** Harding High School, SPPS  
**Abstract:** In plant growth, indole3acetic acid (IAA) plays a vital role in cell division, as well as cell elongation. The hormone is often used by plant researchers to observe plant growth. Along with studying indoleacetic acid, researchers often study tryptophan due to its functions in plant growth during synthesization of proteins. In a previous study, University of Tasmania researchers had studied hydrogen/deuterium exchange on aromatic rings in several indole compounds. In the current experiment, there is an ongoing investigation on hydrogen/deuterium exchange on several IAA and Tryptophan compounds with each sample containing a different number of deuterium. The experiment focuses on testing the effects of changing the pH due to its relation to hydrogens, and changing the conditions the plant hormone compounds by using amino columns. In the experiment, deuterium exchange will be noticeable with the change of mass through a gas chromatography mass spectrometry.
12. **Tsvetelina Baryakova**  
*The Non-Specific Targeting of GL261-luc Mouse Glioma Cells using Self-Assembling ssDNA Nanotubes*  
**Advisor:** Efi Kokkoli  
**Sponsoring Program:** Chemical Engineering  
**Home Institution:** University of Minnesota  
**Abstract:** Traditional chemotherapeutic agents are delivered in a non-specific manner to prevent the mitosis of all rapidly-dividing cells in the body, effectively killing malignant and healthy cells alike. This leads to acute or chronically acquired toxicity that can manifest as severe fatigue, anemia, organ failure, and several other life-threatening complications. In instances where the cancer is fatal, 25% of patients will develop brain metastases at some point. Overcoming the blood-brain barrier is yet another obstacle for traditional, unpackaged chemotherapy drugs, as most are prevented from ever crossing from circulation into the brain parenchyma and the CNS. Nanoparticles are at the forefront of a relatively new branch of medical oncology because these nonviral drug delivery systems can be targeted either passively or actively to tumors to reduce non-site specific cytotoxicity, and have demonstrated potential in serving as colloidal drug carriers to brain. Of interest to us is a modified aptamer-amphiphile created from a hydrophilic ssDNA sequence conjugated with a hydrophobic tail that has self-assembled to form nanotubes. Using confocal imaging techniques, we are interested in seeing if this small “vehicle” will passively be incorporated into luciferase-expressing mouse glioblastoma cells in-vitro via simple diffusion across the cell membrane. Our goal in the future is to hybridize these nanotubes with a specially-engineered aptamer, a highly-stable active targeting molecule that can bind to a unique cell surface protein found to be over-expressed in cancerous tissue, and study their affinity to the desired site.
13. **Jordan Baur**  
*Synthesis and NF- $\kappa$ B Inhibitory Activity of Helenalin-Based Analogues*  
**Advisor:** Daniel Harki  
**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen  
**Home Institution:** University of Minnesota  
**Abstract:** Helenalin, a sesquiterpene lactone found in plants from the *Arnica* family, exhibits anti-inflammatory effects *in vitro* via inhibition of the NF- $\kappa$ B signaling pathway and induces cell death in cancer cells. These biological effects are directly attributed to the  $\alpha,\beta$ -unsaturated carbonyls found in helenalin. Both the  $\alpha$ -methylene- $\gamma$ -butyrolactone and the  $\alpha,\beta$ -unsaturated cyclopentenone of helenalin react with cysteine sulfhydryl groups via Michael type additions. It has been demonstrated that helenalin directly modifies the transcription factor p65 of the p50/p65 NF- $\kappa$ B heterodimer through alkylation of Cys38, which prevents DNA binding. Additionally, it has been hypothesized computationally that helenalin undergoes a second Michael addition with Cys120. Because helenalin's covalent inhibitory properties offer a strategy to regulate aberrant p65 signaling, our group has developed a rapid, 6-step synthesis of simplified helenalin analogues from commercially available starting materials. Our chemical probes closely mimic the NF- $\kappa$ B inhibitory activity of helenalin via cellular reporter assays and provide the opportunity for the development of additional analogues that exploit the unique DNA-binding interface of p65. We have designed and synthesized a number of helenalin-based analogues by varying parameters such as stereochemistry, linker length, and the presence/absence of electrophiles. The synthesis and biochemical evaluation of our helenalin-inspired analogues will be presented.

**14. Brooke Benson**

*Olefins from Biodiesel: Decarbonylation using a Ruthenium catalyst*

**Advisor:** William Tolman

**Sponsoring Program:** Center for Sustainable Polymers

**Home Institution:** Luther College

**Abstract:** The goal of this study is to decarbonylate fatty acid methyl esters (FAMES), primary components in biodiesel, to long chain olefins. Previous efforts to accomplish such decarbonylation used supported metal catalysts at high temperatures (300 °C or higher) and yielded in a mixture of alkenes and alkanes as products. With the intent of improving selectivity for the olefin product by performing the decarbonylation at lower temperatures, we have explored the possibility of a tandem transesterification/decarbonylation reaction under homogeneous conditions. We hypothesized that FAMES could be transesterified with an alcohol featuring a donor/coordinating group to facilitate binding to the metal and hence, subsequent decarbonylation. Initial screening of Lewis acids, ligands, solvents and alcohols using a ruthenium catalyst, Ru<sub>3</sub>(CO)<sub>12</sub>, led to the identification of ZnCl<sub>2</sub>, PCy<sub>3</sub>, DMPU and pyridine-2-methanol as optimal components (Cy = cyclohexyl, DMPU = N,N'-Dimethylpropyleneurea). Under the optimized conditions achieved thus far, a 69 % yield of pentadecene(s) was obtained from the decarbonylation of methylpalmitate using 5 mol % Ru<sub>3</sub>(CO)<sub>12</sub> for 16 h.

**15. Alec Beri**

*Parallel Constrained Tensor Factorization with Fine-Grained Convergence*

**Advisor:** Shaden Smith

**Sponsoring Program:** Computer Science

**Home Institution:** University of Maryland

**Abstract:** AO-ADMM is a state-of-the-art algorithm for constrained tensor factorization. At the heart of AO-ADMM is a set of optimization problems operating on a large dense matrix. These optimization problems iteratively execute a sequence of dense matrix kernels, each of which are parallelized over the rows of the matrix. We reformulate the optimization problems to instead operate on independent row-wise chunks of the matrix. Each chunk can be processed until convergence, totally in parallel, and the numbers of iterations necessary for convergence differs for each chunk. By operating on each chunk individually, the number of iterations per row is and total amount of work done is reduced. Additionally, by operating on chunks in parallel, AO-ADMM only needs to synchronize after all parallel chunking operations have completed. When the chunk size is sufficiently small, all data necessary to operate on a chunk may be found in the cache, reducing computation time further. We noticed speedup of 3x in several large tensors due to reduction of the number of iterations necessary for convergence and speedup of 2x in other tensors due to thread synchronization and improved cache locality.

**16. Jasmin Bretoi**

*Development of a Polymer Scaffold to Promote Cardiac Regeneration*

**Advisor:** Samira Azarin

**Sponsoring Program:** MRSEC

**Home Institution:** Bethel University

**Abstract:** Myocardial infarction (i.e. heart attack) occurs when blood is occluded to the heart, resulting in cardiomyocyte death. Because of the lack of regenerative capabilities in the heart, the damaged myocardium is replaced with non-contractile scar tissue. The aim of our lab is to induce endogenous regeneration of the myocardium by the delivery of proliferation agents to the infarcted area via a polymer scaffold. To be used in the heart, the scaffold must be biocompatible, biodegradable, and reflect the mechanical and electrical properties of the native myocardium. Additionally, the scaffolds must be fabricated in a controlled and reproducible manner. Our goal is to investigate polymers for different aspects of cardiac regeneration. The first aspect of this project was to design polymers for identifying proliferation agents in a neonatal mouse heart. The second aspect is to investigate 3D printing as a method to create scaffolds and to control properties such as pore size, filament dimensions, and geometry. We found that the polymer Pluronic F127 can be used to make a gel for studies of neonatal mouse proliferation and that 3D melt extrusion of polycaprolactone (PCL) results in reproducible scaffolds, whose shape and geometry can be altered.

17. **Brenna Budaitis**

*Investigating Synthetic Routes Toward Optimally Obtaining a Carene-Derived Sustainable Polymer*

**Advisor:** Thomas Hoye

**Sponsoring Program:** Center for Sustainable Polymers

**Home Institution:** University of Michigan, Ann Arbor

**Abstract:** The polymer industry has traditionally relied on the use of petroleum-based resources in the production of commercially available plastics. Current research at the Center for Sustainable Polymers is investigating the use of biomass in hopes of constructing renewable and degradable polymers in order to (1) reduce the dependence on petrochemical feedstocks and (2) decrease society's carbon footprint. Terpenes are one of the largest groups of natural products, comprising of more than 30,000 derivatives, and have had successful applications toward the pharmaceutical, flavor, fragrance, and fuel industries. Among these, 3-carene is the third most abundant terpene derived from turpentine and can be purchased in large quantities at a reasonable price, making it a promising alternative route towards constructing a bio-based polymer. Surprisingly though, little research has been pursued regarding the use of 3-carene as a monomer. To this end, we are working to optimize a synthetic route to a carene-derived  $\epsilon$ -caprolactone that we have successfully polymerized via a ring-opening transesterification polymerization. These syntheses will provide us with better insight into the properties and potential of 3-carene and hopefully help guide the future direction of implementing sustainable polymers developed from natural, renewable resources.

18. **Alejandro Buendia**

*Efficient Computation of the Random Walk Fundamental Tensor using Low Rank Perturbations*

**Advisor:** Daniel Boley

**Sponsoring Program:** Computer Science

**Home Institution:** Columbia University

**Abstract:** A random walk over a strongly connected directed graph (digraph) can be modeled by an irreducible Markov chain. For a fixed target node, the fundamental matrix provides the expected number of passages through intermediate nodes for all pairs of source and middle nodes. Golnari et al. propose a random walk fundamental tensor that generalizes the fundamental matrix for all triples of source, middle, and target nodes. In this work, we introduce an algorithm with  $O(n^3)$  complexity for computing the fundamental tensor of a strongly connected digraph of order  $n$ , improving on Gaussian elimination-based approaches that run in  $O(n^4)$  time. The method is based on applying rank-one updates to the Moore-Penrose pseudoinverse of the digraph's Laplacian to quickly calculate submatrix inverses. This algorithm holds applications in the analysis of networks, which are represented as digraphs, by allowing for fast calculation of hitting times and absorption probabilities. Centrality measures such as betweenness and closeness can be determined from the fundamental tensor and indicate the relative importance of nodes within a network. The algorithm's complexity is verified on synthetic examples of networks. Finally, we show that the algorithm can efficiently calculate properties of strongly connected components of real social networks. This calculation is used to identify the most influential user within a social network.

19. **Dion Casey**, Nikolas Wilkinson, Athena Metaxas  
*Controlling the Polymeric-Anisotropic Particle Flocculation Mechanism*  
**Advisor:** Cari Dutcher  
**Sponsoring Program:** MRSEC  
**Home Institution:** Saint Augustine University  
**Abstract:** Water treatment facilities utilize various purification process to reproduce clean consumable water. Flocculation is the process in water treatment that aggregates and sediments suspended particulates before filtering, generally using. This process utilizes a cationic polyacrylamide, poly(1-carbamoylethylene), polymers that complexes to the surface of anionic particles. Controlling the polymer behavior in flocculation is critical for many applications including, composite material, paper manufacturing, and including composite materials, paper manufacturing, and water treatment. Flocculation behavior is dependent on many parameters including, particulate identity, zeta potential, solution pH, ionic strength, and local hydrodynamics (Sshear ). Here, FfFlocculation performance (final turbidity)turbidity reduction ) was measured as a function of solution added NaCl ionic strength and polymer charge percent , at a constant pH of 6.6 and , hydrodynamic profile, and bentonite concentration of 30 mg/L. The charge percent'spercents used tested are were 1.5%, 10%, 20% and 60%. Increasing ionic strength reduced the optimum polymer dose for all polymer charge percent tested, due to an increase in initial bentonite aggregate size and reduction in electrostatic repulsion. Increasing the polymer charge percent initially from, decreased the optimalum polymer dose., then increased it, possibly due to a change in flocculation mechanism. The charge percent's used are 1.5%, 20% and 60%. Atomic Force Microscopy (AFM) was used to visualize the surface structure of the bentonite aggregates prior to flocculation and to measure the attractive force between the bentonite and polymer for various surface structures and ionic strengths. The porous, edge-face surface structure resulted in the strongest polymer-bentonite interaction. This work sheds light on the complexities of polymer flocculation towards improving reagent polymer dosing and treatment optimization for important applications such as water purification.
20. **Yevedzo Chipangura**  
*Li8ZrO6: A Cathode Material for Lithium-ion Batteries*  
**Advisor:** Andreas Stein  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** University of Minnesota  
**Abstract:** Rechargeable Li-ion batteries are currently in high demand for use in electronics, electric vehicles, medical and energy storage devices. Li-ion batteries are currently being limited by the low specific capacity of the cathode (170-200mAh/g) compared to the anode (1000mAh/g). To compensate for this difference, a greater volume of the battery is dedicated to the cathode. Li8ZrO6 (LZO), a potential cathode material, has a layered structure suitable for intercalation and deintercalation of lithium, high Li-to-mass ratio with a high theoretical specific capacity of 221mAh/g according to computational calculations. In this work, LZO was synthesized by pyrolysis under nitrogen different carbon based lithium precursors: lithium benzoate and lithium acetylacetonate with zirconium precursor. The carbonization yielded an intimately mixing of LZO with a conductive phase, carbon. The grain size of LZO is reduced to 30-50 nm using ballmill. X-Ray Photoelectron Spectroscopy showed a shift of O1s peak during the charging process confirming that oxygen ion near the Li vacancy is oxidized.
21. **Samsam Dirie**, Xin Chen  
*Development of an iron (II) selective electrode through the synthesis of a new phenanthroline dicarboxylate-based ionophore*  
**Advisor:** Philippe Buhlmann  
**Sponsoring Program:** Project SEED  
**Home Institution:** Harding High School, St Paul, MN  
**Abstract:** From detecting iron (II) ions in lake water to diagnosing anemia, the detection of iron (II) in aqueous samples is crucial. This experiment seeks to develop an iron (II) selective electrode that can detect ions in various settings by synthesizing a new ionophore to serve as a carrier compound to selectively detect iron (II) ions in aqueous solutions. To achieve this goal, we plan to synthesize dioctyl 1,10-phenanthroline-2,9-dicarboxylate— a suspected carrier of iron (II)— to be incorporated into the sensor's polymeric sensing membrane. The reaction consists of the combination of alcohol and diacid to create our desired ester product. Future work will search to define a specific range of detection for the sensor, as well as confirm the selectivity for iron (II) versus similar metal ions such as iron (III) or zinc.

- 22. Jennifer Donohue**, Karl Schliep  
*Modeling Pulsed Laser Heating of Multi-Layered Solids*  
**Advisor:** David Flannigan  
**Sponsoring Program:** MRSEC  
**Home Institution:** Binghamton University  
**Abstract:** Ultrafast pulsed laser systems have enabled researchers to investigate processes which occur on femtosecond (fs) timescales. One such application is ultrafast electron microscopy (UEM) which relies on fs laser pulses to initiate reversible processes in defined specimen geometries. Photothermal accumulation and dissipation currently limit the frequency at which the reversible processes can be stimulated. A pulsed laser heating model was developed using the finite difference method to solve the heat equation in the rectangular coordinate system. The model includes a power generation term which simulates the laser heat absorption calculated using standard and experimentally determined optical properties. A radiative boundary condition simulates the vacuum heat exchange through thermal radiation. The model was then calibrated using an aluminum sample. Ultrafast Electron Diffraction (UED) was used to calculate the temperature change in an aluminum specimen. This data was compared to the model-predicted temperatures. The model was then adapted to several specimen geometries including, wedge, flake and rectangular samples. The model allows for the determination of the instantaneous temperature at any point within a multi-layer sample as well as the final steady state temperature at any radial distance after a specified number of pulses. Finally, the model was utilized to predict the temperature in ferrimagnetic terbium cobalt films at which all optical magnetic switching occurred. Further testing of the model using known materials will be used to determine the accuracy of the model-predicted temperatures in wedge and flake specimens. The addition of a third dimension to the model allows for the determination of instantaneous and steady state temperatures at specific specimen depths. However, further optimization of that program will be needed to increase general efficiency.
- 23. Sarah Dotzler**  
*Bimetallic Interactions of Dysprosium and Lutetium Paired with Group 10 Metals*  
**Advisor:** Connie Lu  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** University of Minnesota  
**Abstract:** Group 10 metals such as Ni, Pd, and Pt have been widely explored in catalysis. However, when paired with heavier metals, such as lanthanides, the catalytic activity of the group 10 metals can be enhanced. Bimetallic compounds are now being studied for unique properties in catalysis. Our research has been focused on creating bimetallic complexes of NiLu conjugated with ligands of varying electronic properties as well as MDy compounds with the 3 specified group 10 metals. Details of the synthesis, characterizations, and potential catalytic properties will be discussed.
- 24. Mark Dresel**  
*Phosphate Recycling*  
**Advisor:** Valerie Pierre  
**Sponsoring Program:** MSROP  
**Home Institution:** University of Minnesota  
**Abstract:** Phosphates are vital ions that serve many important functions in the environment as a staple of most lifeforms. Agriculturally, phosphate is one of the limiting factors in our ability to produce food. Unfortunately, the misallocation of phosphates into the water supply leads to an overabundance of these vital nutrients. This overabundance of nutrients, called eutrophication, is responsible for many destructive changes to the ecosystem. Among these changes are low oxygen saturation in the water system due to the overabundance of autotrophs and toxins produced by algae blooms. Additionally, phosphate rock, which is the source of most commercially available phosphate, is exorbitantly high in price and difficult to negotiate politically. Thus, the need arises for an effective solution able to recycle the phosphate currently damaging the environment. Hard metal complexes with hard metal centers provide effective sensing of phosphate in addition to a "catch and release" mechanism, which will allow for the recycling of phosphate. Gd-TRENMAM has been synthesized and has been shown to bind to phosphate in environmental conditions. In addition, this metal complex is selective towards phosphate in the presence of other anions and releases the phosphate at reduced pH. This system is a possible candidate to recycle phosphate.

**25. Ayele Ekue**

*Extracellular Enzyme Activity in Prairie Pothole Lakes*

**Advisor:** Brandy Toner

**Sponsoring Program:** Northstar STEM Alliance

**Home Institution:** University of Minnesota

**Abstract:** Prairie pothole lakes (PPL) in North Dakota play an important role in preserving organic carbon. These wetlands contain sediments which have a high temperature and basic pH, high surface area and biomass (Arnosti et al. 2014; Zeng et al. 2013). Within these PPL sediments, microorganisms produce extracellular (exo) enzymes, which play an important role in carbon cycling (Arnosti et al. 2014). (Currently, there is limited understanding of how physical properties affect the activity of exo-enzymes within lake sediments). In this study we aim to understand how exo-enzyme activity is influenced by mineralogy, organic carbon (OC), and storage techniques. To explore OC-mineral and exo-enzyme mineral interactions, six sediment cores were collected from P1 at the Cottonwood Lake study area near Jamestown, North Dakota, with each undergoing a different storage procedure. Additionally, cores were split and subsampled from the top, middle, and bottom of the core to understand changes in exo-enzyme activity down core. Mineralogy and surface area was investigated through powder X Ray diffraction and Brunauer–Emmett–Teller (BET), respectively. Exo-enzyme activity for carbon, nitrogen, and phosphorus were measured using fluorescent assays.

**26. Anna Folska**

*Analyzing the Different Membrane Interactions 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. The popular CPP, Tat (transactivating transcription factor) peptide, is non-structured, with 8/11 residues being arginine or lysine, providing dense positive charge. It has been shown to enter cells via energy-dependent endocytosis. Pep-1, a 21-residue amphiphilic CPP, traffics cargo to the nucleus once inside. It is known for its fast and strong membrane interaction, superior delivery rates and low toxicity. Pep-1 is thought to directly penetrate cell membranes instead of using an endocytosis pathway, which could lead to higher internalization rates and efficiency of attached drugs due to not having to escape endosomes. The interaction between these CPPs and model lipid membranes is being studied using isothermal titration calorimetry (ITC). Results showed that Tat binds anionic lipid (POPG) membranes but not neutral (POPC) ones, suggesting an electrostatic mechanism. This conclusion was confirmed by an observed dependence of binding constant on buffer ionic strength. Pep-1, however, was shown to bind both POPC and POPG membranes, suggesting different interactions play a role. With these results, the nature of binding between these CPPs and model membranes can be determined, which hopefully sheds light on the different cell uptake mechanisms.

**27. Jessica Freeze**

*Predicting Catalytic Activity for Caprolactone Polymerization through Framework Distortion Analysis*

**Advisor:** Christopher Cramer

**Sponsoring Program:** Center for Sustainable Nanotechnology

**Home Institution:** University of Rochester

**Abstract:** The search for sustainable polymers has made many advances in replacing traditional nonrenewable plastics. In order to compete with traditional polymers, the polymerization rate of the lactide based polymers must be increased. One way this may be done derives from the distortion interaction hypothesis which states a two step mechanism for reaching a transition state. The rate limiting step in the hypothesis is the distortion, which lengthens and weakens the bonds of reactants. Thus, by lowering the distortion energy, one can expect to increase the rate of polymerization reaction. Based on previous studies, the manipulation of the catalyst used in the caprolactone polymerization causes the greatest differences to the distortion energy of the reaction. This study applied modifications to the ligand system of the catalyst in order to analyze the changes in reactivity and to discover a catalyst with minimum distortion energy and thereby, maximum rate of polymerization. Throughout the study, the importance of including the polymerization alkoxide in tests was also examined. Tests were run computationally using DFT. Long term goals include further testing of promising catalysts along the pathway to transition state, followed by experimental testing of the best catalysts for  $\epsilon$ -caprolactone polymerization.

28. **Tom Frost**

*Genetic Editing of HSV-1 with CRISPR/Cas9 to Knockout Viral Envelope Glycoprotein C*

**Advisor:** Stephen Rice

**Sponsoring Program:** UROP

**Home Institution:** University of Minnesota

**Abstract:** Glycoprotein C (gC) is a herpes simplex virus type 1 (HSV-1) envelope glycoprotein thought to play a significant role in the release of progeny virions from the plasma membrane of a host cell. During preliminary studies in a gC-lacking mutant designated d44, reduced progeny titers and lower fractions of released progeny were observed relative to wild-type (WT). Quizzically, larger plaques were formed by d44 as compared to WT HSV-1. In order to evaluate the discrepancy, an independent gC-lacking HSV-1 strain needed to be produced. To generate this mutant, the CRISPR/Cas9 gene editing system was used to induce an early frameshift in the HSV-1 gC gene, resulting in its knockout. pX330, a plasmid containing the CRISPR/Cas9 system, was cleaved with BbsI, separated on an agarose gel, and subsequently isolated. Two 21 base pair DNA target sites for Cas9-mediated cleavage were located in the beginning of the gC gene coding region, and designated Target 1 and Target 2. These targets were cloned into the pX330 plasmid and the resulting plasmids, pX330-gC-T1 and pX330-gC-T2 were sequenced for accuracy. To successfully generate a HSV-1 gC-lacking mutant, HSV-1 DNA was required. HSV-1 DNA was isolated from WT HSV-1 virions and assayed for relative infectivity against known infective HSV-1 DNA. After confirmation of infectivity, HSV-1 DNA and either pX330-gC-T1 or pX330-gC-T2 were transfected into Vero cells and plaque purified. At the time of presentation, the resulting mutant viruses were plaque purified 3 times but were not yet sequenced so it is not yet known if the viruses produced were the correct mutant.

29. **Philipp Gemmel**

*Substrate Scope Study of Tandem Acyl C-O/Aryl C-H Bond Activation*

**Advisor:** Chris Douglas

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Grinnell College

**Abstract:** In the past, organic chemists have put considerable work into developing novel and useful functionalization reactions of aryl C-H bonds to provide tools for organic synthesis of desired molecules. Especially the inert nature of such bonds has made these efforts difficult. Reactions like the Lewis-Acid catalyzed Friedel-Crafts Acylation have become hallmarks in aromatic functionalization. However, the Friedel-Crafts reaction's electron-based regioselectivity has shown to be a challenge. We present a novel, transition metal catalyzed reaction that overcomes the limiting regioselectivity of the Friedel-Crafts Acylation by a proposed Tandem Acyl C-O/Aryl C-H activation favoring less sterically hindered aryl positions. Further advantages of this reaction are a better atom economy, lack of heavy metal byproduct and no required previous functionalization of the reagents, providing us with a greener, more accessible and direct synthesis of biaryl ketone derivatives. In this project, we tested a range of arenes to determine the substrate scope of our reaction to inform future research into optimizing the reaction and to provide new methods for the total synthesis of natural products. The natural product hydroxyphenstatin with its anti-mitotic properties and other members of the phenstatin family are interesting targets further motivating this study.

30. **Francisco Gomez**

*Photoelectron Spectroscopic Characterization of Anionic Complexes*

**Advisor:** Doreen Leopold

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota

**Abstract:** Anion photoelectron spectroscopy was used to study the interactions of anionic complexes containing metal-metal bonds with carbon dioxide. This class of molecule appears in several complexes which exhibited the ability to reduce gases such as nitrogen and carbon dioxide, and carbon dioxide is especially interesting due to its presence in the industrial waste stream. Foundational studies on simple metal dimer complexes were performed in the interest of indicated potential for more complicated catalytic systems which would be able to utilize carbon dioxide. Metal-metal systems which were tested included niobium, cobalt, and iron complexes with tungsten and carbon dioxide. Cobalt and iron complexes using that metal in cathode form were undetected in our system. We were unable to determine conclusively whether this inability to detect the complex were due to poor tuning conditions or due to instability inherent to the complex. The niobium and tungsten system was extremely robust, and the results of the experimentation with this system is reported. Computational modelling with Gaussian was used to identify the geometric structure of observed complexes as well as labeling of energy states and vibrational modes. The electron affinity, as well as the bond dissociation energy, is reported.

**31. Kelsey Harmatta**

*Controlling Resistivity in Barium Stannate*

**Advisor:** Chris Leighton

**Sponsoring Program:** MRSEC

**Home Institution:** Macalester College

**Abstract:** Recent research into Lanthanum doped Barium Stannate ( $\text{BaSnO}_3$ ), both single crystals and thin films have shown the semiconductor to have very high carrier mobility, an essential trait for electronic applications. I will be working with oxygen-vacancy-doped  $\text{BaSnO}_3$  thin films from beginning to end. After making films with plasma deposition, I will use x-ray diffraction to evaluate the quality of the film and the thickness of the films. Once characterized I will pattern the films into Van der Pauw geometry using ion-milling to create devices ready for electrical transport measurements. The prepared devices will be used in ion gel gating experiments to control and alter the carrier density in the film. By placing ion gel across the film and the gates and applying a gating voltage the charge carrier density can be controlled. Ion gel gating has the ability to induce a charge carrier density exceeding  $10^{14} \text{ cm}^{-2}$  in materials. Altering the gating voltage should produce changes in the carrier density which cause changes in the resistance of the films. Applying a positive gate voltage reduced the resistance and applying a negative gate voltage increased the resistance. The resistance differs by two orders of magnitude between a negative gate voltage of 1.5 and a positive gate voltage of 3. When gate voltages of less than 2.5 were applied the average reversibility was a ratio of  $1.07 \pm .15$ .

**32. Bruno Hespanhol**

*Symbiotic bio-remediating biofilms for cleaning nutrient polluted waste waters*

**Advisor:** Bo Hu

**Sponsoring Program:** MSROP

**Home Institution:** University of Minnesota - Department of Bioproducts and Biosystems Engineering

**Abstract:** The purpose of this research is to understand the relationship between the addition of carbon source, the removal of  $\text{NH}_4^+$  and the concentration of  $\text{NO}_3^-$ ,  $\text{NO}_2^-$  and Total Nitrogen and P concentration in the simulated water samples using a mixed culture biofilm, and the production of microbial proteins with respect to different C/N/P ratios.

**33. Kiersten Idzorek**

*Toward Solid-State Reactions Between Nitrile Oxides and Nitriles*

**Advisor:** William Ojala

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** Nitrile oxides are useful in the synthesis of heterocyclic compounds by means of 1,3-dipolar cycloaddition reactions; for example, reaction of a nitrile oxide with a nitrile in solution leads to the formation of a 1,2,4-oxadiazole. We are examining the possibility that nitrile oxides might be capable of co-crystallization with nitriles and that subsequent solid-state cycloaddition might yield a heterocyclic product different from that obtained upon reaction in solution (1,2,5-oxadiazole vs. 1,2,4-oxadiazole). Success of this approach requires a nitrile oxide sufficiently reactive to undergo cycloaddition with a nitrile but not so reactive that it reacts with either the nitrile or with itself (by dimerization) before the incorporation of both components into the crystal. Success also requires an overall similarity in molecular space-filling requirements between the components to allow formation of mixed crystals (solid solutions). Our observation that several nitrogen-containing heterocycles assume crystal structures isomorphous with their corresponding N-oxides suggests that nitriles may be capable of co-crystallization with their corresponding nitrile oxides. Having determined the crystal structure of the relatively hindered 2,6-dichlorobenzonitrile oxide in previous work, we have begun co-crystallization studies using 2,6-dichlorobenzonitrile oxide and 2,6-dichlorobenzonitrile and describe our initial results here.

**34. Chinwenwa Iheme**

*Aerobic Denitrification*

**Advisor:** Satoshi Ishii

**Sponsoring Program:** Northstar STEM Alliance

**Home Institution:** University of Minnesota Twin Cities

**Abstract:** Nitrous oxide, the product of most aerobic denitrification, has a harmful effect on our environment. Denitrification is usually carried out in anaerobic conditions. There are also some bacteria that carry out denitrification in aerobic conditions producing N<sub>2</sub> as a reaction byproduct. In this study, we are going to measure the rate at which N<sub>2</sub>O is reduced by denitrifying bacteria, as well as oxygen consumption rate of the bacteria strains. I grew *Ochrobactrum* sp. strain TS6 and *Pseudomonas* sp. strain S-14, both aerobic denitrifiers, on Lb+ Nitrite media and incubated these cultures at 30°C for 4-5 days. I also grew anaerobic denitrifiers *Azospirillum brasilense* strain Sp7, *Noviherbaspirillum autotrophicum* strain TSA66, and *Pseudogulbenkiania* sp. NH8B on R2A+ nitrate +acetate media and incubated at 30°C 4-5 days. Next, I exchanged all gases in the bacteria cultures for N<sub>2</sub> and incubated at 30°C for 3-5 days. After washing bacterial pellets with 10mM PBS acetate buffer, N<sub>2</sub>O was bubbled into the measurement chamber and with a microsensor, I measured the rate at which N<sub>2</sub>O reduced to constant. I repeated the process using bubbled oxygen into the measurement chamber and measured the oxygen consumption rate. Results from aerobic denitrifiers TS6 and S-14 showed a reduction of N<sub>2</sub>O, however denitrifying rates differed between strains. Measurements for the remaining strains are still underway. Results obtained from my experiment should be useful in further investigation on strain specific -N<sub>2</sub>O removal under aerobic conditions.

**35. Francesca Ippoliti, Jack Queenan**

*Synthesis and characterization of three oleoyl-PEG orthoester micelles for drug delivery*

**Advisor:** Lisa Prevette

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** There are many considerations for the effective delivery of pharmaceuticals within the body, such as solubility, stability during circulation, targeting to specific cells, cellular internalization, intracellular trafficking and proper function once inside. These properties are determined by the chemical structure of the drug molecule. Drug delivery agents can be used to improve upon these properties by packaging the drug, providing reactive sites for targeting ligands and/or interacting with cell surfaces. Often, these delivery agents are micelles that can carry hydrophobic drugs and release their contents in a controlled way. Three new micelle delivery agents were synthesized from polyethylene glycol (PEG) and oleic acid linked through orthoesters. Orthoesters hydrolyze at varying rates in different pH environments and with different structural modifications; therefore, ring size and functional groups were varied. Characterization included determining critical micelle concentrations (CMCs) and orthoester hydrolysis rates using NMR, DLS, and spectrofluorimetry. These orthoester micelles will be further studied for their potential as a delivery agent for the chemotherapeutic doxorubicin to enhance its bioavailability and pharmacokinetics.

- 36. Elianna Isaac**  
*Phase and Size Control of CZTS Nanoparticles through Varying Capping Agents and Tin Oxidation State*  
**Advisor:** R. Lee Penn  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** University of Sioux Falls  
**Abstract:** Solar cells can provide clean energy to reduce the consumption of natural resources and satisfy growing energy demands. The principles of green chemistry can be applied to their production so as to minimize harm to the environment by reducing hazardous waste generated during mining and synthesis of absorber materials. The semiconductor  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) is a promising absorber material for solar cells because it has a band gap suitable for absorbing solar radiation and is composed of non-toxic, earth abundant materials. Both kesterite CZTS and wurtzite CZTS nanoparticles can be synthesized by reacting metal salts with sulfur-containing molecules in ethylene glycol in a microwave-assisted solvothermal synthesis. Materials were characterized using Raman spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction, and electron microscopy. Results demonstrate that both particle size and phase composition depend strongly on the identity of capping agent and the oxidation state of tin employed. Interestingly, syntheses using Sn(II) salts resulted in the formation of larger nanoparticles than for syntheses using Sn(IV) salts. In addition, the use of Sn(II) salts favors the production of the wurtzite phase. While 3-mercaptopropionic acid and thioglycolic acid produced larger nanoparticles, they also inhibited the control of the oxidation state of tin over the crystalline phase produced compared to L-cysteine. However, ethylene glycol was observed on the surface of the nanoparticles probably due to its stronger interactions with the nanoparticles than the capping agents.
- 37. Andrew Jewell**  
*Improving Predictive Models of Bike-Sharing Usage through the use of Meteorological Data*  
**Advisor:** Tian He  
**Sponsoring Program:** Computer Science  
**Home Institution:** Augsburg College  
**Abstract:** Bike-sharing systems are a new, convenient, and environmentally friendly public transportation option for people travelling within large cities. Due to time- and location-based differences in bicycle demand, ensuring each bike station has both enough slots for users to return bicycles and enough bicycles remaining for new users to rent through rebalancing (moving bikes via truck) remains a difficult problem. Current models of the net bike demand per station rely simply on historical and temporal data (the time of day, the day of the week, the week of the year, etc). To improve the accuracy of these models of net demand, meteorological data was incorporated into the existing model of bike demand. Through the use of publically available datasets including temperature, humidity, and weather-condition data, additional patterns of usage can be deduced. Although the historical model provides information about differing usage on weekends and holidays from weekdays, fewer people are likely to ride for pleasure during extreme temperatures or heavy rainfall. Using advanced regression algorithms, this analysis could greatly improve the effectiveness of the existing rebalancing operations, especially on days far from the median conditions.
- 38. Quinn Johnson**  
*A New Measure of Listening Effort in Normal Hearing and Hearing-Impaired Listeners*  
**Advisor:** Peggy Nelson  
**Sponsoring Program:** Northstar STEM Alliance  
**Home Institution:** Carleton College  
**Abstract:** In the deaf and hearing-impaired community, the use of cochlear implants and hearing aids has been widely successful. These devices have been able to restore speech understanding immensely among users. However, as of late there has been a stall in the increase of intelligibility. The cochlear implant (CI) industry has struggled to make improvements in their ability to deliver clear and comfortable speech for users, while people with hearing loss have struggled to find settings that work well for them. Due to this stall in intelligibility, research is now moving its focus toward estimates of listening effort. This study was conducted in an attempt to determine if the reaction time for repeating a word in a basic test of word recognition is a meaningful measure of the effort it takes to understand speech. If it is, it might lead to a clinical use in which hearing aid patients can set their device at the setting which requires the least effort.

**39. Kyle Johnson**

*Investigations of Surface Features Which Inform Cationic Gold Nanoparticle Toxicity to Bacillus Subtilis*

**Advisor:** Christy Haynes

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota-Twin Cities

**Abstract:** As nanoparticles continue to spread into both industry and consumer goods, it rapidly becomes an ecological imperative to understand potential impacts of these particles on environmentally relevant organisms. In order to understand the nanoparticle-cell interactions at a molecular level, we use cell-wall defected mutants of a model gram positive bacterium, *Bacillus subtilis*, to elucidate the key molecular components that govern the interactions. In particular, this work focuses on three mutants with variations on their wall teichoic acid chains (WTA), a prominent surface structure with relevance to reproduction and antibiotic resistance. In interactions with cationic MPNH2 functionalized gold nanoparticles (MPNH2-AuNPs), the mutant with only glucosylated WTAs was found to have the highest level of interaction, yet the differences resulted in little impact in toxicity among the three mutants, most likely due to the mild toxicity of the MPNH2-AuNP. Inquiries regarding the surface charge and more detailed assessment of mutant surface structures are in progress.

**40. Ryan Johnson**

*Solid-State Nitrile Oxide Dimerization: Crystal Structure of 2,3-Dichlorobenzonitrile Oxide*

**Advisor:** William Ojala

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** Nitrile oxides dimerize in solution to form three possible products: a furoxan, a dioxadiazine, or a 1,2,4-oxadiazole-N-oxide. We are using single-crystal X-ray diffraction to determine whether the molecular packing arrangement of the parent nitrile oxide determines which product is formed upon solid-state dimerization. We report here the crystal structure of 2,3-dichlorobenzonitrile oxide, formed by dehydrohalogenation of the corresponding hydroxamic acid chloride. This nitrile oxide crystallizes in the monoclinic space group P21/c with four molecules in general positions in the unit cell. Unlike our previously determined 4-chlorobenzonitrile oxide crystal structure, which includes close oxygen...chlorine contacts but no close chlorine...chlorine contacts, the crystal structure of 2,3-dichlorobenzonitrile oxide includes no close oxygen...chlorine contacts but does include close chlorine...chlorine contacts. A close centrosymmetric approach between neighboring fulminate groups suggests that the "head-to-tail" dioxadiazine or oxadiazole N-oxide dimers might be favored in a solid-state dimerization, but the large molecular motions possible even in the solid state render this conclusion speculative. Future work will involve the identification of the actual solid-state dimerization product as well as preparation of polymorphic forms of the nitrile oxide to determine any dependence of the product obtained on the crystal structure of the parent nitrile oxide.

**41. Nilay Kanova**

*Synthesis of Charge Enhanced TADDOL Catalyst*

**Advisor:** Steven Kass

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Middle East Technical University

**Abstract:** Hydrogen bond catalysts are examples of organocatalysts that utilize hydrogen bonding interactions to accelerate and control chemical reactions. These small, metal-free compounds are relatively simple to synthesize and are more robust and environmentally friendly than other types of catalysts. A specific hydrogen bond catalyst is  $\alpha,\alpha,\alpha',\alpha'$ -tetraaryl-2,2-disubstituted-1,3-dioxolane-4,5-dimethanol (TADDOL), which has been shown to catalyze Diels Alder cycloadditions, N-nitroso aldol and Wittig reactions. Recently, the Kass Group has shown the addition of positive charges into the structures of hydrogen bond catalysts increases their reactivities in nonpolar solvents. The acidity of the cationic hydrogen bond donor is greater than its neutral analogue, which leads to better coordination between the catalyst and substrate in organic transformations. Based on these observations, we have been working towards the synthesis of a positively charged TADDOL catalyst. Once obtained, we will compare its catalytic activity against previously reported TADDOL-catalyzed reactions.

**42. Margaret Klureza**

*Investigating the magnitude and origins of a voltage drop across the electrode | electrolyte interface in thin-film transistors*

**Advisor:** Daniel Frisbie

**Sponsoring Program:** MRSEC

**Home Institution:** Wellesley College

**Abstract:** Electrolyte-gated thin-film transistors (EG-TFT) present an extremely new promising new technology in the field of printed electronics. They are both highly sensitive and able to operate at extremely low voltages. Prior optimization of ion gel-gated EG-TFT devices revealed a persistent voltage drop that occurred across the gold gate electrode | ion gel electrolyte interface, limiting the overall efficiency. Initially, it was believed that this occurred due to a gold-specific interaction with the ion gel. Subsequent testing was done by utilizing alternate materials for the gate electrode, including platinum and the organic conductor PEDOT, in the hopes of both reducing the voltage drop and gaining insight into its origin. The devices were fabricated by using photolithography instruments in the Minnesota Nano Center to pattern electrodes onto silicon wafers. An aerosol jet printer was then used to print the semiconductor poly(3-hexylthiophene) and an electrolytic ion gel onto the electrode/silicon substrate. Characterization of the devices through IV curves revealed that the voltage drop was not unique to gold electrodes. Instead, those made with platinum showed nearly identical results to the gold. PEDOT electrode EG-TFT devices did show an improvement in efficiency, but further study is required to determine the underlying cause of the material-specific variation in efficiency.

**43. David Kraus**

*Pharmacokinetics of Human IL-1ra after Intraperitoneal and Intracerebral Injections of Kineret in Rats with Infantile Spasms*

**Advisor:** Lisa Coles

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota College of Pharmacy -Center for Orphan Drug Research

**Abstract:** Infantile spasms (IS) are epileptic seizures in infants and young children, which often lead to the emergence of other types of seizures, cognitive deficits, and neurodevelopmental disabilities. The current treatments are often ineffective and associated with numerous adverse effects. Thus, the long-term goal of this project is to identify a new therapy for IS that can effectively and rapidly achieve sustained suppression. One potential drug candidate is Kineret (Anakinra), a recombinant, non-glycosylated form of the human interleukin-1 receptor antagonist (IL-1ra). Objective: The objective of this work is to characterize the pharmacokinetics of the anti-inflammatory drug, Kineret in rat pups induced with infantile spasms following intraperitoneal (i.p.) and intracerebral (i.c.) dosing. Methods: Rat pups received either a single i.c. dose (298.6 ug) of Kineret or vehicle, or multiple i.p. doses (597 ug) of Kineret, one every 12 hours. Blood and brain samples were collected and human IL-1ra concentrations were measured using Quantikine® ELISAs. Results: Peak IL-1ra concentrations within brain samples were observed between 1 hour and 4 hours following the i.c. injection. IL-1ra levels were predominately higher in rat brain compared to rat plasma samples after i.c. injection. Following multiple i.p. doses, brain concentrations increased, but were between 10 to 170 times lower in concentration than in the plasma. This suggests that there was limited Kineret uptake in the brain. In addition, plasma concentrations were over 5 times greater after the 6 hours following multiple doses compared to the same time after a single dose even though the trough concentration returned to baseline. This suggests that perhaps a priming effect occurred resulting in increased IL-1ra activity after the subsequent exposure. Conclusion: This work demonstrates that while i.p. dosing results in increased IL-1ra brain concentrations, brain uptake is minimal. I.C. dosing resulted in increased brain concentrations of IL-1ra, however, it is not practical for clinical use. Future work includes evaluating other routes of administration in an attempt to attain similar brain concentrations as i.c. dosing.

**44. Anna Krieger**

*Electrochemical Detection of Chemical Messenger Secretion from Malarial Platelets*

**Advisor:** Christy Haynes

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Gustavus Adolphus College

**Abstract:** Blood platelets are small, anuclear, cell-like bodies that regulate processes such as thrombosis via secretion of molecular chemical messengers. Platelet exocytosis also plays a critical role in blood-relevant diseases such as malaria, a parasitic infection with no vaccine and increasing drug-resistance that disproportionately affects underprivileged youths in Africa. The Haynes lab has developed novel analytical techniques to characterize both bulk and single platelet secretion events. In this work, high performance liquid chromatography and carbon-fiber microelectrode amperometry, among other techniques, will be used to characterize blood platelet secretion in the context of malarial infection in an established mouse model to elucidate platelet functions that may be a target in future malaria treatment.

**45. Elizabeth Krinkie**

*Adhesion Quality Comparison of Ziegler-Natta and Metallocene-Catalyzed Polyolefins*

**Advisor:** Chris Macosko, Frank Bates

**Sponsoring Program:** MRSEC

**Home Institution:** Purdue University

**Abstract:** Polyolefins are polymers that are produced by the polymerization of alkenes with the general formula  $C_nH_{2n}$ . In our research, we tested the adhesion strength of the laminate between two different polyolefins: polyethylene (PE) and isotactic polypropylene (iPP). The overall goal of our project was to better understand what is happening during the adhesion process of PE and iPP to find a model to maximize the adhesion force between these two polyolefins. For our procedure a hot press was used to melt and form films of PE and iPP and then used to laminate the two films together. In order to determine the adhesion strength of the laminate, a solids analyzer rheometer performed a peel test by calculating the force required to delaminate the two polyolefins. From our results we are able to compare the differences between two catalyst methods used to produce polyolefins: a traditional method known as Ziegler-Natta and a more recently developed process which uses a single-site catalyst called metallocene. We predicted that the metallocene-catalyzed polyolefins would exhibit stronger adhesion than the Ziegler-Natta-catalyzed polyolefins due to interfacial entanglements of the polymers in the molten state. In our results we found metallocene pairs exhibited almost three-fold greater adhesion strength than the Ziegler-Natta pairs. Published literature states that in Ziegler-Natta-catalyzed polyolefins an accumulation of an amorphous polymer at the interface inhibits some interfacial entanglement. Interfacial differences, such as the crystallization of the metallocene laminate, can be observed using transmission electron microscopy (TEM) imaging. These are the beginning phases of research that could one day develop a method for blending these two immiscible polyolefins.

**46. Maria Francine Lapid**

*Effects of Window Size on Perceived Interior Spaciousness of a Room in Virtual Reality*

**Advisor:** Victoria Interrante

**Sponsoring Program:** Computer Science

**Home Institution:** Texas A&M University

**Abstract:** This experiment explores how the addition of a window or a painting, in an otherwise empty room, affects a subject's perceived interior spaciousness of the room in an immersive virtual reality environment. The results of this experiment aim to provide insight into the science behind the art of effective architectural design. A total of 30 rooms, --varying in window shape, window size, room size, painting shape, painting size, and view --were modeled with Autodesk Maya 3D modeling software and Unreal Engine 4. We will ask eight participants to qualitatively judge the spaciousness of each room based on a carefully modeled Likert scale that ranges from 1 to 7. 1 represents a very small room and 7 represents a very large room. In addition to subjects rating the room size on the Likert scale, subjects will also be asked to perform blind walking from one side of the room to the other to quantitatively measure the perceived depth. For this experiment, we hypothesize that the the addition of a window will increase the perceived spaciousness and depth of the room, with larger windows having a greater impact. We use the paintings, matched in color and luminance to the views through the windows, as a control condition to better disambiguate the effect of the view of external space that the window provides from the concurrent color and luminance differences within the window frame with respect to the wall.

**47. Virginia Larson**

*Synthesis of Ligands and Titanium Imido Complexes for Pyrrole Catalysis*

**Advisor:** Ian Tonks

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Wheaton College

**Abstract:** Pyrrole is a common motif found in many natural compounds and is desired in many organic syntheses. The Tonks group seeks to develop titanium imido complexes that will regioselectively catalyze pyrrole synthesis via 2+2 addition of an alkyne in the titanium imido bond, a second insertion of alkyne to form a 6 membered metallacycle, and reductive elimination of pyrrole. The imido is regenerated from a diazene. The first step in the catalytic cycle, 2+2 addition of the alkyne, resembles hydroamination. Therefore, ligands were chosen that perform regioselective hydroamination. This known selectivity will help determine the regioselectivity of the second alkyne insertion. For this project, two hydroamination ligands were selected: N,N-di(pyrrrolyl- $\alpha$ -methyl)-N-methylamine (dpma) and 2-methyl-2-(2-pyridyl)propane-1,3-diamine (mppa). These are both LX2 type ligands, a subset of hydroamination ligands not yet explored by the Tonks group. Dpma prefers markovnikov, while mppa displays anti-markovnikov selectivity. Moreover, the four and six membered metallacycles, both postulated intermediates in our catalytic cycle, have been isolated with the mppa titanium complex.

Dpma ligand was synthesised through a one-step Mannich reaction between a pyrrole, acetone, and ammonium chloride. The corresponding titanium imido complex was made by salt metathesis with n-Butyl Lithium and the titanium precursor Ti(NTol)Cl<sub>2</sub>py<sub>3</sub>. The identity of the complex was confirmed by NMR. This complex will be applied towards catalysis of pyrroles. Mppa ligand was synthesized through a multi-step literature synthesis. Mppa will be put on titanium by either salt metathesis or direct substitution.

**48. Maggie Lau**

*New Lactone Monomers from Oxidation of Substituted Phenols*

**Advisor:** Marc Hillmyer

**Sponsoring Program:** Center for Sustainable Polymers

**Home Institution:** University of Tennessee-Knoxville

**Abstract** Polymers are used in a wide variety of applications, such as adhesives and plastic bags. However, they are mostly derived from petroleum which makes them unsustainable. To continue meeting the demand for polymers without destroying the environment, we are interested in developing renewable and biodegradable polymers. Here, we aim to synthesize two new lactone monomers: d-decapenta-e-caprolactone and trimethyl-e-caprolactone. The former is attractive because its precursor can be obtained from hydrogenation of cardanol, an inexpensive byproduct of the cashew processing industry; the latter can potentially be used to access a biodegradable polyester that is structurally similar to polypropylene, a major commodity plastic. To synthesize the lactones, we hydrogenate their corresponding alkyl-substituted phenols and investigate how green chemicals, such as bleach and oxone, can be used to oxidize the hydrogenated phenols to obtain the desired lactone monomers. The chemical composition of the monomers are determined using gas chromatography-mass spectrometry and <sup>1</sup>H NMR. Finally, we polymerize trimethyl-e-caprolactone using ring opening transesterification polymerization and characterize the resulting polytrimethylcaprolactone.

- 49. Victoria Longley**  
*Synthesis and Analysis of Bipyridine Ruthenium Complexes*  
**Advisor:** Wayne Gladfelter  
**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen  
**Home Institution:** University of Minnesota - Twin Cities  
**Abstract:** Two heteroleptic bipyridine ruthenium complexes for use in dye-sensitized solar cells were synthesized and characterized by NMR, mass spec, fluorescence, and UV-Vis spectroscopy. The two dyes contain two 4,4'-dipiperidino-2,2'-bipyridine (pipbpy) ligands and either a 4,4'-bis(diethylphosphonate)-2,2'-bipyridine (PETbpy) or a 4,4'-bis(phosphonic acid)-2,2'-bipyridine (POHbpy) ligand. The phosphonate-bearing ligands were chosen to anchor the complexes to the surface of a semiconductor such as TiO<sub>2</sub> or ZnO. The ligands were synthesized according to known procedures. The ruthenium complexes were prepared in a stepwise fashion. Initially, the two pipbpy ligands reacted with RuCl<sub>3</sub>·nH<sub>2</sub>O to form [Ru(pipbpy)<sub>2</sub>Cl]Cl. After reduction of the metal, this intermediate was reacted with the bipyridine bearing the two phosphonate ester groups and precipitated as the [Ru(pipbpy)<sub>2</sub>(PETbpy)](PF<sub>6</sub>)<sub>2</sub> using Na[PF<sub>6</sub>]. Acid hydrolysis converted the phosphonate ester groups into the phosphonic acids. Using a combination of electronic absorption spectroscopy, fluorescence spectroscopy, and potentiometric titrations, the complex acid-base behavior of the new ruthenium compounds were studied and will be discussed. Fluorescence measurements were used to assess the ability of 3.0 nm ZnO nanocrystals to quench the excited states of the two complexes.
- 50. Javier Lopez-Hernandez**  
*Synthesis of Antibiotic Metal Ions Complexed with a Tripodal 6,6 Linear Catecholate*  
**Advisor:** Valerie Pierre  
**Sponsoring Program:** MRSEC  
**Home Institution:** University of Puerto Rico at Humacao  
**Abstract:** Antibiotic resistance has become the biggest health threat around the world. In 2013, over 2 million illnesses and 23 thousand deaths were caused by antibiotic resistance. The overused and misused of antibiotics without professional oversight leads to natural mutagenic resistance of the bacteria. During their virulence period the microorganism require a 10<sup>-6</sup> M iron concentration, nevertheless the host exhibit a 10<sup>-24</sup> M iron concentration. To full fill their need for iron they produce siderophores, small molecular weight organic compounds which have high affinity for metal ions, especially iron. There are two types of siderophores: Aerobactin and Enterobactin. Enterobactin, which is the one with most affinity for iron (Fe), is formed by two specific structures: tri-lactone and three catechol. The tri-lactone is the structure that can be modify to obtain new analogues and the three catechol allow the metal-binding by coordinating bonds. Previous research has shown uptake of Enterobactin analogues by the bacteria. Also, triccatecholamide analogs of Enterobactin with metal ions, such as Gallium and Indium has been investigated as radiopharmaceuticals showing an increment in the stability of the metal-binding. Inspire by Enterobactin structure, we have develop a library of metal ion complex (Fe<sup>+3</sup>, Ga<sup>+3</sup>, Cu<sup>+2</sup>, Zn<sup>+2</sup>, Sn<sup>+2</sup>, Co<sup>+2</sup> and Ni<sup>+2</sup>) analogues which are exemplify with the synthesis of the 6,6 linear catecholate.
- 51. Khao Nou Lor, Bryan Jones, Titu Devamani, Romas Kazlauskas**  
*Stabilization of an  $\alpha/\beta$ -Hydrolase (Salicylic Acid Binding Protein 2 from Tobacco)*  
**Advisor:** Romas Kazlauskas  
**Sponsoring Program:** Project SEED  
**Home Institution:** Johnson Senior High School, SPPS  
**Abstract:** Although  $\alpha/\beta$ -hydrolases are proven to be vital enzymes for biocatalysis, their applications for industrial purposes may be limited by their stability. For example, enzymes used in laundry detergents must withstand the 50-60 C water used to wash clothes. In this stability study, plant esterase, salicylic acid binding protein 2 (SABP2), was used as an example  $\alpha/\beta$ -hydrolase. SABP2 showed typical stability to heat inactivation. To increase its stability, the DNA of SABP2 was altered in two different locations (140P and 189V) by replacing amino acids with proline and valine, changing the protein sequence. These two mutants, along with the original protein sequence of SABP2, were heated at 60°C for 15 minutes, and then tested for their kinetic activity afterwards. They were also tested for their esterase activity by varying the concentration of substrate used. With a better understanding at which mutant is most stable against heat and which concentration of substrate changes the protein's activity the least, SABP2 may be used as a more stable enzyme for future industrial purposes.

52. **Malik Majette**

*Data-driven Simulation and Evaluation of Virtual Social Environments*

**Advisor:** Dr. Stephen Guy

**Sponsoring Program:** Computer Science

**Home Institution:** North Carolina State University

**Abstract:** Modeling virtual humans in settings to intelligently interact and instinctively gesture is an active research area with broad applications. In our research we focus on the combination of virtual reality, facial animations, and architectural evaluation to present a realistic immersion in ancient structures that have deteriorated, and no longer support the initial magnitude of occupancy. Specifically, the Pnyx, an ancient Athens structure said to be the birthplace of democratic assemblies, is currently unable to actualize these archaic events to tourists due to its decay. We developed a virtual program to represent gatherings in the Pnyx that naturally condense towards a speaker's podium and make a variety of facial expressions in response to each other. Constructing this model presented a computational challenge in large simulations since the authenticity of human emotion is difficult to invoke in graphical simulations, and there is no previous data of how the Athenians organized or to support the claim that the structure had capacity for 16,000 men. We address these issues using a data-driven approach to simulate intelligent agents in the Pnyx based on the concept of a universal power law governing pedestrian behavior. In our model large crowds can enter into the structure while conforming to natural behaviors such as avoiding collisions, natural dispersion, and social space. Furthermore, in collaboration with doctors from the UMN Otolaryngology Department we collect and evaluate facial features across a large sample, which is utilized to reproduce genuine emotions in virtual agents. With real-world pedestrian interactions and data-driven facial animations our model provides a convincing and accurate representation of democratic assemblies from the beginning of human recording.

53. **Christine Marquette**

*Identification of New Shape Memory Alloys with Satisfaction of the Cofactor Conditions*

**Advisor:** Richard James

**Sponsoring Program:** MRSEC

**Home Institution:** University of Minnesota-Twin Cities

**Abstract:** Shape memory alloys exhibit many desirable characteristics. The defining characteristic is their ability to withstand extreme deformation and then regain their original shape with the addition of heat. As a shape memory alloy undergoes phase transformations, its properties and crystal structures change, but the entire process is reversible up to a certain number of cycles. How many cycles it can undergo is known as its fatigue life and is determined by its reversibility. For a material to be considered a shape memory alloy, it must satisfy certain conditions called the cofactor conditions. If the cofactor conditions are satisfied, the alloy will have an improved fatigue life compared to other materials. Since there are few materials that have been proven to be shape memory alloys, we will identify potential new materials that satisfy the cofactor conditions, and thus, new shape memory alloys. We will use an arc melt furnace to weld the metals together and physically make the alloy. The alloy will then be placed in a furnace and quenched to give it shape memory properties. Once the alloy is made, we will perform X-Ray diffraction on it to determine its lattice parameters, which can be used to determine if the alloy satisfies the cofactor conditions. If it does not, its metals' compositions will be adjusted as need be, until the alloy satisfies the cofactor conditions.

54. **Andres Marroquin, Peng Xu, Dr. Bharat Jalan**

*Carrier Density Control of 2DEGs NTO/STO Heterostructures*

**Advisor:** Bharat Jalan

**Sponsoring Program:** MRSEC

**Home Institution:** The University of Texas - Rio Grande Valley

**Abstract:** Extremely high carrier density ( $\sim 10^{15} \text{ cm}^{-2}$ ) has been achieved by NdTiO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures, grown via the hybrid molecular beam epitaxy approach. It has been shown that such electronic transport behavior can be controlled by intentionally changing the valence states of NdTiO<sub>3</sub>, by changing cation stoichiometry of NdTiO<sub>3</sub>. Preliminary experiments show that NdTiO<sub>3</sub> is sensitive to air, and oxygen atoms can fill in the interstitial sites and oxidize Ti<sup>3+</sup> in NdTiO<sub>3</sub>, resulting in a metal-to-insulator transition. This project will focus on rapid thermal annealing (RTA) of NdTiO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures under O<sub>2</sub> and forming gas, and characterize structure using High Resolution X-Ray Diffraction (HRXRD) and Atomic Force Microscopy (AFM). We will also study the effects of RTA on the electronic transport properties using Physical Properties Measurement System (PPMS). The correlation will be investigated between thermal treatment, crystal structure and the electronic transport properties.

55. **Kevin Marroquin**

*Calculation of the singlet-triplet gap for C3H3- and C5H5+ using Multiconfigurational Pair Density Functional Theory .*

**Advisor:** Laura Gagliardi

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Universidad del Valle

**Abstract:** The new Multiconfigurational Pair Density Functional Theory (MC-PDFT) method is a theory that combines multiconfiguration wave function theory with density functional theory (DFT). It is as accurate as multireference methods, but it has a cost more affordable and comparable to DFT. It was used to calculate the energy difference between the singlet and triplet states ( $\Delta E_{ST}$ ) of two different systems, the C3H3- and the C5H5+. These systems are all radicals and are being studied because they have experimental interest and are challenging for theory. In the literature a wide range of values for the  $\Delta E_{ST}$  can be found and it is unclear which is the correct one. The values obtained using a multireference method followed by second order perturbation theory, CASPT2, are used as reference to be compared with the ones obtained with MC-PDFT. For the C3H3- the CASPT2 and MC-PDFT calculations were performed, giving both low  $\Delta E_{ST}$  results suggesting that the singlet and the triplet are almost degenerate states. For the C5H5+ the CASPT2 and MC-PDFT gave similar  $\Delta E_{ST}$  values, which demonstrates that the MC-PDFT can give accurate results at a more affordable cost.

56. **Nik Martinneau**

*The Development of Ovine Distal Alveolar Lung Tissue Using the Additive Manufacturing Technique: Freeform Reversible Embedding of Suspended Hydrogels.*

**Advisor:** Angela Panoskaltzis-Mortari

**Sponsoring Program:** Northstar STEM Alliance

**Home Institution:** Minneapolis Community and Technical College

**Abstract:** Main Objective: The need for human organs designated for transplantation far overshadows our current supply. For this reason, there is an urgency to develop more efficient, successful and reproducible methods for providing solutions to this pertinent, global issue. Producing organs using hydrogels, iPSCs and 3-dimensional printers is a relatively new process to the world and shows endless promise in this respect. Methods: F.R.E.S.H., a term coined by the process' inventors at Carnegie Mellon University, stands for Freeform Reversible Embedding of Suspended Hydrogels. This method has shown promise in increasing the structural support systems of printed tissue. Results and conclusion: Inconclusive. May or may not have data by time of exposition. If insufficient data is produced, I will fashion my presentation to extrapolate on the intricacies of FRESH and lyophilization methodology.

57. **Dylan Masi**

*Flame Synthesis of Aluminum-Doped Zinc Oxide*

**Advisor:** Chris Hogan

**Sponsoring Program:** MRSEC

**Home Institution:** University of Massachusetts Amherst

**Abstract:** Transparent conducting oxides are highly functional in electro-optical devices including thin film solar cells, flat panel displays, LEDs, and sensors. Indium-doped tin oxide is commonly used as an electrode in many of these applications due to its high conductivity and transparency. The main challenge with transparent conducting oxides is cost; indium is expensive to harvest, and indium-doped tin oxide films are typically synthesized on a large scale with magnetron sputtering. The properties of an alternative material, aluminum-doped zinc oxide, were examined, as well as a more cost-effective synthesis method for creating transparent conducting oxide films. An aerosol flame reactor was developed to produce aluminum-doped zinc oxide nanoparticles. Flame synthesis is easily scalable for industrial applications, it can be carried out at atmospheric pressure, and it produces homogeneous films. X-Ray Diffraction was used to confirm the lattice structure, material composition, and size of the particles after flame synthesis. A new online instrumentation technique using a Differential Mobility Analyzer coupled with an Aerosol Particle Mass Analyzer and a Condensation Particle Counter was used as an alternative to Transmission Electron Microscopy for characterizing particles. This research determined the effects of various precursor ratios of zinc and aluminum on the properties of the final nanopowders.

- 58. Christopher McDonough**  
*How to optimize a Neural Network for Neutrino Physics*  
**Advisor:** Marvin Marshak  
**Sponsoring Program:** Physics REU  
**Home Institution:** University of Minnesota  
**Abstract:** The field of Particle Physics and in particular Neutrino Physics is calling for more and more advanced detectors to output even more data. In order to analyze the absurdly large amount of data the detectors can output some sort of computing process is needed. The NOvA project uses a convolutional neural network which is kind of artificial intelligence that proves to be successful at tasks such as image analysis. Convolutional neural networks are currently a big deal in the Computer Science community and the topic of a lot of research due to their effectiveness at image analysis. Since it's such a fresh topic of research many things are unknown about them such as effective structures for certain types of image analysis and likely it will be specific to your project such as NOvA. The topic of my research is to help improve and understand the neural network used in the NOvA by changing and modifying anything from simple parameters to the more obscure things such as the structure of the network.
- 59. Sam Merlus**  
*Biosynthesis of novel monomers*  
**Advisor:** Kechun Zhang  
**Sponsoring Program:** Center for Sustainable Polymers  
**Home Institution:** Miami Dade College  
**Abstract:** We have engineered *E. coli* to produce a family of monomers that can potentially provide similar properties to petroleum-based products. The goal is to create biochemical products are renewable, cost-effective, and environmentally friendly. Our products include dipicolinic acid (DPA) and several related structures. These compounds resemble petroleum-derived phthalates, such as isophthalate which is used for Nomex™ fire resistant gloves. Our compounds are produced engineering the lysine pathway. Previous work on this project has successfully isolated DPA, a naturally produced compound found in high concentrations in *Bacillus subtilis* endospores.<sup>1</sup> In this project we used traditional metabolic engineering techniques to design pathways for the production of two more lysine derivative products. Once the pathway is validated, the engineered strains will be used for fermentation and production of new monomers.
- 60. Kyle Miller**  
*Replacing lead in organic-inorganic perovskite for a more sustainable solar cell*  
**Advisor:** Russell Holmes  
**Sponsoring Program:** MRSEC  
**Home Institution:** University of Puget Sound  
**Abstract:** Perovskites are crystals of the formula  $\alpha\beta X_3$  where  $\alpha$  and  $\beta$  are large and small cations, respectively, and X is an anion bound to both cations. Organic-inorganic perovskites have an organic  $\alpha$  cation, typically methylammonium ( $\text{CH}_3\text{NH}_3$ ). Since 2006, perovskite photovoltaic cells have experienced an unprecedented increase from 2.2% to 22.1% power conversion efficiency, now rivaling more established architectures such as CIGS (cadmium indium gallium diselenide) and CdTe (NREL 2016). Despite their excellent optical absorption and low rates of non-radiative recombination, perovskites have yet to see widespread commercial adoption in photovoltaic devices. The presence of lead in the most efficient and well-studied organic-inorganic perovskite ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) is a major inhibitor of commercial feasibility. To address health and environmental safety concerns surrounding the manufacture and disposal of devices containing lead, this investigation attempts to find a less toxic alternative to lead for the  $\beta$  cation. Based on Goldschmidt's tolerance factor, density functional theory (DFT) simulations, and similar compounds synthesized in literature, barium was selected as the  $\beta$  cation replacement candidate. We attempt to synthesize perovskites of the formula  $\text{CH}_3\text{NH}_3\text{BaI}_3$  with a two-step vapor-assisted solution process and a single-step solution process. Neither process produced an identifiable perovskite but the solution process yielded unknown and dynamic spectral features when exposed to air. Further investigation is required to confidently identify the source of the spectral features. While it is unlikely that the target perovskite was obtained in this study, significant progress was made in finding and refining synthesis and characterization techniques.

61. **Gunnar Nelson**

*Low Intensity UV Treatment of Zinc Oxide Nanocrystal Thin Films*

**Advisor:** Eray Aydil

**Sponsoring Program:** MRSEC

**Home Institution:** Creighton University

**Abstract:** Zinc Oxide nanocrystal thin films show great potential as a cheap, highly conductive, and transparent semiconductor. A disordered nanocrystal structure allows for both hyper rapid film production and tunable properties via nanocrystal size. However, hydroxyl electron traps are found on the surface of the thin film. These electron traps decrease conductivity by trapping the free electrons found in the Zinc Oxide film. These electrons result from oxygen vacancies in the nanocrystal. Previously, this problem was solved by covering the film with ~7nm of Aluminum through atomic layer deposition. However, this solution does not align with the hyper rapid film production scheme. We have seen that films exposed to low intensity UV light (~365nm) showed a decrease in hydroxyl group signal in FTIR measurements in a glove-box environment. A localized surface plasmon resonance (LSPR) corresponding to a free carrier density on the order of  $10^{19}$  cm<sup>-3</sup> is seen after only a few seconds of UV exposure. This indicates that electrons are freed as the hydroxyl traps are removed. If a film is then exposed to air, the hydroxyl group signal shows again in FTIR measurements. We see, with various UV exposure times, the mechanics of this phenomena. This UV exposure effect is juxtaposed with how heat effects LSPR to better outline the differences. A hypothesis for this UV exposure mechanics involving surface restructuring is proposed.

62. **Maria Neuzil**

*Structures and Properties of Crystalline Benzonitrile Oxides*

**Advisor:** William Ojala

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** Nitrile oxides are compounds containing the fulminate group, composed of a carbon atom triple bonded to a nitrogen atom that is single bonded to an oxygen atom. These compounds are useful in solution reactions, particularly in 1,3-dipolar cycloadditions, but their solid-state properties and reactivity have been understudied. We are interested in examining the parent nitrile oxide and its three possible solution-phase dimers — the furoxan, the dioxadiazine, and the 1,2,4-oxadiazole-N-oxide — to see if there is a correlation between the product of the solid-state dimerization and the packing arrangement of the parent nitrile oxide. We have obtained the infrared spectra of a selection of nitrile oxides and their dimers, including 4-nitrobenzonitrile oxide and 2-chlorobenzonitrile oxide, which indicate that we have successfully synthesized these parent nitrile oxides and also potentially a corresponding oxadiazole-N-oxide. To confirm these results, samples have been submitted for analysis by single-crystal X-ray diffractometry. Our ongoing work will include obtaining a complete set of solid-state molecular packing arrangements (crystal structures) for the parent nitrile oxides and their dimers in the 2-nitrobenzonitrile oxide, 3-nitrobenzonitrile oxide, 4-nitrobenzonitrile oxide, and 2-chlorobenzonitrile oxide series.

63. **Suong Nguyen**

*Synthesis and Investigation on the Reactivity of the Allylic Azide System*

**Advisor:** Joseph Topczewski

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** University of Mississippi

**Abstract:** Chiral amines are present in a wide range of natural products, drug candidates, and catalyst ligands. While there have been extensive studies on the synthesis of chiral amines, there are not many methods for the preparation of chiral  $\alpha,\alpha$ -disubstituted amines that are in general use. The majority of available syntheses are limited to some specific substrate motifs. Included in this work is an efficient method to prepare allylic azides which can be used as precursors to make chiral  $\alpha,\alpha$ -disubstituted amines via direct catalytic reaction. In addition, the research also focuses on examining the reactivity of allylic azides system, including catalytic epoxidation and hydrogenation reactions.

- 64. Christian Oswood**  
*Synthesis of Pyranoarene Derivatives via Enal Trapping of HDDA-Generated Benzyne*  
**Advisor:** Tom Hoyer  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** St. Olaf College  
**Abstract:** Benzyne can be trapped by a variety of agents to create complex chemical motifs. HDDA-generated benzyne can be created under relatively mild conditions. When an enal is used as a trap, the result is a substituted pyranoarene resulting from a mechanism involving an ortho quinone methide intermediate. Various exocyclic enals were synthesized and tested as traps for a specific HDDA substrate. Endocyclic enals were also tested, but were not able to function as traps.
- 65. Russell Pekala**  
*Understanding Neural Networks in Caffe*  
**Advisor:** Marvin Marshak  
**Sponsoring Program:** Physics REU  
**Home Institution:** University of Minnesota  
**Abstract:** Unavailable
- 66. Spencer Peloquin**  
*Planetarium Exploration of the Human Heart*  
**Advisor:** Daniel Keefe  
**Sponsoring Program:** Computer Science  
**Home Institution:** University of Wisconsin Stout  
**Abstract:** We developed a virtual tour of the human heart in a planetarium environment to give immersive and highly scale-able educational experiences to museum visitors. While graphics software has been used for projects ranging from planets and 3D volume rendered skulls, we employed Unity to address several challenges unique to rendering of the human heart. Unity allowed us to implement a Bezier Spline rapidly and obtain points for the camera to travel along smoothly and a fish eye lens to bend our image to project correctly on . Unity also allowed use the crucial use of a 3D texture. For our heart we had over 450 pictures of horizontal slices of a cadaver's heart as well as a corresponding mesh. To texture it we used Unity's 3D Texture, which acts like a box you fill with color and according to where the mesh is inside that 3D space. We could process the pixel of our images as layers for the 3D texture to exactly color the heart as accurately as possible. Current challenges still exists however such as matching the experiences of other planetarium software such as Uniview while making sure it's versatile to update for many projection platforms.
- 67. Merrick Pierson Smela**  
*Synthesis and Characterization of Fluorescent Compounds for OLED Active Layers*  
**Advisor:** Thomas Hoyer  
**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen  
**Home Institution:** University of Minnesota  
**Abstract:** Organic light-emitting diodes (OLEDs), which electrically excite highly conjugated compounds to emit visible light, are a promising technology for lightweight and flexible displays. However, the efficiency of OLEDs, especially that of blue ones, has much room for improvement. Therefore, it is necessary to develop new compounds for OLED active layers. These compounds must be highly emissive in the visible range. Furthermore, because OLED active layer production involves vapor deposition, suitable compounds must also be stable to heat. Substituted dibenzofurans show promising characteristics in these areas, and the hexadehydro-Diels-Alder reaction provides a convenient way to produce a wide variety of compounds of this type. A total of ten such compounds were synthesized, and their fluorescent properties and thermal stability were evaluated. Among the dibenzofurans, it was found that fluorescence depended on molecule planarity and ring substituent electronegativity. Replacing side-chain methyl esters with benzyl esters altered absorptivity only at very short wavelengths, but diminished fluorescence across the whole spectrum. The analogous dibenzothiophene showed little fluorescence, whereas the benzonaphtho[2,1]furan fluoresced more intensely and at longer wavelengths than the parent dibenzofuran. All compounds had good thermal stability, and five had fluorescent properties promising enough to warrant their use in prototype OLEDs.

68. **Jordan Potter**

*Optimizing a Convolutional Visual Network*

**Advisor:** Marvin Marshak

**Sponsoring Program:** Physics REU

**Home Institution:** Kenyon College

**Abstract:** Classification of neutrino interactions has become an increasingly important topic of research with a drastic increase of data to be considered. Physicists in the NOvA (Numi Off-Axis Nu<sub>e</sub> Appearance) collaboration have turned to an algorithm called deep learning to classify these events. This artificial neural network is loosely based on the neurons in a human brain to apply different convolutional and pooling filters to identify the image. For neutrinos the net will classify the image as a  $\nu_e$  or  $\nu_\mu$  charged current event, neutral current event or cosmic ray. This summer I examined optimizing the CVN (Convolutional Visual Network) used by NOvA through changing different parameters of the network and the architecture of the net. The importance of this research is that an optimized network can classify data more efficiently and accurately. This result in turn will allow better confirmation of charged current neutrino events.

69. **Janna Quick**

*Absorption of colloidal silicon nanoparticles with sterically hindered ligand surfaces*

**Advisor:** Uwe Kortshagen

**Sponsoring Program:** MRSEC

**Home Institution:** College of Saint Benedict

**Abstract:** Silicon nanocrystals have photoluminescent properties that make them useful tools for many electronic and optical applications. These luminescent properties must be further researched to increase their efficiency and adaptability. The specific aspect that will be investigated is finding the molar extinction coefficient of specific silicon nanocrystals with attached ligands. I will achieve this by collecting absorbance spectra of colloidal silicon nanoparticles with 1-dodecene on the surface, a long sterically hindered carbon chain. These nanoparticles are synthesized using a nonthermal plasma reactor, which passivates the silicon completely with hydrogen. Keeping air-free conditions, the 1-dodecene is attached using a hydrosilylation reaction. Taking absorbance spectra of these particles will allow for ample data to utilize the Beer-Lambert law, and the molar extinction coefficient can then be calculated. The coefficient can then be converted to reflect the extinction coefficient and the concentration on the atomic level. Using this calculated coefficient, it will be possible to calculate the concentration of the particles suspended in solution without having to estimate concentration by weight. This is useful because often times the weight estimation is difficult due to solubility/solvent obstacles. This technique will allow for a more precise means of measuring the concentration of the colloidal silicon nanoparticles, as well as polymers with the silicon nanoparticles embedded inside of them.

70. **Steven Roach**

*GroupStart: Incorporating Group Projects into MOOCs*

**Advisor:** Haiyi Zhu

**Sponsoring Program:** Computer Science

**Home Institution:** Macalester College

**Abstract:** Massive Open Online Courses (MOOCs) give students free access to high quality, educational content on a global scale. They provide an online learning environment where diverse groups of students can satisfy their academic interests. However, most MOOCs rely on individual activities, which means collaborative activities such as group projects are difficult to implement. Many challenges exist in designing a MOOC group project such as establishing group accountability, accounting for high attrition rates, and allowing for the vast diversity of MOOC students. While many effective group communication and task management systems currently exist, few software platforms focus on online group projects. We introduce GroupStart; an experimental web application that seeks to facilitate the formation of groups as well as the establishment of familiarity among group members in a MOOC group project. We implement different group formation algorithms to test levels of homogeneity and heterogeneity within groups based on different attributes. In an effort to establish familiarity among group members, we provide a platform for students to create a shared document to establish their group purpose, goals, and communication methods. We will use GroupStart to test different mechanisms for establishing group accountability in the early stages of online group work.

71. **Cristobal Rodriguez**

*Cell attachment and proliferation on Cellulose nanocrystal composite nanofibers*

**Advisor:** Theresa Reineke

**Sponsoring Program:** MRSEC

**Home Institution:** University of Texas Rio Grande Valley (UTRGV)

**Abstract:** Cellulose nanocrystal (CNC) is a kind of nanoparticle that could be obtained easily from cellulose by acid hydrolysis. Due to its high elastic modulus, large surface area, high aspect ratio, and good biocompatibility, it is attracting wide research interest. In this work, cellulose nanocrystal with surface tethered dopamine will be utilized to generate cellulose nanocrystal reinforced composite nanofibers that could also be functionalized through dopamine based reactions. The combination of cellulose nanocrystals and biomolecules suggest potential applications to enhance cell attachment and proliferation properties on nanofibers spun through forcespinning method. Human dermal fibroblasts neonatal (HDFn) cells were cultured and seeded onto nanofibers to test cell attachment. An MTT-assay and hemocytometer was conducted for a quantitative cell proliferation analysis. Fluorescence microscopy was conducted using Mito-Tracker Red (MTR) for mitochondrial and DAPI for nucleus morphology. Both MTT-assay, hemocytometer, and fluorescence microscopy showed low cell attachment and viability. With the consideration of cellulose nanocrystal affecting the surface properties of nanofibers. A new nanofiber matrix material was used through different dip coating cellulose nanocrystal concentrations, in order to test the cellular behavior of fibroblasts cells on modified nanofibers and unmodified ones.

72. **Kevin Sanchez**

*Utilizing the Transmission Electron Microscope (TEM) beam broadening to identify elements in materials*

**Advisor:** Andre Mkhoyan

**Sponsoring Program:** MRSEC

**Home Institution:** University of Puerto Rico at Mayagüez

**Abstract:** The TEM beam broadening occurs due to the interaction of the electrons and the atoms of the specimen. This effect has always been present in TEM analyses and has been a concern for many researchers in the areas of materials science and engineering. This beam broadening depends on the material's composition and structure, the thickness of the specimen and the energy of the electron beam. The TEM beam broadening was modeled and observed through both nanocrystals and amorphous solids of different elements to ultimately define a general relationship between the radius of broadening and the atomic number of the elements. These calculations were conducted by computer simulations, specifically with the Multislice method. This method simulates how the electron probe propagates through the sample in a number of slices. With the computational work, the preliminary results showed that with increasing atomic number the radius of broadening increases; the beam will broaden more in heavier elements. Further simulations with more elements should be conducted, considering thermal vibrations and the position and energy of the beam. Hence correlating the beam spreading with the atomic number in order to introduce an alternative way of identifying elements in materials with the TEM.

73. **Jennifer Sanchez, Leo Oquendo**

*Synthesis and characterization of sugar based surfactants*

**Advisor:** Marc Hillmyer

**Sponsoring Program:** MRSEC

**Home Institution:** The University of Texas Rio Grande Valley

**Abstract:** Surfactants have a variety of uses including applications in the petroleum industry, membranes, biological systems, detergents and formation of nanostructures. These derivatives are amphipathic, meaning they are composed of both hydrophilic and hydrophobic groups. In this work, surfactants composed of sugars and longer alkyl chains will be used to study the ability of these derivatives to produce nanostructures by induced macrophase separation in the system. The synthesis of this type of surfactant derivative was achieved first by reacting allyl bromide with 1-octene using Grubbs [G2] as a catalyst to produce 1-bromo-2-nonene. The second step involves the reactions of D-Glucose with 1-bromo-2-nonene using Sn to produce an unsaturated derivative. In the next step this derivative will be hydrogenated using Pt/C catalyst to achieve the final surfactant derivative. Characterization of the products is obtained by <sup>1</sup>H NMR, <sup>13</sup>C NMR, infrared spectroscopy (IR), and mass spectrometry (MS). The self-assembly properties of this surfactant and the formation of nanostructures will be studied using thin films.

**74. Jonathan Schultz**

*Surface-Enhanced Femtosecond Stimulated Raman Spectroscopy: Toward Ultrafast Vibrational Signatures from Single Molecules*

**Advisor:** Renee Frontiera

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota Twin Cities

**Abstract:** Spectroscopic interrogation of molecules on the timescale of individual vibrations is critical for understanding the reactive trajectory of countless photo-active systems. In particular, the utility of a structurally sensitive method, femtosecond stimulated Raman spectroscopy (FSRS), has been proven through ultrafast mechanistic studies ranging from biological systems to materials for solar energy harvesting. These experiments illustrate the importance of elucidating the early reactive characteristics of systems spanning numerous chemical disciplines. However, previous investigations using FSRS have been limited to samples in bulk and with large Raman cross sections. This restraint imposes the need for ensemble measurements, which average data across a collection of molecules and therefore mask dynamics hidden within single molecules. Accordingly, I present efforts to unite FSRS with surface-enhanced Raman scattering (SERS), a technique capable of visualizing single molecule vibrations. Thus far, with surface-enhanced femtosecond stimulated Raman spectroscopy (SE-FSRS), I have obtained ultrafast vibrational signatures from an ensemble of molecules approximately seven orders of magnitude less in number than that required for bulk measurements. I will further discuss trends regarding the electric field dependence of SE-FSRS in relation to normal SERS, a topic valuable to the spectroscopic community. With the ability to probe the ultrafast behavior of single molecules, SE-FSRS will allow researchers to reveal dynamics of systems previously shrouded by molecular ensembles.

**75. Marian Shaw**

*Entropic Filter for Recovering Long DNA*

**Advisor:** Kevin Dorfman

**Sponsoring Program:** MRSEC

**Home Institution:** New York University

**Abstract:** Long DNA molecules are crucial for genome technologies such as whole-genome mapping and cell engineering. However, samples of long DNA are often contaminated by small DNA from shearing and other small biomolecules that present obstacles in sequencing. Using photolithography and reactive ion etching, we have fabricated an entropic trap-based-electrophoretic device in glass to filter out precious DNA molecules longer than a desired length from an impure mixture. After fine-tuning the device by altering the strength of the electric fields, the design of the channels, and the heights of the well and slit regions in an entropic trapping configuration, long DNA is trapped in the device at the nanoslit-microchannel interfaces, while short DNA passes through. In the future, performance of the new filtration method will be quantified by running the filtered and impure sample through pulsed-field gel electrophoresis (PFGE). Ideally, the sample of long DNA produced from the device should not have bands smaller than a certain length. The PFGE system is new for the lab. We have performed numerous PFGE control experiments to determine optimal parameters and DNA concentration for distinct separation and to understand the system's limitations. The tunable entropic filter offers an efficient method for sample preparation of long DNA that can be used in subsequent genome applications.

76. **Violet Sheffey**

*Synthesis of Degradable Polyester Elastomers*

**Advisor:** Guilhem De Hoe

**Sponsoring Program:** Center for Sustainable Polymers

**Home Institution:** University of New Mexico

**Abstract:** Plastic waste contamination has become an increasingly global dilemma. In order to combat the effects of non-degradable plastics on our environment, methods to synthesize degradable cross-linked elastomers have been developed. The objective is for these polyester elastomers to compete with conventional elastomers (e.g. rubber bands) in terms of mechanical performance. Post polymerization cross-linking was used to afford films of varying molecular weights (approx. 10, 20, and 30 kg/mol). It has been demonstrated that the mechanism for film synthesis does not require a catalyst. Also, the effects of varying the amount of carbonate functional groups from the cross-linking agent to the amount of hydroxyl groups present in the polymer were explored. It was found that varying these stoichiometric ratios had profound effects on the degree of cross-linking of the film samples up until a ratio of 2:1. Ongoing work with these polyester elastomers includes scaling up the film synthesis to films of larger diameters and obtaining mechanical property data. This data shall then be compared against that of a conventional rubber band. Future work shall also revolve around blending polymers of differing molar masses into a single film and the studying the subsequent effects of the resulting mechanical properties thereof.

77. **Michael Stodolka**

*Solid-State Structures and Reactivity of Halogenated Benzonitrile Oxides*

**Advisor:** William Ojala

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** Halogenated benzonitrile oxides are compounds bearing both a halogen atom and a fulminate group on a benzene ring. Because these compounds are useful in 1,3-dipolar cycloadditions, their solution chemistry has been studied extensively; however, their solid-state chemistry, including their potential dimerization into a furoxan, a dioxadiazine, or a 1,2,4-oxadiazole N-oxide, has not yet been investigated in detail. The primary focus of our project is to investigate the solid-state 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. As part of our efforts to elucidate the role of molecular packing in the enhanced reactivity of the 3-chloro isomer and to determine the product(s) of solid-state dimerization, we have now grown crystals suitable for single-crystal X-ray diffraction of the compound likely to be the corresponding furoxan, obtained from solution in the absence of the pyridine or triethylamine catalysts that favor the other possible dimers, and we have submitted these crystals for analysis.

78. **Emily Swanson**

*Self-Assembly of Monolayers on Graphene with Pyrene and Cyclodextrin Derivatives*

**Advisor:** Phil Buhlmann

**Sponsoring Program:** UMN Chemistry- Lando

**Home Institution:** Elon University

**Abstract:** : In this work, graphene was functionalized through self-assembly of pyrene and cyclodextrin derivatives driven by  $\pi$ - $\pi$  stacking interactions. Graphene was grown on copper sheets by chemical vapor deposition. The pyrene derivatives that were used for functionalization were pyrene, 1-pyrenemethanol, 1-pyrenemethylamine, 1-pyreneacetic acid, *N,N*-diethyl-1-pyrenemethylamine, and methyl 1-pyreneacetate. The perbenzylated  $\alpha$ -,  $\beta$ -, and  $\gamma$ -cyclodextrins were also synthesized and used for self-assembly. The functionalized graphene substrates were characterized using contact angle goniometry. By varying the concentration of each derivative in the self-assembly solutions, a relationship between surface coverage and concentration was found, providing the minimum concentration needed for the assembly monolayers on graphene without forming multilayers. These compounds will be used to prepare sensor arrays for early disease detection.

**79. Jeremy Swartz**

*Synthesis of a Renewable, Degradable Thermoset Polymer*

**Advisor:** Jane Wissinger

**Sponsoring Program:** Center for Sustainable Polymers

**Home Institution:** University of Florida

**Abstract:** The main goal of the Center for Sustainable Polymers is to design polymers that are derived from renewable resources instead of petroleum, a nonrenewable resource. Isosorbide, which is derived from glucose, is the main chemical used as the foundation for our research. When reacted with succinic anhydride in a microwave reactor, a diacid forms that acts as one of our monomers. A thermoset polymer can be formed when this monomer is reacted with glycerol, which is derived from vegetable oil. This class of polymers demonstrates excellent thermal and mechanical properties. When we incorporate poly(ethylene oxide) (PEO), a 300 g/mol polymer, into our polymers, the flexibility of the polymers can increase. Castor oil is a triglyceride that hopefully can act as a completely renewable comparison to PEO and give the polymers similar mechanical properties. Tensile testing was performed to investigate the effects of both PEO and castor oil on the polymers. This polymer experiment has been implemented in the undergraduate teaching laboratory as well. The experiment is divided into three parts: monomer synthesis, polymer synthesis, and degradation testing. The responses from the students about the experiment were very positive and encouraging as to the future success of the experiment in the teaching lab.

**80. Adinda Syahmansyah**

*Biological Regeneration of Zeolite and Surfactant Modified Zeolite (SMZ) for Nitrogen Removal in Synthetic Domestic Wastewater*

**Advisor:** Bo Hu

**Sponsoring Program:**

**Home Institution:** Bioproducts and Biosystems Engineering

**Abstract:** The removal of nitrogen in wastewater is important to avoid the phenomena of algae bloom in water bodies. Currently the removal of nitrogen in most of wastewater treatment plants rely on the nitrification/denitrification process. The use of zeolite and Surfactant Modified Zeolite (SMZ) as carrier materials might help the biological nitrification/denitrification process. In this work we used zeolite and SMZ to evaluate i) the removal rates of ammonium and nitrate in batch tests ii) the chemical and biological regeneration efficiency using 3M NaCl and denitrifying/nitrifying bacteria iii) the capacity of adsorption using synthetic wastewater. We are currently operating a Sequential Batch Reactor (SBR) with a 1 hour cycle (15 mins anaerobic, 30 mins aerobic and 15 mins settling time) with 10 hours of Hydraulic Retention Time (HRT). We are planning to add SMZ into SBR in order to decrease the HRT. Our results show that zeolite has a better removal capacity than SMZ, but different selectivity. In addition, we have demonstrated that zeolite and SMZ can be bio-regenerated using bacteria. The use of SMZ to help the biological process warrants additional research.

**81. Corey Tesdahl**

*Implementing Scalable Hypergraph Processing Frameworks:*

*A Comparison Between MESH and HyperX*

**Advisor:** Abhishek Chandra

**Sponsoring Program:** Computer Science

**Home Institution:** Normandale Community College

**Abstract:** Graphs are mathematical models which show the relationship between objects. The objects are represented by vertices and their relationships are indicated by edges connecting the vertices. Hypergraphs, a generalization of graphs, have been shown to be a powerful and efficient modeling foundation for group interactions. Scalable systems to support hypergraph computation are beginning to emerge. The design and implementation of these systems has a critical effect on runtime performance. Here we present our findings of a runtime performance comparison between two hypergraph processing frameworks, MESH and HyperX. In order to achieve scalability hypergraph processing frameworks need to distribute hypergraph representations across multiple computers. Several partitioning policies exist which distribute a hypergraph representation onto a cluster of computers. Choosing which partitioning algorithm to use for a given hypergraph representation has a significant impact on runtime. In our experiments we execute several different partitioning strategies that are available in MESH alongside HyperX's one-size-fits-all approach to partitioning. After partitioning has taken place we execute a Label Propagation algorithm on each system. We then evaluate the run times of both partitioning and algorithm execution to compare MESH's performance to that of HyperX. We do this on several different real world datasets which differ in their structure.

**82. Tong Thao**

*Effects of Window Size on Perceived Interior Spaciousness of a Room in Virtual Reality*

**Advisor:** Victoria Interrante

**Sponsoring Program:** MSROP

**Home Institution:** University of Minnesota Twin Cities

**Abstract:** This experiment explores how the addition of a window or a painting, in an otherwise empty room, affects a subject's perceived interior spaciousness of the room in an immersive virtual reality environment. The results of this experiment aim to provide insight into the science behind the art of effective architectural design. A total of 30 rooms, --varying in window shape, window size, room size, painting shape, painting size, and view --were modeled with Autodesk Maya 3D modeling software and Unreal Engine 4. We will ask eight participants to qualitatively judge the spaciousness of each room based on a carefully modeled Likert scale that ranges from 1 to 7. 1 represents a very small room and 7 represents a very large room. In addition to subjects rating the room size on the Likert scale, subjects will also be asked to perform blind walking from one side of the room to the other to quantitatively measure the perceived depth. For this experiment, we hypothesize that the the addition of a window will increase the perceived spaciousness and depth of the room, with larger windows having a greater impact. We use the paintings, matched in color and luminance to the views through the windows, as a control condition to better disambiguate the effect of the view of external space that the window provides from the concurrent color and luminance differences within the window frame with respect to the wall.

**83. Paul Trisko**

*Identification of Specific Readers of Epigenetic Modifications in Human Bronchial Epithelial Cells using a Quantitative Proteomics Approach*

**Advisor:** Natalia Tretyakova

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota - Twin Cities

**Abstract:** Precise control of the levels of gene expression is achieved via epigenetic modification of DNA. C5 methylation of cytosine in DNA at CpG sites in promoter regions results in a decrease of gene expression through binding of methyl CpG binding proteins that recruit HDACs, resulting in chromatin remodelling. Methylcytosine (mC) can be oxidized by the TET family of proteins to hydroxymethylcytosine (hmC), formylcytosine (fC), and carboxylcytosine (caC). mC oxidation to hmC causes changes in protein binding and reactivates gene expression. fC and caC are also hypothesized to change protein-DNA binding and may possess unique epigenetic functions. In the present work we investigated the ability of selectively modified, synthetic DNA strands to pull down proteins from HBEC nuclear extract. We selected a section of the WTH3 promoter which is controlled by methylation of a single CpG site and synthesized modified DNA duplexes containing mC, hmC, fC, or caC at that site. The DNA was incubated with nuclear extract, washed to remove non-specific binders, and bound proteins were eluted. These proteins were digested, TMT-labeled, and analyzed on an Orbitrap Fusion mass spectrometer. We identified 671 proteins binding to our DNA with 9, 7, 29, 41, and 2 unique binders to C, mC, hmC, fC, and caC respectively. Our results indicate that each epigenetic modification selects a different profile of specific readers which may lead to unique signaling effects.

**84. Kamal Tusa**

*Neuromodulation of orexin neurons and the role of microglia in cognitive function*

**Advisor:** Tammy Butterick

**Sponsoring Program:** Northstar STEM Alliance

**Home Institution:** UMN

**Abstract:** Obesity increases the risk of Alzheimer's disease (AD) and cognitive decline. Neuroinflammation, accompanied with a progressive neuronal loss, is known to be heightened in cognitive decline and obesity. The risk of neuroinflammation and cognitive impairment is aggravated by chronic consumption of high fat diets (HFD) rich in saturated fatty acids such palmitic acid (PA). Palmitic acid can directly stimulate microglial (brain immune cells) and increase pro-inflammatory cytokines. Orexin-A (OXA) a neuropeptide can reduce inflammation and neurodegeneration. The immunomodulatory role OXA in the hippocampus and in cognitive decline is unknown. We hypothesized that OXA effects on cognition are due in part by immunomodulation of microglia. To test this, we pre-treated immortalized mouse microglia with OXA (300 nM) and then challenged with PA (0.1 mM; 4h). Gene expression for arginase-1 (anti-inflammatory marker; via qRT-PCR) and TNF- $\alpha$  secretion (via ELISA) were measured. In O/A3 mice (deficient in OXA) we tested cognitive function using a two-way active avoidance memory task. OXA attenuated PA induced TNF- $\alpha$  secretion ( $p < 0.0001$ ) and upregulated arginase-1 ( $p < 0.001$ ). O/A3 mice showed a significant impairment in cognitive performance as compared to wild-type mice ( $p < 0.05$ ). Future studies will use a rodent pharmacogenetic model of neuromodulation (designer receptors exclusively activated by designer drugs; DREADDs), to directly activate OXA neurons. We will determine if increased orexin signaling will reduce HFD-induced cognitive decline via reduced microglial inflammation. These results would support a pivotal role for OXA immunomodulation in the context of obesity and cognitive decline.

**85. Devon Urness**

*Kinetic Analysis of the Alternating Copolymerization of Epoxides with Cyclic Anhydrides*

**Advisor:** William Tolman

**Sponsoring Program:** UROP

**Home Institution:** University of Minnesota - Twin Cities

**Abstract:** Copolymerization of epoxides and cyclic anhydrides have provided an exciting new route to aliphatic polyesters with varied properties. In efforts to improve the efficiency of the catalytic process of this copolymerization, an understanding of the mechanism is desired. Previous studies performed with butylene oxide (BO) and a bicyclic anhydride (CPMA) indicated that the order of CPMA in the rate law is negative, which is suggestive of an inhibition by the anhydride in the mechanism. This effect is further witnessed by the rate of reaction over time, which increases instead of decreases as monomer concentration drops. The goal of this project was to change the anhydride to further probe how the anhydride effects the rate law and mechanism of the copolymerization focusing on a change from a bicyclic anhydride to a cyclic anhydride (CHA). Experiments with CHA indicated that the rate between runs with the same equivalents of CPMA and CHA did not display a noticeable change. Also, when the equivalents of CHA was varied between reactions, it was found by initial rates and COPASI fitting that there was a negative order similar to that observed for CPMA. This indicates that changing the anhydride does not affect the rate law and therefore the mechanism of anhydride inhibition.

**86. Tommy Vang**

*Dual-site Diels-Alder Reactions Using Various Heterocycles*

**Advisor:** Wayland Noland

**Sponsoring Program:** Project SEED

**Home Institution:** Washington Technology Magnet High School, SPPS

**Abstract:** Synthesis of 1-methylindole and substituted thiophene was proposed in order to compare the reactivity of sites in its conjugated system. The starting material, 1-methylindole, was reacted with 2-acetylthiophene to make the alcohol product. The alcohol product will be dehydrated by an acid catalyzed dehydration to yield the diene product. The diene is to be reacted with a dienophile to yield a Diels-Alder adduct. From the reaction, whichever isomer is in higher yield will tell which site on the diene is more reactive. NMR, TLC, and Mass Spectrometry will be used to help identify the final product. The purpose of this experiment is to synthesize novel compounds with sulfur and nitrogen groups, which will be tested for biological activity by NIH (National Institute of Health).

- 87. Xatziri Viveros**, Jonathan Schultz  
*Effects of Iron (III) on varying size particles of akaganeite*  
**Advisor:** R. Lee Penn  
**Sponsoring Program:** Project SEED  
**Home Institution:** Washington Technology Magnet School, SPPS  
**Abstract:** The understanding of iron oxides and their interaction with the environment is useful with the understanding of the pollutant reduction schematic. Akaganeite particles of various sizes were synthesized with aqueous Fe(III) at a pH seven with a carbonated buffer. The synthesis was let to sit for different times, the aqueous solution was centrifuged, let to dry and the particles were then analyzed with X-ray Diffraction. The data obtained from the akaganeite synthesis with the X-ray Diffraction was used to analyze how particles transform from akaganeite, lepidocrocite, Goethite and Magnetite when Fe(III) was added in various amounts. The results obtained suggest that the transformation of akaganeite to a different iron oxide occurred due to destabilization-recrystallization
- 88. Nicole Wagner**  
*Quantifying the Environmental Sensitivity of the <sup>19</sup>F Chemical Shift in Model Systems and Proteins*  
**Advisor:** William Pomerantz  
**Sponsoring Program:** UMN Chemistry- Lando  
**Home Institution:** Edinboro University of Pennsylvania  
**Abstract:** Incorporation of fluorine into proteins via fluorinated amino acids allows fluorine to be used as a biological probe for studying protein-ligand interactions by <sup>19</sup>F nuclear magnetic resonance spectroscopy (NMR). The magnetically active <sup>19</sup>F nucleus is environmentally sensitive, and as such, the microenvironment in a folded protein can dramatically alter the chemical shift. To simulate different microenvironments, trends in fluorine chemical shifts in selected nonpolar, polar protic, and polar aprotic solvents were observed using isomers of fluorinated p-cresols and indoles, which serve as small molecule analogs of the amino acids tyrosine and tryptophan, respectively. For each isomer in both protic and aprotic solvents, chemical shift was plotted against solvent dielectric constant. Based on these results, we are now incorporating fluorinated isomers of tyrosine and tryptophan into the protein Brd4 to compare the chemical shift variability within a folded protein to the effects observed with the small molecule analogs.
- 89. Alan Wang**, Ben Brummel  
*Molecular Dynamic Simulations of Water within a Lipid Bilayer*  
**Advisor:** Johnathan Sachs  
**Sponsoring Program:** Biomedical Engineering  
**Home Institution:** Mounds View High School, Arden Hills, Minnesota  
**Abstract:** Electroporation is a well known and often used technique for introducing molecules into cells through pores in cell membranes created by an electrical field. When the pores close, water may become trapped between the leaflets of the lipid bilayer. The goal of this project is to better understand the process of electroporation at the molecular level by conducting molecular dynamics simulations of water trapped within a lipid bilayer. This project is composed of two parts. The first part is molecular dynamics simulations of different amounts of water trapped between the leaflets using coarse-grained molecules from the Martini force field. The second part is a potential of mean force (PMF) calculation of a single water molecule with respect to a lipid bilayer. The PMF calculation was performed at the atomistic level using a GROMOS force field for increased accuracy. All simulations were conducted using the GROMACS software package. We will describe the results and their implications.

90. **Hannah Weissman**

*Creating a Self-Updating Global AA Meeting List*

**Advisor:** Lana Yarosh

**Sponsoring Program:** Computer Science

**Home Institution:** Wellesley College

**Abstract:** Alcoholics Anonymous (AA) is a grass-roots fellowship, hosting thousands of meetings for recovering alcoholics around the world. Each local chapter maintains their own website with a list of upcoming meetings. This has resulted in there being no global AA meeting list, or even a state-wide meeting list. Therefore, we purpose creating a self-updating global AA meeting list by combining automated scraping of local chapters websites, machine learning algorithms for classification and data mining, and crowdsourcing where automated methods fail. In this poster, we present our pipeline for creating a self-updating AA meeting list. Firstly, we scraped, via the scraped Selenium, aa.org to obtain the urls of all the local chapter sites. Next, we are attempting to scrape each local site to obtain all the urls listed on that site, however this is proving to be much more difficult than anticipated. While we are working on perfecting the scraping code, we are also working on finding the best classification algorithm for determining whether a particular page contains a list of meetings. We are comparing a variety of machine learning algorithms, provided by the WEKA tool, for this task. For those pages in which our code is not able to produce high accuracy we will use crowdsourcing. The last step will be to identify the meetings within the meeting page, by extracting the meeting information through a combination of machine learning and crowdsourcing. My contribution to the pipeline has been helping to improving the accuracy of scraping the local websites and determining which WEKA classification algorithm is most accurate for our data.

91. **Thomas Wheeler**

*Monoligated Aryl Oxide Complexes of Titanium: Donor Properties and Catalysis*

**Advisor:** Ian Tonks

**Sponsoring Program:** UMN Chemistry- Heisig Gleysteen

**Home Institution:** University of Minnesota Twin-Cities

**Abstract:** The synthesis of a monoligated titanium aryl oxide is accomplished by salt metathesis in benzene using the sodium salt of 2,6-diisopropylphenol  $\{[(CH_3)_2CH]_2C_6H_3ONa\}$  and a bridged halide imido,  $ToIN=TiX_2Py_2$  ( $X=Cl, Br, I$ ) to produce  $ToIN=TiOC_6H_3[(CH_3)_2CH]_2XPy$ . Further salt metatheses allow for the installation of other x-type donors: OPh ( $OC_6H_5$ ) Pyr ( $NC_4H_4$ ) OBz ( $OC_6H_8$ ) DA ( $N(CH_3)_2$ ) and Fluoride (F). The donor values covered by these X-type ligands is varied to enhance the visibility of ligand donor ability upon catalysis, and preliminary catalytic experiments for hydroamination, pyrrole formation, and alkyne trimerization are shown.

92. **Samantha Whitcomb**

*Solid-State Chemistry of Reactive Nitrile Oxides*

**Advisor:** William Ojala

**Sponsoring Program:** University of St Thomas- Chemistry

**Home Institution:** University of St. Thomas

**Abstract:** Nitrile oxides dimerize in solution to yield three possible products, depending on the reaction conditions: a furoxan, a dioxadiazine, or a 1,2,4-oxadiazole-N-oxide. We are examining the solid-state chemistry of benzonitrile oxides that should be capable of solid-state dimerization. Here we describe our studies on compounds relevant to the solid-state chemistry of two particular nitrile oxides: 4-methylbenzonitrile oxide and 3-nitrobenzonitrile oxide. In previous work we determined the crystal structure of the bis(4-methylphenyl) furoxan; we have now found through hot-stage microscopy that this compound undergoes a phase transition to a second, high-temperature polymorph, which we are currently attempting to obtain independently by crystallization from solution. We are also attempting to co-crystallize this furoxan with its bis(4-chlorophenyl) analogue to determine whether the phase transition can be influenced by solid solution formation. In this 4-methyl series we have also now determined the crystal structure of the bis(4-methylphenyl)dioxadiazine, which has a severely nonplanar central ring. In addition, we have determined the crystal structure of the bis(3-nitrophenyl)furoxan, which, like the 4-methyl analogue, is disordered about the approximate twofold axis through the molecule. Characterization of these dimers will be useful in determining the outcome of solid-state dimerization of the parent 4-methylbenzonitrile oxide and 3-nitrobenzonitrile oxide.

- 93. Thomas Wieser**  
*Decreased Cytotoxic Acetylated and Phosphoryl Cholinated G5 Poly(amidoamine) Dendrimer as Promising Gene Delivery Agent*  
**Advisor:** Lisa Prevette  
**Sponsoring Program:**  
**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. G5 poly(amidoamine) dendrimer (PAMAM) is a spherical, branching polymer with 128 terminal amines which can be used as gene delivery agent. DNA binds to G5 PAMAM via electrostatic interactions between the positively charged terminal amines of PAMAM and the negatively charged phosphate backbone of DNA. Unmodified G5 PAMAM, however, is cytotoxic. Previous studies show that the cytotoxicity of G5 PAMAM can be decreased by attaching neutral acetyl groups or zwitterionic 2-methacryloyloxyethyl phosphoryl choline (MPC) to the terminal amines. G5 PAMAM was conjugated in different end group ratios with acetyl groups and MPC to study their effect on binding pDNA. Electrophoretic mobility shift assays were used to study pDNA binding to acetylated PAMAM (Ac-P) and phosphoryl choline PAMAM (PC-P). Increasing the degree of acetylation leads to decreased pDNA binding, with 100% acetylation preventing association of pDNA. PC-P conjugates have been synthesized and characterized by NMR, but pDNA binding remains to be studied.
- 94. Jamie Wooding**  
*3D Printing of Co-Continuous Immiscible Polymer Blends for Hierarchically Porous Tissue Scaffolds*  
**Advisor:** Christopher Macosko  
**Sponsoring Program:** Center for Sustainable Polymers  
**Home Institution:** Rutgers University  
**Abstract:** Co-continuous immiscible polymer blends are unique in that they are composed of two phase-separated polymers that form an interpenetrating network throughout one another. When one polymer phase is selectively extracted from this blend, a porous polymer results. Recently, fused deposition modeling, commonly referred to as 3D printing, has been lauded for its great ease in fabrication and ability to allow for rapid, low-risk prototyping. In this research, fused deposition modeling is, for the first time, employed to print a co-continuous immiscible polymer blend of polystyrene and polylactic acid into a structure suitable for tissue engineering applications. Since the co-continuous morphology of the immiscible polymer blend remains after printing, the polystyrene phase can be selectively extracted, developing a biocompatible, hierarchically porous PLA tissue scaffold that successfully maintains its original printed geometry. This porous PLA scaffold exhibits a unique interconnected, fibrous morphology that may present better functional capabilities for specific tissue engineering applications.
- 95. Kenny Xiong**  
*Diels Alder Synthesis of 1-Methylindole and Substituted Thiophene*  
**Advisor:** Wayland Noland  
**Sponsoring Program:** Project SEED  
**Home Institution:** Washington Technology Magnet School, SPPS  
**Abstract:** In this project, an exploration experiment was done to compare two Diels-Alder products. Both of the Diels-Alders were to be synthesized to see which of the two compounds would have the most reactive diene. So for the experiment, the starting materials were synthesized by reacting imidazole with benzenesulfonyl chloride. From this reaction, the percent yield was 74%. The starting material was then lithiated and reacted with 2-acetylindole. The starting material also was to be lithiated and reacted later with 3-acetylindole separately from the 2-acetylindole. After the alcohol synthesis, two dienes were to be synthesized using an acid catalysed dehydration. Eventually, the two dienes would have been reacted with dienophile to synthesize two Diels-Alder products to see which Diels-Alder site is preferred. Unfortunately, there was no reaction between the starting material and the acetylated indole, so the alcohol was not synthesized. The Diels-Alder with the most reactivated diene would have been offered for biological testing by the National Institute of Health.

96. **Yomar Zayas-Ortiz**

*Synthesis Optimization and Characterization of Tin Sulfide (SnS) NanoSheets*

**Advisor:** Eray Aydil

**Sponsoring Program:** MRSEC

**Home Institution:** University of Puerto Rico at Humacao

**Abstract:** Thin nanosheets of tin (II) sulfide (SnS) have substantial applications in electronic devices and energy storage technology such as lithium ion batteries. In addition, tin (II) sulfide has low toxicity and a reasonable natural abundance. When tin (II) sulfide is exfoliated into thin nanosheets, it exhibits a wide optical band gap of 1.3 eV, making it useful as a semiconductor in photovoltaic cells. To synthesize tin (II) sulfide nanosheets, conventional-hydrothermal syntheses were made using tin (II) chloride and thiourea (sulfide source) in a Parr reactor, producing Tin (II) sulfide. Synthesized tin (II) sulfide was exfoliated using sonication and was centrifuged at different speeds to separate the nanosheets from the bulk tin (II) sulfide. The identification and characterization of the resulting tin (II) sulfide involved the use of the Scanning Electron Microscope (SEM), Raman Spectroscopy, UV-visible spectrophotometry and X-Ray diffraction. Atomic Force Microscopy (AFM) was used to detect the exfoliated tin (II) sulfide nanosheets.

**Poster Presentations for RET Participants  
Listed Alphabetically by Presenting Author**

97. **Sarah Atkins**

*Using Dystopian Literature to Enhance Student Engagement of Chemistry*

**Advisor:** Christy Haynes

**Sponsoring Program:** MRSEC

**Home Institution:** University of Minnesota

**Abstract:** It has been suggested that student engagement increases with the use of cross-curricular academic lessons that are designed to relate to students' interests and are perceived as challenging, yet also match their skill level. Dystopian literature is popular in teen leisure reading and as a natural connection to current teens can be used as a platform for cross-curricular lessons that allows students to relate general chemistry concepts. Lessons developed for the 2015-2016 academic year for general chemistry students integrated dystopian literature to cover key general chemistry concepts. These lessons were intended to promote critical thinking, reading comprehension, and application of chemistry concepts to dystopian literature while providing students an experience that initiated critical thinking of the world in terms of chemistry and connection of their high school academic subjects to each other and to the world around them. Pre- and post-assessments were used to evaluate the effectiveness of this interdisciplinary approach to chemistry. This project focuses on using data from the 2015-2016 academic year to make changes to improve student engagement with this method for the 2016-2017 academic year. In addition, with the assistance of a high school language arts teacher, appropriate level texts are being selected that meet the Minnesota language arts curriculum standards. One of these new texts is a technology dystopia and will be used in conjunction with microfluidics and acid-base chemistry.

**98. Cassandra Knutson, Cassidy Javner**

*Polymeric Medical Sutures: An Exploration of Polymers and Green Chemistry*

**Advisor:** Jane Wissinger

**Sponsoring Program:** MRSEC

**Home Institution:** White Bear Lake High School

**Abstract:** Green chemistry involves the creative design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. There is a need to teach and train future chemists to apply the principles of green chemistry to develop sustainable solutions that address the needs of our society and economy. A lab experiment was further developed that utilizes medical sutures as a platform to explore polymers, intermolecular forces, and the twelve green chemistry principles. In the first part of the experiment students mimic the creation of medical sutures by drawing the polymer polycaprolactone of varying molecular mass into threads. In the second part students test the tie-ability and tensile strength of their sutures while comparing them to actual medical sutures. The students explore green chemistry principle ten, Design for Degradation, as they test the degradability of the polycaprolactone and actual sutures in part three. In part four the students design an experiment to explore green chemistry principle seven, Use of Renewable Feedstocks, as they melt-blend additions of renewable polylactic acid and assess changes to the draw-ability, tie-ability, tensile strength, and degradability of the sutures. In addition to developing the medical suture experiment this project included learning about green chemistry and its applications in the classroom through a course offered by Beyond Benign. The contents from this course will be transferred to a three-day workshop that will be offered to teachers during the summers of 2017 and 2018.

**99. Emily McDonald**

*Investigating Genetically Modified Foods in a High School Classroom*

**Advisor:** Ben Hackel

**Sponsoring Program:** MRSEC

**Home Institution:** Shakopee High School

**Abstract:** DNA extraction experiments are common in high school biology classrooms. However once the extraction has been performed students do not get the opportunity to perform laboratory techniques such as PCR or gel electrophoresis due to the lack of resources in the high school classroom. Biotechnology and genetic engineering are concepts covered in the high school classroom. This experiment was developed so students will get the opportunity to learn about genetic engineering through the extraction of DNA from a variety of foods that they consume on a daily basis. After the extraction students are given the opportunity to carry out a PCR reaction to identify if the food they choose contains food products that have been genetically modified. Students will compare the DNA sequences that were amplified by their PCR to the DNA sequence of a plant that does not contain genetically modified genes through the observation of a gel electrophoresis. This experiment is done to show students lab techniques that scientists use on a daily basis in order to analyze DNA. They are also learning how genetically modified foods are made and which foods contain genetically modified genes.

**100. Alouisa Thames**

*Characterization and Classification of Breast Cancer Cell Lines using PCR*

**Advisor:** Ben Hackel

**Sponsoring Program:** MRSEC

**Home Institution:** University of Minnesota

**Abstract:** In this lab designed for high school students grades 11-12, students are exposed to the idea of cancer cell classification by the presence or lack thereof of marker protein expression. In particular, the lab investigates the expression of the estrogen receptor, the progesterone receptor and the human epidermal growth factor receptor in three cancer cell lines. The cell lines chosen have known molecular profiles with regard to the expression of the aforementioned protein markers, but are given as "unknowns" to students.