Abstracts

Astronomy & Astrophysics

A1 – The reflection effect for eclipsing binaries
Author: Jeffrey Gropp
Advisor: Dr. Andrej Prsa

Using a database of eclipsing binaries or EBs (stars which pass in front and temporarily block each other out) from the Kepler space telescope we searched for star systems which displayed characteristics corresponding to the reflection effect. The reflection effect is essentially the brightening of one star due to irradiation by its companion. We discovered 40 candidates amongst the nearly 5000 EBs in the database. With these candidates we plan to analyze the parameters and properties of each system using the "PHysics Of Eclipsing Binaries" (PHOEBE) modeling program. Using a variant of the "Markov Chain Monte Carlo" (MCMC) method, we will statistically analyze our solutions to find the best fitting parameters. With these parameters we will attempt to find commonalities to help us determine more about the reflection effect.

A2 – The old novae as supernova type Ia progenitor candidates: DN gem
Author: Amanda Findlay
Advisor: Dr. Edward Sion

Little is known about how a nova explosion affects the rate of mass transfer in a cataclysmic binary system and the subsequent evolutionary behavior of the accreting white dwarf during post-nova quiescence. We present a synthetic spectral analysis of the archival IUE far ultraviolet spectra of the post-nova, DN Gem (Nova Gem 1912). The mass of the white dwarf has been estimated to be approximately 0.92 solar masses (Dobrotka 2008), and has an orbital period of 0.127844 days (Peter & Thorstenson 2006). The system's orbital inclination is approximately 30 degrees (Darnley 2012) while various distance estimates range from 450 to 1900 parsecs. Interstellar reddening of the spectra was removed with E(B-V) = 0.15. Our synthetic spectral analysis utilized optically thick, steady state accretion disk models and white dwarf model atmospheres that we constructed using TLUSTY and SYNSPEC (Hubeny 1988, Hubeny & Lanz (1995)). Our input parameters were the white dwarf mass, inclination and a range of accretion rates for which we found the best-fitting model. We report the results of our model fitting, the mass transfer rate 115T years after its nova explosion and compare DN Gem with other post-novae at comparable times past their nova outburst.

A3 – Precovery of eclipsing binaries: identifying eclipse timing variation among Kepler eclipsing binaries in KELT

Authors: Valerie Bernstein, Dr. Joshua Pepper
Advisor: Dr. Joshua Pepper

Eclipsing binaries (EBs) offer the opportunity to precisely measure the dynamics of multi-body systems. When an EB is gravitationally bound to a third star in a hierarchical configuration, the times and durations of the eclipses can be perturbed, providing information about the orbits and properties of the stars. The Kepler Eclipsing Binary Catalog provides light curves and physical properties of over 2500 classified eclipsing binary systems observed over approximately four years by the Kepler spacecraft. Observations of part of the Kepler field by the KELT survey span approximately seven years. By cross-matching Kepler EBs with light curves from KELT, we obtain a longer time baseline on which to probe eclipse variations, although with lower photometric precision than Kepler. Comparison of the matched EBs can reveal eclipse timing variation in KELT data that could lead to the modification of models used to anticipate past and future events. This work lays the groundwork for extending this process to EBs observed by the K2 mission, which has 80-day observing campaigns, and thus will benefit much more from the extended baseline of KELT.

A4 – Secret lives of cepheids: photoelectric photometry of bright cepheids - searching for evolutionary changes

Author: Mike Toce
Advisor: Dr. Edward Guinan

Classical Cepheids (Cepheids) are one of the most important classes of variable stars. From the Leavitt (Period-Luminosity = P-L) Law, these stars serve as crucial "standard candles" for determining the cosmic distance scale and measuring the Hubble Constant (H0). Also, Cepheids play a fundamental role in the calibration of Type Ia supernovae, which indicate that the expansion of the Universe is accelerating, and also infer the existence of dark energy (Riess et al. 2011). Cepheids are also important astrophysical laboratories for probing the internal structure, stellar atmospheres and evolution of moderate mass ($\sim 4 - 15\ M_\odot$) stars and Type II SN progenitors, for Cepheids above $\sim 8M_\odot$. The study of Cepheids provides valuable information about convective core overshooting, mass loss, rotation and helium core burning for moderate mass, evolved stars. Studies of changes in their pulsation periods and amplitudes reveal evolutionary changes too subtle to detect directly, and understanding these various characteristics of Cepheids is crucial to their use as high-precision standard candles.

To this end, the Villanova Secret Lives of Cepheids (S.L.C.) program was initiated several years ago. This program is a comprehensive study of Cepheid behavior, evolution, pulsations, atmospheres, heating dynamics, shocks and winds. The program now spans almost the entire electromagnetic spectrum, from recently acquired X-ray observations (XMM-Newton and Chandra), to FUV/UV spectra (HST, IUE and FUSE), to the ground-based photoelectric photometry.

As part of this S.L.C. program, photoelectric photometry is being carried out of small sample of bright Cepheids. The observations are being made using the 14-inch reflector telescope at Villanova Campus Observatory. The observations are being made using SBIG photoelectric photometer equipped with standard Johnson BVRI filters. Photometry is being carried out of the following stars along with their spectral type, period, and visual mag: X Cyg (F7Ib, ~16.39d, 6.47mag), DT Cyg (F7.5Ib, ~2.5d, 5.82mag), S Sge (G5Ibv, ~8.38d, 5.36mag), FF Aql (F6Ib, ~4.47d, 5.38mag), Eta Aql (F6Iab, ~7.18d,3.80mag), Delta Cep (F5Iab, ~5.37d,3.75mag)The primary science objectives are to obtain light curves to investigate possible evolutionary changes from small variations in luminosity, light amplitude and pulsation period.

We place special emphasis on the classical Cepheid X Cyg, its characteristics stated above. Szabados' 1991 paper showed a phase jump in X Cyg's O-C (Observed-Calculated) diagram which indicates a sudden change in pulsation period. X Cyg holds priority in our observations as we attempt to affirm or deny this pulsation period change. We combined the Villanova photometry with complementary B, V and Near-IR photometry conducted from nearby Allentown by Wasatonic.

A5 – Dating the stars next door: ages and coronal X-ray emissions of nearby K-stars

Authors: Marcus Katynski, Dr. Edward Guinan, Dr. S. Engle
Advisor: Dr. Edward Guinan

Stellar age is a very important physical property of a star but among the most difficult basic physical property to reliably determine. Due to the long timelines on which stars evolve, their observable age-dependent physical properties (such as stellar luminosity, temperature and diameter) change very slowly and are thus very difficult to determine. One possible means to estimate the age of a star is from its rotational period; it is known that as a star ages, it loses angular momentum due to magnetic braking and its rotation slows down. However, a star's rotational period is typically difficult to measure photometrically (or spectroscopically) for older, less active stars since they rotate slowly and their star spots and active regions are smaller and less prominent. For this reason, measuring the coronal X-ray activity of a star is an appealing alternative to measuring the rotation. Coronal X-ray activity is powered by a star's magnetic dynamo, the strength of which depends on the star's rotation, so rotation and X-ray emission are fundamentally related. The relevant difference is that X-ray fluxes are far easier to measure and importantly available for many stars. During the 1990's the ROSAT X-Ray Satellite carried out an all-sky survey of thousands of X-ray sources including hundreds of nearby stars, producing a large archival library of X-ray data. Most stars in the solar neighborhood are included in this important X-ray archive (see HEASARC: heasarc.gsfc.nasa.gov/).

Utilizing these and other available X-ray data, we determined the relation between coronal X-ray emission and stellar age of nearby K-type stars. K-type stars (also known as orange dwarfs) are cooler, less luminous and slightly less massive than the Sun (masses ~60-85% of the sun's mass). These K-type stars are important because of their long lifetimes and relative stability and appear to be favorable candidates for hosting potentially habitable planets. By collecting data on coronal X-ray emission from K-type stars with ages independently determined by methods such as asteroseismology-

age-mass relations, verified membership to clusters or moving groups with known ages, or stars in multiple systems where its companion has a known age, we were able to calibrate a precise relation between X-ray luminosity and age. We have applied this relationship to nearby K-stars (within ~7 parsecs, or approximately 23 light years) with measured X-ray fluxes to estimate their ages. Several of these stars host planets. We discuss these results and future plans for this research.

A6 – Modelling stellar light curves
Author: Griffin Werner
Advisor: Dr. Andrej Prsa

An issue in the theory of low-mass stars is the discrepancy between predicted and observed radii of M-type stars. Using data that have been accumulated from the Kepler space craft and Kitt Peak National Observatory on eclipsing M-type stars, we will model the light curves and radial velocity curves of these systems using fundamental parameters (mass, radius, luminosity, and temperature). We will then compare these models to the observed curves and fit them in order to obtain the actual values of the masses and radii of stars in eclipsing binary systems. Getting to the position where we will be able to model the light curves accumulated by Kepler, a full and complete understanding of the modelling program PHOEBE and an understanding of Markov chain Monte Carlo sampling was necessary in order to comprehend the accuracy of our models. This summer, we learned how to use the modeling program PHOEBE and practiced modeling curves that have already been solved in the literature. We then wrote a python program using MCMC to find the error in the solutions of our models and compare them to those in the literature. Our goals moving forward are to start modelling the Kepler data, and use our program to find the uncertainties in the parameters of the systems.

A7 – Photometry of the variable bright red supergiant Betelgeuse from the ground and from space with the BRITE nano-satellites
Authors: Robert Minor, Dr. Edward Guinan, Dr. Richard Wasatonic
Advisor: Dr. Edward Guinan

Betelgeuse (Alpha Orionis) is a large, bright, luminous semi-regular red supergiant of spectral class M1.5-2Iab. It is the 8th brightest star in most filters and the brightest star in the infrared. Betelgeuse is 30,000 times more luminous than the Sun and 700 times larger. It is an evolved star with an estimated age of ~8 +/- 2 Myr. Betelgeuse will end its life in a Type II supernova (anytime from now up to about a million years). When it explodes, it will most likely shine with the intensity of a full moon and possibly visible during the day. However, it is too far away to cause and significant damage to Earth.

Photometry of this important pre-supernova star has been ongoing at Villanova for nearly 45 years. These observations are being used to monitor and define the complicated brightness variations of this star. Semi-regular periodic light variations have been found with characteristic periods of 385 days up to several years. These light variations are used to study its unstable atmosphere and resulting

complex pulsations. Over the last 15 years, the star has been observed by Wasatonic who has accumulated a large photometric database.

The ground-based observations are limited to precisions of 1.5%, and due to poor weather, limit observations to typically 1-2 times per week. However, with the recent successful launch of the BRITE Nano-satellite system (http://www.brite-constellation.at) during 2013-14, it has been possible to secure high precision photometry of bright stars, including Betelgeuse, continuously for up to 3 months. Villanova has been invited to participate in the BRITE guest investigators program and has been awarded observing time and data rights for over a dozen bright stars, including Betelgeuse. BRITE blue and red observations of Betelgeuse were carried out during the November-February 2013-14 season and the 2014-15. These datasets have been made available to Villanova and have been combined with contemporaneous photometry from Wasatonic. The red data from BRITE were found to not be useable due to saturation, but the blue data is useable. The BRITE datasets were combined with our ground-based V, red, and near-IR photometry. Problems were uncovered with the some of the BRITE data, but they were resolved for the most part. We present and discuss the results obtained so far.

Biochemistry

A8 – The importance of research: how cell culture density changes the effect reactive oxygen species have on activation of the antioxidant response element

Author: Anna Briker
Advisor: Dr. Aimee Eggler

In periods of oxidative and electrophilic stress in cells, the Nrf2 transcription factor binds to antioxidant response elements (AREs) located upstream of a battery of genes encoding for cytoprotective proteins. Upregulation of these cytoprotective proteins by Nrf2 is believed to contribute to the prevention and amelioration of chronic diseases, including cancer, heart disease, diabetes, and neurodegenerative diseases. Thus, a greater understanding of Nrf2/ARE activation has significant implications for preventative medicine. During normal cellular conditions, Keap1, the repressor protein of Nrf2, is bound to Nrf2, targeting it for ubiquitination and degradation. Electrophiles, including many found in foods, covalently modify Keap1, preventing it from targeting Nrf2 and thus allowing Nrf2 protein to accumulate and target AREs. Nrf2-activating compounds show promise for disease prevention. A number of these compounds also cause the production of H2O2 and other reactive oxygen species (ROS) in the cell, which could contribute to ARE activation. However, there are conflicting results in the literature as to the degree of importance that ROS generated by Nrf2 activators play in activating ARE. We hypothesize that H2O2 activates the Nrf2/ARE pathway minimally on its own, but significantly enhances ARE activation in conjunction with an electrophile.

We tested this hypothesis by treating cells with the electrophile sulforaphane and H2O2 and used an ARE-reporter plasmid to monitor ARE activation. After passaging and plating the cells at the

optimal confluency (80%), we observed that cells treated with H2O2 showed minimal ARE activation, but H2O2 in combination with sulforaphane resulted in synergistic ARE activation. However, we found that that the confluency of the cells during passaging and plating can change the effects of addition of ROS on ARE activation. When the assay is repeated with cells passaged at low confluency, H2O2 does not appear to cause synergistic ARE activation. Additionally, when the assay is repeated with cells passaged at high confluency, H2O2 on its own activates ARE, and in conjunction with sulforaphane synergistic effects of H2O2 are not observed. Possible causes for the effect of cell confluency during passaging and plating on ARE activation are discussed. In the future, we will closely monitor confluency of cells at plating as well as at harvest, so that we may continue to investigate the effects of ROS on ARE activation with minimal confounding variables.

A9 – Lithium ion battery ab intio simulations
Author: William Yoquinto
Advisor: Dr. Ryan Jorn

Lithium-ion batteries can be used to store energy. Studying the chemistry involved in the operation of battery can lead researchers to finding optimal operational parameters. Using ab intio molecular dynamics the electrolyte, consisting of ethylene carbonate (EC) and lithium hexafluorophosphate (LiPF6) in the battery cell is, was modelled interacting with various solid electrolyte interface configuration (SEI). The SEI consisted of varying concentrations of lithium fluoride (LiF) or lithium carbonate (Li2CO3) in dilithium ethylene dicarbonate (LiEDC). Additionally bulk simulations were run on just the SEI layer.

A10 – Synthesis of Nrf2/ARE activators mimicking a natural product structural motif
Authors: Rishi Chauhan, Sally Zhou, Dr. Aimee Eggler, Dr. Konstantinos Agrios
Advisor: Dr. Konstantinos Agrios

Electrophilic molecules are an important defense mechanism against oxidation, and thus serve a noteworthy function in preventing cellular damage in the cases of many diseases, such as Parkinson's disease and Alzheimer's. Our project aims to synthesize an analog of Dysidaminone 16 (DA 16), a sesquiterpene aminoquinone isolated from South China Sea Sponges. Natural product DA 16 has been suggested to be a promising Nrf2/ARE activator. The DA 16 structure involves two components: a hydrophobic segment and an electrophilic segment. Our synthetic strategy for the DA 16 analog was based on separately synthesizing the hydrophobic segment from trans-1-decalone, and the electrophilic segment from guaiacol. The two suitably functionalized and protected synthetic intermediates were coupled successfully via a Suzuki reaction.

A11 – Determining the role of ROS in the activation of Nrf2/ARE-regulated genes by qPCR

Author: Alexandra Elder
Advisor: Dr. Aimee Eggler

The transcription factor Nrf2 has been proven to play a key role in the defense and protection of cells against harmful oxidative stresses. It functions by binding to a gene sequence called the antioxidant response element (ARE), which is located upstream on the DNA of more than 20 known genes that encode cytoprotective proteins. When the cell is subject to electrophilic and oxidative stress, these cytoprotective genes are upregulated in order to eradicate the potentially destructive agents within the cell.

The first step in the activation of Nrf2, and subsequent transcription of necessary cytoprotective genes, is the reaction of an electrophilic inducer molecule with a repressor. Some commonly known inducer molecules include sulforaphane, a naturally occurring phytochemical commonly found in cruciferous vegetables, and celastrol, another naturally occurring phytochemical found in the roots of the thunder god vine. In addition to these phytochemicals, several oxidizable diphenols are known inducers of the transcription of ARE-regulated genes.

There is a controversy within the field pertaining to the role of reactive oxygen species (ROS) formed by the redox cycling of oxidizable polyphenols in the activation of Nrf2. When diphenols are oxidized, they are transformed into their electrophilic form, and are capable of deactivating the repressor of Nrf2. In addition, ROS are generated. Various groups have shown ROS generated by Nrf2 activators are important for triggering the Nrf2 pathway. In contrast, there is evidence within the field that ROS generated by oxidizable diphenols do not in fact play a role in the induction of ARE-regulated genes. Additionally, some ARE's have an added regulation by the transcription factor Bach1. One such ARE-regulated gene is HO-1(heme oxygenase 1). Bach1 is a repressor that inhibits the binding of Nrf2, and is inactivated in the presence of ROS.

The goal of my summer research was to elucidate the role that reactive oxygen species play in the transcription of several ARE-regulated genes through the use of quantitative polymerase chain reactions (qPCR). Quantitative PCR is a useful tool in the comparison of mRNA accumulation in the cell under different treatment conditions. We were testing the hypothesis that there is a synergistic, or more than added, activation of ARE-regulated genes upon the combined treatment with an electrophile and ROS.

The experiments included four treatment conditions: sulforaphane, hydrogen peroxide (ROS source), sulforaphane+hydrogen peroxide, and a DMSO control. The results of my qPCR experiments have shown that, not only does ROS enhance the activation of HO-1 by an electrophile; it has a synergistic effect on the transcription of this highly regulated cytoprotective protein. In addition, ARE reporter has shown the same synergistic effect, as well as western blot of HO-1 accumulation. The goal of my project is to determine whether this observed synergy is also seen for other ARE-regulated genes that are not highly regulated by Bach1. The mRNA transcripts tested thus far are HO-1, AKR1C1, AKR1C2, GCLC, and GCLM, and we plan to test NQO1 next.

A12 – The role of ZC3H8 in breast cancer cell invasion, phenotypes, and in transcription through the little elongation complex

Authors: Jani Swiatek, Keith Danielson, John Schmidt, Dr. Janice Knepper
Advisor: Dr. Janice Knepper

Cells induced to overexpress ZC3H8 have increased tumor aggressiveness in terms of proliferation and migration but little is understood of its mechanism of action. High throughput studies have shown that ZC3H8 may be a component of the little elongation complex which is involved in transcription of small noncoding RNAs. A cDNA encoding ICE1, a protein the Little Elongation Complex, was cloned so the association of ZC3H8 and ICE1 could be confirmed. Because of ZC3H8's role in transcription, all of the RNA in human breast cancer cells overexpressing ZC3H8 was sequenced. MEMO1 was found to be overexpressed 4.16 fold and has been shown to be a gene responsible for increased migration of cancer tumor cells. Using PCR and quantitative PCR, its levels have been shown to decrease in cDNA from cells with decreased expression of ZC3H8 when compared to their unaltered counterparts. The same experiments have been carried out with cDNA from cells overexpressing ZC3H8; levels of MEMO1 in the cDNA were increased compared to the unaltered cDNA. Further confirmation of these results is necessary to solidify these conclusions. MEMO1 has also been cloned into a vector, pcDNA3.1, which was used to transfect, or add, additional MEMO1 into cells lacking ZC3H8. This will determine if it will rescue the cancerous phenotype especially in terms of migration and if levels of ZC3H8 will increase in response to MEMO1's addition. Future work will include determining the effects of the MEMO1 transfection of the cells lacking ZC3H8 as well the relationship between ICE1 and ZC3H8. The effect of reducing expression of MEMO1 in ZC3H8 overexpressing cells will also be studied to determine if it will decrease migration. With these experiments we hope to better understand the mechanism of ZC3H8's s effect on cancer as well as MEMO1's role in relation to ZC3H8 in cancer aggressiveness.

A13 – Effects of aromatic paddle mutations on the 26s proteasome

Author: Matthew Oleksak, Dr. Daniel Kraut
Advisor: Dr. Daniel Kraut

The Proteasome is a central component of the eukaryotic cell's protein degradation process. The three major components of the 26S proteasome are two 19S regulatory caps located on opposite ends of the 20S core component. To begin the degradation process, the target protein must be tagged with a poly-ubiquitin chain. Once ubiquitinated, the protein is recognized by one of the regulatory caps. Upon recognition the protein enters into the opening of the cap, which is surrounded by six Rpt subunits. These Rpt subunits translocate the protein into the core component where it can be degraded. Each Rpt subunit contains an aromatic paddle with a central tyrosine residue that faces the pore and "paddles' the substrate toward the 20S core. Our objective is to determine if there is a link between these aromatic paddles and the proteasome's processivity. Processivity is calculated by comparing the amount of fully degraded protein and the amount of partially degraded protein.

Mutations to these six subunits were made by Rafael Jedilinski, a former member, and these mutations were tested using a degradation assay with different substrates. Multiple substrates were used to determine which substrate domains promoted or inhibited processivity. Using parameters developed by Dr. Daniel Kraut we determined that the aromatic paddle mutations are affecting the degradation process. Oddly, we found that the mutated proteasomes were more processive than the wild type proteasome. However, in most cases we found that the mutants had slower degradation. We determined that it is possible that the mutant proteasomes interact with the substrate in slower, but more deliberate way making them more processive, but slower than the wild type. To further study the effects of these mutations we have begun making proteasomes that contain multiple Rpt subunit mutations. We hope that these mutants will shed more light on the role of each of the aromatic paddles, and the processivity of the proteasome.

A14 – Cloning, expressing, & purifying D.melanogaster Keap1

Author: Prabhjot Kaur
Advisor: Dr. Aimee Eggler

Nrf2 is a transcription factor of the leucine zipper family, and together with Keap1, as its specific repressor, signaling through the body this system defends against electrophilic and oxidative stress in the body. The Nrf2/ Keap1 system is activated when electrophiles modify Keap1 cysteines, allowing the repression of Nrf2 to be relieved. Nrf2 signaling upregulates cytoprotective genes through the antioxidant response element (ARE). Thus, Nrf2/ Keap1 signaling in humans allows for the prevention of diseases including cancers, and cardiovascular, metabolic, inflammatory and neurodegenerative diseases. Since the D. melanogaster Keap1 is 38.1% identical in sequence to the Keap1 found in the human body, it can be used as a good model system to compare to the human Nrf2/ Keap1 system. However, the D. melanogaster system does not have a cysteine corresponding to human Keap1 C151, a major sensor of ARE-activating electrophiles. In our research, we want to comprehend the mechanism that Drosophila Keap1 uses to sense electrophiles, so that long-term we will be able to better understand the role the Nrf2 system plays in the biological functions of the fly. Over the course of the summer, I attempted to purify the D. melanogaster Keap1 (dKeap1) gene, which is cloned and optimized into a protein expression vector.

Over the summer, I worked with the two D. melanogaster Keap1 isoforms (776 and 744 amino-acids long) and two vectors, pET15b and pGEX, focusing primarily on purifying the dKeap1-744 isoform. During the spring semester, dKeap1-744 was successfully cloned and expressed, and this summer I attempted to purify the dKeap1 protein. The batch purification method utilized the glutathione tag in frame with Keap1 via the pGEX vector, and a GST tagged resin. Induction times were varied from 37˚C to 25 ˚C in an attempt to produce higher yield levels. Unfortunately, purification by either glutathione gravity column agarose resin or magnetic resin produced low yields shown by SDS PAGE. Also, attempts to clone dKeap1-776 into the pGEX vector using Gibson Cloning are described.

Biology

A15 – Is deep soil decomposition inoculum-limited?
Authors: Megan Foley, Dr. Adam Langley
Advisor: Dr. Adam Langley

The purpose of this study was to examine inocula composition as a determinant of deep soil decomposition. A reciprocal soil inocula transplant incubation was performed to assess the ability of three distinct microbial communities to decompose over the course of six weeks. Communities were isolated at three depths (0-10cm, 10-20cm, >60cm) from a core taken from a brackish marsh. Communities were then used to inoculate vials containing autoclaved homogenized soil with a headspace treatment of either N2/O2 or N2 gas. Shallow soil microbes (0-10 cm) were found to respire at a greater rate than deep soil microbes (>60cm) across soil substrate and headspace treatments. The headspace treatment N2/O2 was found to correlate with higher respiration rates across inocula type than the N2 treatment. This study suggests the potential of microbes to decompose varies across communities with depth.

B16 – Regulation of wago-1: an examination of the regulatory architecture that governs Argonaute protein expression in Caenorhabditis elegans
Authors: Erin Rosenberg, Dr. Elaine Youngman
Advisor: Dr. Elaine Youngman

Across eukaryotes, thousands of small, noncoding RNA molecules silence or license gene expression via their interactions with Argonaute proteins through RNA interference (RNAi) and related processes. Since its discovery in 1998, RNAi has emerged as an important contributor to genetic regulation and has been utilized as an invaluable tool for functional genomics and medical therapeutics. Despite the important role RNAi plays in the regulation of gene expression, little is known about how the Argonaute effector proteins involved are regulated. As a foray into understanding the regulation of the Argonaute protein network, we have chosen to examine the developing germ line of the nematode Caenorhabditis elegans, where at least five Argonautes are expressed in overlapping patterns. Presumably because the genome is being prepared for passage to the next generation and is relatively inaccessible to transcription factors, gene expression in the germ lineages of many animals – including C. elegans – is thought to rely heavily on posttranscriptional regulation. We therefore hypothesize that proper patterns of Argonaute expression in the germ line will depend both on promoter sequences and the 3' – untranslated region (3'UTR). Using molecular cloning methods combined with cutting-edge genome engineering based on the CRISPR/Cas system, we are using a green-fluorescent protein (GFP) reporter transgene strategy to test this hypothesis. This past summer, I generated a series of four reporter constructs that will allow me to individually assess contributions to regulation of the Argonaute protein wago-1, which plays an important role in both in developing sperm and oocytes. I have designed and constructed CRISPR sequences to guide

integration of these transgenes into a defined locus on Chromosome II known to support germline expression, and am currently performing microinjection to establish transgenic worm strains. Analysis of these strains by florescence microscopy will allow me to test the specific hypothesis that wago-1 is regulated at the transcriptional level in developing sperm and the post-transcriptional level in developing oocytes, similar to known regulatory mechanisms for other genes in the C. elegans germline. This research will provide the first insight into the mechanisms that regulate Argonaute protein expression during germ cell development, and will also advance methods for generating CRISPR-integrated reporter transgenes in C. elegans.

B17 – Investigating the potential regulators of DAF-16, a FOXO3a conserved transcription factor, in C. elegans

Authors: Paul Regan, Prem Patel, Safae Bennani
Advisor: Dr. Matthew Youngman

The process of aging in living organisms is associated with changes in gene expression. The insulin signaling pathway is one of the major cellular signaling pathways responsible for these age-related changes. In the nematode Caenorhabditis elegans, the insulin/IGF-1 (insulin growth factor) signaling pathway plays an important role in stress resistance and longevity. DAF-16, a FOXO3a conserved transcription factor that is part of the insulin/IGF-1 pathway, is known to mediate responses to stress in younger animals and it becomes activated in an age-dependent manner in adults, even in the absence of stress. However, the mechanism by which DAF-16 is activated specifically during aging remains unclear. Previous studies have uncovered potential regulators of DAF-16 that may bind directly to DAF-16 or influence which genes the transcription factor activates as part of the stress response. We used a reverse genetics approach to ask if these known potential regulators of DAF-16 are responsible for modulating its transcriptional activity during aging in C. elegans. When worms were infected with the bacterial pathogen Pseudomonas aeruginosa, RNAi-mediated knock down of SMK-1, AAK-2, and TORC-1 caused adult worms to be more susceptible to infection, while RNAi-mediated knock down of HCF-1 resulted in longer-lived adults. These data suggest a mechanism in which DAF-16 transcriptional activity is highly regulated during aging, with both activators and repressors playing important roles. Since many stress-related pathways in C. elegans have human homologs, understanding the regulation of DAF-16 could have implications for human stress responses and age-related diseases. With the human homolog of DAF-16, FOXO3a, being strongly linked to longevity, it is possible that lifespan in humans has a highly regulated genetic component as well. The phenomenon of cofactors interacting with transcription factors later in life might be a pattern that will be seen in future aging studies.

B18 – Developing a field-based protocol for measuring songbird exploratory behavior

Authors: Breanna Bennett, Sarah Polekoff, Dr. Robert L. Curry
Advisor: Dr. Robert L. Curry

Exploratory behavior is a frequently studied component of animal personality. European ornithologists have developed a standardized aviary approach for use with passerines such as parids. Accumulated research using this protocol has shown that Great Tit exploratory behavior is repeatable, heritable, and strongly correlated with other behavioral and demographic variables. We aimed to develop a proxy method for use in a field situation that would avoid logistic requirements and regulatory headaches associated with keeping birds in captivity overnight. Using backyard songbirds in southeastern Pennsylvania, we released mist-netted individuals directly into a commercially available "screen house" containing two sets of perches; we video-recorded movements and vocalizations for 5 min, and then analyzed data using principle components analysis (PCA). This method was effective: across our sample of > 30 birds (Carolina Chickadee, Tufted Titmouse, White-breasted Nuthatch, and American Goldfinch), we found substantial within- and between-species variability and within-individual consistency: PC1 (accounting for > 50% of variation) scores depended on number of movements and conversely on latency to perch on various walls and perches, while PC2 scores reflected change over the duration of the test. We plan to use this system to investigate whether exploratory behavior is a component of personality in Carolina chickadees, Black-capped chickadees, and their hybrids.

B19 – Investigating lymphoid tissue inducer cells on the inhibited development of Peyers patches in Ly-6A transgenic mice

Authors: Brandon Chu, Gabrielle Faragasso, Dr. Anil Bamezai
Advisor: Dr. Anil Bamezai

Peyer's patches (PP) are mammalian secondary lymphoid organs associated with the gut and located on the mesenteric side of the small intestine. Microfold cells (M cells) present in Peyers patches facilitate uptake of foreign antigens and components of the gut flora. PP also house cells that initiate innate and adaptive immune responsiveness to foreign antigens. Foreign antigens transported into the Peyer's patches are sensed by cells of adaptive immunity (B and T lymphocytes) either directly or after their internalization/endocytosis by phagocytes and other antigen presenting cells. We have previously shown that the Peyer's patches of Ly-6A (Sca-1) transgenic mice appear to be significantly reduced in size, underdeveloped, or have disappeared altogether. To further our investigation, we focused on lymphoid tissue inducer (LTi) cells, which originate from the fetal liver and travel to the gut early in embryogenesis and are vital in the formation of Peyer's patches. Immunohistochemistry was performed on E18.5 Ly-6A (Sca-1) transgenic and wild type mice to compare expression of the LTi cell associated proteins LTα1β2 and ROR-ϒt. LTα1β2 is a heterotrimeric extracellular ligand on LTi and binding of the ligand to its receptor, LTβR on mesenchymal cells serves as a vital step in PP formation. ROR-ϒt is a nuclear hormone receptor on LTi cells that is also vital for the development

of Peyer's patches, though the exact mechanism of action is still unclear. Preliminary FACS analysis revealed that Ly-6A transgenic mice exhibited lower levels of LTi cells than wild type mice in the fetal liver.

B20 – Examining the role of DAF-18, a PTEN homolog, on age-dependent regulation of DAF-16
Author: Prem Patel
Advisor: Dr. Matthew Youngman

The genetic theory of ageing looks directly at the impact of genes on the regulation of lifespan. Caenorhabditis elegans have an insulin-signaling/DAF-2 pathway that is evolutionarily conserved throughout animals and has implications on stress and ageing. Insulin-like peptides initiate a phosphorylating cascade in the DAF-2 pathway, which ultimately phosphorylates DAF-16 and inhibits the ability for stress response. In adult worms, DAF-16 is activated even in the absence of acute stress. This project looks upstream of DAF-16 in the pathway at DAF-18, a homolog to the phosphatase PTEN in mammals, to determine the impact of DAF-18 on the transcriptional activity of DAF-16 throughout ageing in normal, healthy, and unstressed worms. RNAi knockdown of daf-16, daf-18 and various other controls on worms, coupled with slow kill assays (SKA) with Pseudomonas aeruginosa and fluorescent imagery, showed that daf-18 knock-down by RNAi phenocopies daf-16 both with respect to increased susceptibility to bacterial infection and with regard to the expression levels of an in vivo reporter for DAF-16 transcriptional activity (lys7::GFP). The phenocopy shows that DAF-18 is necessary in adult worms to allow for DAF-16 to reach its transcriptional targets for stress response. The mutation of PTEN in humans is linked to prostate cancer due to overexpression of AKT and ETS targets, thus the increased knowledge on DAF-18 increases the ability to understand PTEN regulation.

B21 – Downregulation of DZIP1L in Fliz1 transfected tumor cells
Author: Gerard Walker
Advisor: Dr. Dennis Wykoff

Upregulated Fliz1 expression is associated with invasive phenotype in epithelial cells. In examining the regulatory effects of Fliz1 upregulation, RNA Seq analysis of Fliz1 transfected and un-transfected cells showed a 26 fold downregulation of DZIP1L in Fliz1 transfected cells. The function of DZIP1L is uncharacterized, yet conserved DAZ interacting and zinc finger domains may indicate similar function to DZIP1, which is involved in the proliferation stimulating Hedgehog signaling pathway. I hypothesized that Fliz1 represses DZIP1L expression, and that DZIP1L deregulation contributes to the phenotypic effects of Fliz1 overexpression. In human cell lines, the hDZIP1L sequence was unable to be amplified using rt-PCR while mouse mDZIP1L sequence was amplified and showed visibly higher expression in FLIZ1 un-transfected cells. However, qPCR of transfected and un-transfected Comma D cDNA showed no significant difference in DZIP1L expression. Western blot analysis of

Fliz1 transfected and un-transfected HeLa, T47D, and Comma D cell lysates showed no difference in protein expression, and the bands in all cases were sized lower than expected at 60 kDa rather than 87 kDa. Comparisons between Fliz1 transfected and un-transfected cells at both the DNA and protein level showed no consistent Fliz1 repression of DZIP1L; yet the abnormal protein sizes detected by western blot could indicate the prominence of an alternate DZIP1L splice variant. Future investigation of DZIP1L and its role in normal and tumorigenic mammary cell function will involve overexpression of mDZIP1L into Comma D cells to elucidate DZIP1L localization and effects, if any, on invasive phenotypes in cells.

B22 – Investigating the role of siRNAs in producing memory of pathogen exposure in C. elegans.
Author: Laura Meissner
Advisor: Dr. Elaine Youngman

In defiance of the laws of traditional Mendelian inheritance, it has been observed the experience of parental generations can lead to alterations in their progeny's genome. Examples of such experiences is environmental changes, such as starvation, which can cause heritable, epigenetic effects on gene expression in the roundworm Caenorhabditis elegans (C. elegans). The somatic cells of this organism can respond to environmental influences and alter gene expression through mechanisms involving regulatory RNA molecules, known as endogenous small interfering RNAs (siRNAs) (Fire, et al., 1998). It has been previously demonstrated that C.elegans can learn to avoid the pathogenic soil bacterium Pseudomonas aeruginosa (P. aeruginosa) after exposure for four hours to the pathogenic bacteria through a mechanism involving alterations in serotonin expression in specific chemosensory neurons (ADFL and ADFR). Given the recent discovery of the role neurons play in directing siRNA to the germline to produce epigenetic changes, we hypothesized that the observed modifications C. elegans exhibit in its olfactory preferences after exposure to pathogenic bacteria will be heritable and involve a siRNA pathway. To test for heritability, worms were raised either in the presence of both pathogenic P. aeruginosa (PA14) and non-pathogenic Escherichia coli (OP50), or on OP50 alone. F1, F2, and F3 progeny of these trained naïve populations were tested for pathogen avoidance without ever having themselves been exposed to the pathogen. Strikingly, we have found that after five or more generations of repeated exposure to the pathogenic PA14, the learned pathogen avoidance behavior is stably inherited for at least 3 generations. To determine whether siRNAs are involved in olfactory learning in this system, we are currently testing whether mutant strains defective in endogenous siRNA production can learn to avoid pathogen. In addition, deep sequencing of the RNA from trained and untrained animals will be carried out and analyzed to identify learning-associated changes in mRNA and small RNA expression.

Center for Peace & Justice, Economics

B23 – The implementation and funding of Bolsa Família: a focused analysis on conditional cash transfer in education policy as it applies to the political-economic structure of Brazil

Author: Alexandra Robinson
Advisor: Dr. Miron Wolnicki

Using data and previous research from the World Bank and the Ministry of Social Development in Brazil, this research sought to quantitatively and qualitatively examine the impact of Bolsa Família in Brazil. Bolsa Família is the largest conditional cash transfer in the world in terms of size and money spent per year. Conditional cash transfers are a type of welfare program that seeks to offer short-term relief to the poor and extreme poor while also ensuring that conditions regarding health and education of children are met to end the inter-generational transmission of poverty. Although this research primarily sought to understand the inception and evolution of the Bolsa Família program from the municipal to national level, common problems found within the Bolsa Família program included supply-side constraints and political party clientelism to gain power by offering welfare with only short-term relief to the masses. Some of the supply-side constraints include a lack of teachers and classrooms for the beneficiaries of the Bolsa Família program. In conclusion, this research found that there are still holes within the Bolsa Família program that prohibit recipients from working their way out of poverty through better education and health.

Center for Peace & Justice

B24 – Geographical intersection: concentrated race, incarceration and food insecurity

Author: Anna Boyd
Advisor: Dr. Brighid Dwyer

Race and low socioeconomic status are concentrated factors for a person's life outcome. They are both geographically positioned in similar areas. Furthermore, the areas most targeted by mass incarceration are impoverished city centers that have been redlined to create racially-homogeneous neighborhoods. Food deserts occur in both urban and rural communities, but are usually found in the extremes of both. This paper uses previously collected data and articles to investigate the geographical proximity of race, neighborhoods most susceptible to mass incarceration, and food deserts.

Chemistry

B25 – Investigation of La0.80Sr0.20Ga0.80Mg0.20O3-δ solid oxide fuel cell electrolyte material
Author: Tim Marshall
Advisor: Dr. Bryan Eigenbrodt

Declining sources of combustible fuels have motivated the search for alternative devices, such as Solid Oxide Fuel Cells (SOFC)'s, that are capable of utilizing these fuels with increased efficiency. Chemical processes and electrochemical power production of these devices is often limited by the electrode and electrolyte materials. In an attempt to improve SOFC power generation, a new electrolyte material was synthesize as an attempt to lower the activation energy of oxide migration from the cathode to the anode. The material being studied is the perovskite La0.80Sr0.20Ga0.80Mg0.20 O3-δ (LSGM) based electrolyte material. This material was generated using three separate syntheses routes, which were compared electrochemically, spectroscopically and microscopically. Using the synthesized lanthanum-doped ceria (LDC) buffer layer, Ni-LDC anode and commercially available lanthanum strontium manganite (LSM) cathode sets of functional LSGM supported SOFC were tested using X-Ray Diffraction (XRD), Electrochemical Impedance Spectroscopy (EIS), Linear Sweep Voltammetry (LSV) and Scanning Electron Microscopy (SEM).

B26 – Synthesis and characterization of [Fe(bpy)3]2+ (bpy = 2,2'-bipyridine) and [Fe(bpy(OMe)2)3]2+ (bpy(OMe)2 =4,4' –Dimethoxy-2,2'-bipyridine)
Author: Daniel Zuschlag
Advisor: Dr. Jared Paul

The Paul lab is interested in the development of effective catalysts for water oxidation, a reaction necessary for the storage of solar energy and artificial photosynthesis. While the lab works primarily with ruthenium as the transition metal center of potentially catalytic coordination compounds, we have not synthesized or studied iron compounds as often. Iron, which like ruthenium is a group 8 transition metal, has the potential to form cheap, effective catalysts for water oxidation. Before catalyst design is attempted, it is important to understand the electrochemical and spectroscopic effects of different ligands on iron coordination complexes. Polypyridyl ligands in particular have unique spectroscopic and electrochemical effects on transition metal centers due to their ability to absorb light.

[Fe(bpy)3]2+ (bpy = 2,2'-bipyridine) and [Fe(bpy(OMe)2)3]2+ (bpy(OMe)2 =4,4' –Dimethoxy-2,2'-bipyridine) were synthesized and characterized. Synthesis of the desired product was confirmed in both cases with NMR and x-ray crystallographic tests. The electronic and spectroscopic properties of these complexes were studied using cyclic voltammetry and UV/Visible spectroscopy. The complexes were studied in both acetonitrile and aqueous solutions.

B27 – Measurements of triclosan in a southeastern Pennsylvania watershed
Authors: Garrett Waligroski, Dr. Amanda Grannas
Advisor: Dr. Amanda Grannas

Triclosan (5-chloro-2 (2,4,-dichlorophenoxy)phenol-TCS) is an antimicrobial agent used in shampoos, soaps, medicated cosmetics, and other commercial products including textiles and plastics, to prevent microbial growth. The presence and concentration of TCS was tested for in water samples collected along the Brandywine River by method of water extraction. Due to the fact that TCS is a common chemical ingredient in many consumer products, its presence in aquatic ecosystems is significantly high. In the study presented, the concentration of TCS in natural water samples from thirteen different locations will be determined using GC-MS analysis to assess the occurrence and fate of TCS in the aquatic environment. Extractions of the standard TCS aqueous solution showed method extraction efficiencies of 95%. Thirteen environmental samples were obtained and tested from twelve sites, with TCS concentrations ranging from 0.1311 to 274.4 ng/L. The concentration of TCS at each of the thirteen sites is reported as the main results for this research.

B28 – Synthesis of anti-virulence compounds for the treatment of chronic infections caused by Pseudomonas aeruginosa
Author: Celina Santiago
Advisors: Dr. Alexander Titz, Ines Joachim

The summer of 2015, I had the opportunity to go to Germany and do chemistry research in a laboratory in Saarbrücken, Germany. The research focused on finding anti-virulence compounds, which would create a promising new drug target mechanism. The synthesis of drugs to treat new and reemerging diseases has slowed in the past two decades. Owing to an increase in multi-resistant species of microbes, finding treatments that can be effective in the long run has become extremely important. The goal of the Helmholtz Institute for Pharmaceutical Research in Saarland has taken on the task of developing novel drugs for a wide variety of infectious diseases. One important target is the bacterium Pseudomonas aeruginosa. Colonization of this bacteria is common in hospital settings owing to a high percentage of hospital acquired infections. Pseudomonas aeruginosa is also the main cause of chronic lung infections in cystic fibrosis patients. A vital key mechanism that the bacterium uses to establish these infections is biofilm formation aided by two bacterial Lectins, LecA and LecB. Carbohydrate-based inhibitors have been shown to disrupt biofilm formation and are a promising treatment for Pseudomonas linked infections.

B29 – Synthesis and characterization of isogemichalcone analogs: potential aromatase inhibitors
Authors: Sean Longson, Alicia Angelbello, Melissa Morales, Dr. Eduard Casillas
Advisor: Dr. Eduard Casillas

Isogemichalcones B and C, metabolites of Broussonetia papyrifera, have modest inhibitory effects against aromatase. The compounds offer promising therapeutic treatment against breast cancer especially for postmenopausal women. Utilizing a recent synthetic route, substitutions to a phenyl group are being prepared to study the effect of stereoelectronic properties in inhibition. Modifications to key reactions in the synthesis of the isogemichalcones have been optimized to prepare analogs (CH3, H, CF3, F, and Ar). Furthermore, current compounds have been characterized by 1H and 13C NMR spectroscopy, IR spectroscopy, melting point, mass spectrometry, and combustion.

B30 – Scaffold-hopping of multicationic amphiphiles yields three new classes of antimicrobials
Authors: Myles A. Mitchell, Anthony A. Iannetta, Dr. Kevin P.C. Minbiole
Advisor: Dr. Kevin Minbiole

Quaternary ammonium compounds (QACs) are a vital class of antiseptics; recent investigations into their construction are uncovering novel and potent multicationic variants. Based on a trisQAC precedent, we have implemented a scaffold-hopping approach to develop alternative QAC architectures that display 1-3 long alkyl chains in specific projections from cyclic and branched core structures bearing 3-4 nitrogen atoms. The preparation of 30 QAC structures allowed for correlation of scaffold structure to antimicrobial activity. We have identified QACs with limited conformational flexibility that have improved bioactivity against planktonic bacteria as compared to linear counterparts. We also confirmed that resistance, evidenced by an increased MIC for MRSA compared to MSSA, can reduce efficacy up to 64-fold for monocationic QACs. Differentiation of antimicrobial and antibiofilm activity, however, was not observed, suggesting that these compounds utilize a non-specific mode of eradication.

C31 – Synthesis of a cyclopropl glycoside donor for the Lipid A disarcharide
Authors: Hannah Curran, Dr. Robert Giuliano
Advisor: Dr. Robert Giuliano

Lipid A is a component of Gram-negative bacterial endotoxin that is responsible for toxicity and also adjuvant activity toward protein and carbohydrate antigens. The core structure of lipid A consists of two β-linked glucosamines with attached acyl chains. Lipid A synthesis is studied due to its potential use in vaccines. Our approach to the synthesis of the lipid A disaccharide is based on the coupling of a cycloproplglycoside and a diol acceptor. Lipid A synthesis is currently possible but the use of a cyclopropyl donor requires more study and is theoretically a more efficient way to generate Lipid A.

The cyclopropyl glycoside has been generated but has yet to be successfully used in the coupling reaction.

C32 – Natural product-derived quaternary ammonium compounds with potent antimicrobial activity
Authors: Maureen Joyce, Megan C. Jennings, Celina N. Santiago, Madison H. Fletcher
Advisor: Dr. Kevin Minbiole

Quaternary ammonium compounds (QACs) bearing long alkyl chains are classical examples of amphiphiles, displaying a variety of interesting physical properties, such as the capacity for micelle formation and gelation.1 QACs also enjoy extensive precedent and applications in bacterial cell membrane disruption, leading to their widespread use as antiseptics.2 Both synthetic QACs and peptide-based amphiphiles (notably, antimicrobial peptides or AMPs3) are prevalent, however, there are relatively few QACs in scaffolds of natural products that are not peptide-based.

C33 – Synthesis of 9-desmethyl-(-)-diplopyrone
Author: Jonathan Grecco
Advisor: Dr. Robert Giuliano

The chemical (+)-diplopyrone, is a toxin that comes from the fungus Diopldia mutilaa. This toxin is responsible for a decline in cork oak trees in parts of southern Europe, leading to a large, negative impact both economically and environmentally. The structure of diplopyrone, however has only come from spectroscopic data and theoretical calculations of its optical properties; naturally occurring diplopyrone is dextrorotatory. As of now, there has been no syntheses of this chemical. Thus, a synthesis of enantiomeric desmethyl (-)-diplopyrone is proposed, with its basis in the chemistry of carbohydrate-derived C-glycosides. If successful, this could eventually lead to the synthesis of (+)-diplopyrone and its desmethyl analog.

C34 – Modeling sodium battery electrolytes and electrode interfaces at varying concentration using classical molecular dynamics
Author: Jessica Wahlers
Advisor: Dr. Ryan Jorn

Sodium battery electrolytes are being studied as an alternative to lithium batteries since there is a larger abundance of sodium which would make batteries more cost effective. Using Classical Molecular dynamics, sodium battery electrolytes comprised of diglyme (C6H14O3) and sodium triflate (CF3SO3Na) were modeled to study the structure of the materials as well as their transport properties. Force fields were developed for the electrolyte based on quantum chemical calculations and were subsequently used to calculate the density, radial distribution functions (RDFs), solvation structure,

and diffusion coefficient for sodium electrolyte species. These properties were then compared for a 0.5 M solution, 1.5 M solution, 2 M solution and a 3 M solution. The solvent-induced separation of the salt pair was noted to be greatly reduced in contrast to a prototypical lithium ion salt as a result of differences in the counter-ion charge distribution. In addition to studying bulk properties, the electrolyte/electrode interface was also considered by implementing an image charge method to incorporate an electric field. The results for distributions of electrolyte species as a function of distance from the electrode were then compared at each of the varying concentrations. The electrode simulations showed similar results to current lithium systems comprising of ethylene carbonate (C3H4O3) and lithium hexafluorophosphate (LiPF6).

C35 – Spectroelectrochemical studies of Ruthenium complexes containing the 4,4'-dimethoxy-2,2'-bipyridine ligand
Author: Erin Peterson
Advisor: Dr. Jared Paul

Ligands with multiple protonation states have tunable electronic properties based on changes in pH, which could lead to controlling catalysis. Therefore, understanding the structural and electronic properties of these types of complexes at a fundamental level is of great interest. However, with these complexes existing in multiple states, it is useful to build complexes that are similar in nature, but without the pH-dependence. Therefore, we are interested in the study of metal complexes with methoxy-substituted bipyridine ligands in order to compare to hydroxyl-substituted bipyridine ligands that exist in multiple protonation states. To this end, this summer I studied polypyridyl ligands containing methoxy groups. I report here the electrochemical and spectroelectrochemical studies of [Ru(bpy)2(44'bpy(OMe)2][Cl]2 (bpy = 2,2'-bipyridine; 44'bpy(OMe)2 = 4,4'-dimethoxy-2,2'-bipyridine) and [Ru(44'bpy(OMe)2)3][Cl]2. These studies reveal consistent reduction potentials of 0.89 V vs AgCl for [Ru(bpy)2(44'bpy(OMe)2][Cl]2 and 0.67 V vs AgCl for [Ru(44'bpy(OMe)2)3][Cl]2. In addition, spectroelectrochemical studies show consistent decrease in the MLCT band paired with an increase in a new LMCT absorbance band of these complexes when oxidized at different pH values.

C36 – Synthesis and characterization of [Ru(phen=O)2bpy][PF6]2, and [Ru(phen=O)2(bpy(OMe)2)][PF6]2 (bpy = 2,2'-bipyridine; OMe=4,4'dimethoxy-2,2'bipyridine; (phen=O) =5,6' phenthroline- 1,10' dione)
Author: Ashley Arcidiacono
Advisor: Dr. Jared Paul

Current trends in the inorganic field of anticancer research have focused on strong electron-withdrawing complexes as powerful anticancer agents. As a lab, we are interested in synthesizing such complexes that have the ability to serve as anti cancer agents. To this end, we have studied the 1,10' phenathroline-5,6' dione ligand when coordinated to a Ruthenium metal center with additional

polypyridal ligands. We report the synthesis and study of Ru(phen=O)2Cl2 , [Ru(phen=O)2bpy][PF6]2, and [Ru(phen=O)2(bpy(OMe)2)][PF6]2 (bpy = 2,2'-bipyridine; OMe=4,4'dimethoxy-2,2'bipyridine; (phen=O) =5,6' phenthroline- 1,10' dione). Verification of synthesis and electronic properties of the resulting complexes were studied using cyclic voltammetry, UV/visible spectroscopy, infrared spectroscopy, and Nuclear Magnetic Resonance (NMR).

C37 – Synthesis, characterization, and the coordination chemistry with select lanthanide nitrates of di(2-pyridinyl)phenylphosphonate and oxide derivatives.
Author: Carina Fairfield
Advisor: Dr. Scott Kassel

The synthesis of the ligand, di(2-pyridinyl)phenylphosphonate (OP(OPy)2Ph) was completed in a one pot synthesis from triethylamine, hydroxypyridine, and phenylphosphonic dichloride in THF at reflux. The coordination chemistry of lanthanide(III) nitrates (Ln = NdIII, SmIII, YbIII) with OP(OPy)2Ph was investigated. Additionally, preparations of N-oxide derivatives of the ligand were attempted. Compounds and complexes were characterized by X-ray crystallography, IR, UV-vis, and 1H/31P NMR spectroscopy, and electrochemistry.

Computing Science

C38 – Persuasive human-computer interaction for environmental sustainability: encouraging the use of hydration stations through a mobile application
Author: Emma Chin
Advisor: Dr. Robert Beck

Human-computer interaction (HCI) is integral to how information is received and processed by the user, and is thus especially useful in encouraging certain behavioral changes. Our research looks specifically at the field of persuasive HCI and how its techniques can be used in conjunction with environmental sustainability. We focus specifically on how to better monitor and encourage the use of Villanova's hydration stations, which are widely available throughout the campus. We aim to achieve this through the development of a mobile application.
Firstly, several theoretical models were developed based on an increasing number of users per week, assuming the introduction of a computer device in these hydrations stations. In order to assess current patterns of water usage, weekly bottle fill data was gathered over the course of 11 weeks. Our next focus was to develop a way to remotely collect usage data from the hydrations stations and use this data in the implementation of persuasive HCI techniques. Bar-code readers will be used to identify unique bottles and update the system on individual bottle fills. Within the mobile application, this data will then be used to create customized water consumption 'itineraries' for each user; tracking and notifying the user on his or her progress throughout the day. We anticipate a steady increase in number

of bottle fills per week with the introduction of the mobile application, and hope to extend this persuasive HCI technique to other areas of environmental sustainability.

C39 – Improving the energy efficiency of data centers
Authors: Michaela Wilkins, Jeffrey Moreno
Advisor: Dr. Aaron Wemhoff

Data centers consume approximately 2-3% of the nation's electricity, so improvements in energy efficiency can have an impact on energy sustainability. Two projects, focusing on improving the energy efficiency of data centers, are (1) the conversion of data center equipment component models into an open-source programming language, and (2) the visualization of data center airflow data, generated from computational fluid dynamics (CFD) simulations, using the CAVE facility on campus. The first part of our work involved the conversion of several equipment component models from the Villanova Thermodynamic Analysis of Systems (VTAS) data center analysis software. During this we converted MATLAB code to C so that they could be more available to the data center research community. To ensure that the C code was correctly implemented and gave the same outputs, test files for both MATLAB and C were created. Each component model consisted of four files, the MATLAB component and test files, and the C header and test files. Following this we worked on visualization in the CAVE. The goal is to create a life sized data center and find the best way to visualize the data within the data center. We started by using the commercial CFD software 6SigmaDC to model velocity distributions and airflow temperatures, which would be used directly in the data center. The open-source software Vizard was then implemented for visualization in the CAVE.

Computing Science, VSB

C40 – Real-time data visualizations within a cave automatic virtual environment
Author: Stephen Werpehowski
Advisor: Dr. William Wagner

Immersive systems are becoming a more prevalent aspect of the daily user's life. Although these systems offer unprecedented advances in virtual reality, it is reality itself that is less commonly incorporated into the virtual world. We propose a methodology for real-time data integration within the virtual world for receiving, analyzing and visually interpreting data. This implemented methodology interacts seamlessly with the Oculus Rift as well as a Cave Automatic Virtual Environment. Further, our methodology allows for interfacing with robotics from within the virtual world.

Engineering

C41 – Automated analysis of fluorescence images of micropatterned cells
Authors: Karl Chandeck, Dr. Jens O.M. Karlsson
Advisor: Dr. Jens O.M. Karlsson

The objective of this research project was to develop MATLAB code to automatically analyze images of cells that are attached on micropatterned substrates, to produce morphometric and statistical data. Specifically, the cells were patterned to grow within circular islands of diameters ranging from 80 μm to 225 μm (with anywhere between 1 and 100 cells per island), and were visualized by fluorescence microscopy, using a nucleic acid probe to stain the cell nuclei. Our image analysis algorithm combines multiple image processing techniques that by themselves would not result in accurate segmentation of the images (due to challenges inherent in the diversity of the image histograms caused by variations in image quality and differences in staining intensity between cells in the same image). The finished code is able to identify the cell nuclei in an image (with minimal error rate), without requiring the parameters of the algorithm to be customized for individual images. Upon successful image segmentation, the algorithm also counts the number of cells found in each island, and provides data on the positions and sizes of the cell nuclei.

C42 – Application of sorption-enhanced catalysis to ethanol reforming
Authors: Jacky Ho, Charles Pong, Dr. Justinus Satrio, Dr. Charles Coe
Advisor: Dr. Justinus Satrio

Biomass is probable the best resource in the next emerging carbon-neutral energy era for producing large scale quantities of renewable hydrogen (H2). A potential source for H2 is the bio-oil resulting from fast pyrolysis of biomass. Conventional production of H2 from solid coal or biomass involves gasification to produce synthesis gas (syngas) followed by multiple reaction steps each requiring different catalysts. It has been shown that it is possible to replace the complete multistep process for producing hydrogen by steam reforming with a much simpler process that allows the steam reforming (SR) and water gas shift (WGS) reactions to occur in a single step. This is accomplished using a combined catalyst and sorbent materials with the sorbent being capable of removing CO2 from the reaction gas mixture and driving the SR and WGS towards completion. We are working to develop improved sorption enhanced catalyst/sorbent composites to produce hydrogen in excess of its equilibrium amounts at much milder conditions from oxygenates that are found in bio oils.

The initial focus of the research is reforming ethanol to hydrogen at mild conditions in a single step using a mixed sorbent/catalyst. A fixed bed reactor equipped with both liquid and gas flows was commissioned at Villanova thus establishing a capability to do reforming studies. After condensing the residual steam and any liquid products from the reactor the non condensable gases were analyzed using an IR analyzer that was in tandem with a mass spectrometer. A homogenous mixture of a Ni-based reforming catalyst and granular CaO were used for the initial studies. At the same time, fixed

bed reactor studies in a micro-reactor were carried out at CCNY using Pt-based catalysts in a powdered form. Studies of ethanol reforming carried in both reactors have confirmed that the presence of known CO2 sorbents can effectively improve the hydrogen selectivity in reforming ethanol. In addition compaction studies in attempts to make granular forms of composite sorbents have shown that there is a large change in the CO2 sorption rates if the powders are simply pressed.

Preliminary results for studies using homogeneous mixtures of CaO with either a Pt/Al2O3 catalyst or Ni-based catalysts will be shown and compared to catalyst alone results. In addition, results from using a composite CaO/Pt/Al2O3 catalyst in the same reactor system. As expected, both the composite and mixed catalysts produced more hydrogen than the control systems showing that the enhanced sorption approach could be successfully applied to the reforming of ethanol. At 560ºC the sorption enhanced catalyst containing 7% CaO on a 1%Pt/Al2O3 gave a 25% enhancement in the hydrogen production. These proof- concept studies provide a foundation for additional studies using improved CO2 capture adsorbents where the total yield of hydrogen is expected to increase.

C43 – Graphene synthesis for graphene polymer nanocomposite of increased thermal conductivity
Authors: Kolby Koeck, Dr. Calvin Li
Advisor: Dr. Calvin Li

Graphene is one of the most promising materials in the past 5 years for its exceptional mechanical, electrical, and thermal properties. Graphene is derived from natural graphite by means of chemical reactions, exfoliation, and thermal reduction. Graphene as a single monolayer of carbon atoms can be incorporated into various polymers to create a polymer nanocomposite that enhances the base properties of the polymer. To create graphene, an improved exfoliation method is conducted to synthesize graphite to create graphene oxide then reduce it to create graphene. Analysis techniques, such as TEM imaging observations, are then used to characterize the structure of graphene oxide and graphene at the nanoscale, measuring the thickness, area, and amount of folding of the layers. Then, the folding and size are interpreted are used to make hypotheses regarding the relative advantages adding graphene as a filler to polyurethane would have to increase the thermal conductivity over the base polymer for use in small scale thermal management. Overall, through a simple synthesis graphene can be produced from graphite with optimal characteristics for many nanoscale applications.

C44 – Changing DNA plasmid structure through inclusion of specific sequence repeats
Authors: Adam Butchy, Dr. William Kelly, Dr. Jacob Elmer
Advisor: Dr. William Kelly

DNA is a reoccurring theme in life. It provides the recipe for continuing life through providing the instructions for protein synthesis and RNA construction but we still know so little about it! Recently, epigenetics has taken a step forward in better understanding the effect of DNA structure on gene

expression; specifically, the attachment of chemical groups on histones that pack and organize DNA. This project takes another route.

Instead of focusing on histones, particular sequence repeats were inserted into a bacterial plasmid to examine the effect of particular DNA sequences on DNA structure. The sequences used in this project were selected based on their occurrence in nature, namely, they cause the genetic disorders of Huntington's Disease and Fredrich's Ataxia. These two particular sequences are known to create tertiary DNA structure through repetitive sequences in the primary structure of DNA.

This project explores the potential benefits of these DNA anomalies by exploring the effect of these DNA sequences on the size and shape of a bacterial plasmid through atomic force microscopy and scanning electron microscopy. These conformational changes, once confirmed, will then be tested to determine whether or not these structures have a significant effect on transgene expression in gene therapy. In addition, this project would like to take one step further into more commercial application by exploring the potential use of these complexes as a means to aid in DNA separation and purification using commercially available resins.

C45 – Mechanical properties of human lumbar intervertebral disc tissues under transient hyperphysiologiv loading conditions: a pilot study

Authors: Samantha E. Kalup, John F. DeLucca, Dawn M. Elliot, Dr. David Jamison
Advisor: Dr. David Jamison

In certain occupations, exposure to transient hyperphysiologic non-acute (THPNA) mechanical shocks is common, stemming from operating certain equipment and vehicles. For individuals frequently exposed to these types of shock, rates of lower back pain and accelerated disc degeneration have been shown to be higher. However, mechanical properties of individual disc tissues are still largely unknown and therefore mechanisms of lumbar spine injury from THPNA loading remain elusive. Therefore, the objective of this pilot study was to measure mechanical properties of human lumbar nucleus pulposus (NP) and extra-fibrillar annulus fibrosus (AF) under THPNA loads using a confined compression testing protocol and constitutive analyses. Successful completion of this work may lead to a better understanding of disc behavior and ultimately identify damage mechanisms from this type of occupational loading.

D46 – Rational design of cost-efficient CO2 electro-reduction catalysts with hybrid tungsten carbide/graphene systems

Author: Zachery Smith
Advisor: Dr. Rees Rankin

The use of conventional fossil fuels and their associated technologies is facing increasing pressure from sources including environmental concerns, national security interests, and dwindling abundance of natural supplies. Fuel and energy-chemical sources of the future will – by default – require new

technologies to be brought to market sustainably. One potential route to achieve the selective and sustainable synthesis of commodity, energy, and fuel related chemicals is through the use of novel techniques and materials in heterogeneous catalysis and electrocatalysis. The ability to predictively design such novel catalyst materials and reaction schemes in silico has come to fruition recently with the rapid increase in low-cost computing workstations and HPC servers, combined with ever-more-accurate quantum chemistry/ ab initio calculation tools.

Through the use of a High Performance Computing Cluster (HPC) running Medea-VASP (an ab initio density functional theory {DFT} code), we worked in an attempt to attain a viable catalyst or electrocatalyst for the reduction of CO2 to value added commodity chemicals or fuels such as CH4 or CH3OH). Specifically we looked at the effectiveness of using hybrid tungsten carbide(WC)/graphene electrocatalysts for CO2 electroreduction (in a simulated aqueous media). Our results have so far shown that the WC/graphene electocatalyst has an electronic structure that should make it a good electocatalyst for CO¬2. The benefits of developing such a technology would be profound both with respect to neutralizing the escalation of the world's energy budget, as well as mitigating further emission of greenhouse gases such as CO2 which may disproportionately impact the developing world nations through manmade climate change.

D47 – Influence of mineralization on cortical bone mechanical properties
Authors: Theresa Thompson, Dr. Ani Ural
Advisor: Dr. Ani Ural

Osteoporosis is defined as a disease that shows low bone mass and micro-architectural deterioration of bone tissue leading to skeletal fragility and is the underlying cause of over 9 million fractures each year [1,2]. However, bone mass is not sufficient to accurately identify individuals who may experience fragility fractures and it has been acknowledged that mineralized collagen fibrils, which are the building blocks of bone at the nanoscale level, have significant contributions to bone fragility, however, experimentally quantifying this effect has lacked studies. There are two main factors at the nanoscale which have been proposed to affect bone fracture: mineralization and cross-linking [3]. An increase in mineralization, which is high in osteoporosis patients, may cause an increase in bone fragility by increasing the brittleness of bone [3]. The goal of this study is to quantify the effect of mineralization on the mechanical properties of bone in hopes to better understand the way bone fractures at the nanoscale.

D48 – In-vitro experimental study of nanopartical polymer coating for drug delivery and release
Author: Gillian Krautman
Advisor: Dr. Calvin Li

Composite nanoparticles have become a focus in improving targeted drug delivery methods to reduce toxicity and side effects of drugs. The composite nanoparticles of this study consist of a ferromagnetic

core, a drug load, and a polymer shell. The polymer shell is made by poly-lactic-co-glycolic acid (PLGA), a Food and Drug Administration (FDA) approved polymer, through two different methods of two different concentrations and two different preparation temperatures. When preparing the composite nanoparticles for drug delivery study, A solution of Bovine Serum Albumin (BSA) in phosphate buffer, which is the dummy drug in this study, will be prepared before incorporating in a PLGA and ethyl acetate solution, which offers the polymer shell. Then, the ferromagnetic cores (Fe2O4 nanoparticles) are dispersed into the solution to generate composite nanoparticles with BSA drug load and PLGA polymer shell. The final composite nanoparticles are in the range of 50-300 nm (TEM images), but intend to agglomerate together to create larger particles up to 1 micron in size.

To determine the effectiveness of the composite nanoparticle for drug delivery, a release study is conducted. Two batches of composite nanoparticles were studied to see how the two different methods, nanoprecipitation and a modified emulsification technique, differ in their release of protein over time. At set times, samples were taken, placed in a microplate with the appropriate BSA standards and copper sulfate working reagent The plate was then placed in a microplate reader to measure the absorbance of the protein from the nanoparticles.

The absorbance over time of each batch were plotted and compared among trials. The concentration versus absorbance was also plotted to determine how the concentration of the sample affects the release rate as well. Many of the samples had a quick initial release, and then leveled out. The final particles tended to sinter together to create larger particles between 1000-6000nm in diameter, determined though TEM analysis.

Based on the images and absorbance values gathered from these trials, it can be determined that because of the non-uniformity and larger sizes of nanoparticles from the nanoprecipitation method in comparison to the emulsification technique, the latter is the more effective method for producing nanoparticles out of the two procedures. Based on the images gathered in the different emulsification trials, it can also be determined that changing the concentration of PLGA does not have significant impact on the size of particles nor did it create more isolated particles. Lastly, preparation temperature also does not seem to have much effect on particle size, although the future testing this over a larger temperature distribution could have different results. Exploration of more methods for creating and isolating particles would be the next step in continuing the field of targeted drug delivery.

D49 – Experimental study of mesoporous silica coated magnetic nanoparticles on thermomagnetic energy conversion

Author: James Sutherland-Foggio
Advisor: Dr. Calvin Li

Thermal therapy of severe illnesses has been utilized since before 1927 when Heinrich Wieland won the Nobel Prize in Chemistry, inducing a fever in patients to treat cardiovascular diseases. As technology progressed, control of the heat delivery became more refined. In the late 20th century, nanoparticles were first demonstrated as an efficient means of both delivering drugs and thermal energy to the body. In targeted drug delivery, a silica interlayer provides stability, biocompatibility,

and increased specific adsorption rate (SAR) of ferromagnetic nanoparticles. The purpose of this study was to determine the thermo-physical properties of solid and mesoporous silica nanospheres to aid in design of the silica layer of iron-core nanoparticles for targeted drug delivery. Synthesis of solid silica was performed through a modified Stober method. Through variation of solvent concentrations, particles of size 175nm and 30 nm were achieved. Synthesis of mesoporous silica nanoparticles through extremely dilute surfactant solution yielded particles of 200 and 60 nanometers. The particles were characterized using BET N2 adsorption techniques to measure specific surface area and pore volume. Mesoporous silica exhibited significantly larger pore volume, 0.392 cm3/g, than silica of comparable size, 0.041 cm3/g. Both mesoporous silica and solid silica particles in 0.84% silica water solution generated heat exceeding that of pure water with SARs of 1.45 W/g and 1.69 W/g respectively. This research concludes that mesoporous silica provides increased surface area over solid silica nanoparticles and comparable SAR.

D50 – DNMT inhibition and transgene expression

Author: Evan Kurt
Advisor: Dr. Jacob Elmer

Current gene therapy treatments require several follow-up treatments, since the host cells that are transfected quickly target and degrade the foreign DNA used in gene therapy. One of the enzymes that cells use to target foreign DNA is DNA methyltransferase (DNMT), which silences genes by methylating their promoters. The DNMT targets specific CpG motifs ("C's" followed directly by a "G") in key bacterial sequences. To reduce plasmid methylation, DNMT inhibitor drugs can be added to the cells. These drugs either inhibit the DNMT directly by acting as a cytosine analogue, or they can replace a cofactor in the reaction sequence.

Multiple groups have previously shown that one DNMT inhibitor – 5-Aza-cytidine – can effectively enhance gene therapy by preventing DNA methylation, but it is rather expensive. We sought to identify a cheaper alternative by screening four new DNMT inhibitors (Procainamide, Caffeic acid, Chlorogenic acid, and Hydralazine HCl) at various concentrations (0.001 - 100 uM). The effectiveness of each inhibitor was determined a luciferase assay was run. Based on the relative luminescence data, Caffeic acid and Chlorogenic acid were more effective than 5-Aza. To determine the toxicity of the drugs, an MTT cell proliferation assay was used. All of the drugs tested were less toxic than the 5-Aza control when at concentrations greater than 0.1 uM. Overall, Caffeic acid was the best in both assays, particularly at 0.1 uM, and followed by Chlorogenic acid at 1.0 uM. Also important, Caffeic acid costs less than 5-Aza for the amount provided by the supplier.

Based on the first phase's data, the next step was to determine the extent that the drugs would be effective. From another summer project, overlap-extension PCR was used to replace the luc2 gene in pGL4.50 with the GFP (green fluorescent protein) gene from the pEF-GFP plasmid. Both GFP gene-containing plasmids were transfected in PC3 cells with the best performing concentrations of each drug. The fluorescent microscopy provided data over two weeks, with the drug replaced every two days. The result was that both the original pEF-GFP plasmid and the modified pGG4.50 plasmid

differed in expression over time, with the pEF-GFP having a stronger fluorescence overall. For both, however, Caffeic acid, Chlorogenic acid, and DMSO+polyplex control had the most fluorescing cells.

Overall, the goal is to continue identifying those drugs and concentrations which work best for expression and cell viability. Further trials of the drugs at the selected concentrations will be continued to better refine the trends observed. Currently, the research is focusing on Caffeic acid at 0.1 uM and Chlorogenic acid at 1.0 uM in the SK-BR-3 cells. The long-term goal for the DNMT inhibitor project would be to look at the methylation of the plasmids with and without drug, in order to confirm the mechanisms by which each one works.

D51 – The effect of spatial separation on 2D temperature mapping using thermographic phosphors

Authors: Andrew Meluch, Daniel Stenders
Advisor: Dr. Garrett Clayton

It is critical to perform analysis of surface temperatures in virtually all engineering applications in order to improve efficiency and safety. Most recent studies have focused on the observation of temperature distribution within solid, flat, homogenous surfaces. There are many instances, however, where this type of set-up would not produce accurate results due to physical or other restrictions. This project uses phosphor thermometry to map the two-dimensional temperature distribution of two samples separated by a small gap. Both samples were heated to different known temperatures using independent heating sources. Continuous pulses of light from a laser were captured, concentrated and refined using mirrors, lenses and filters. These pulses were focused onto the samples. Lifetime based, pixel-by-pixel imaging was performed using a high-speed camera. The experimental setup was completely enclosed, ensuring that all measurements were taken in complete darkness. Images were analyzed by LabVIEW software, resulting in two-dimensional color representations of the surface temperature distribution. The experiment was repeated at varying temperature gradients to determine the effect of the small gap between the heating plates.

D52 – Comparing the effects of feedstock on the yields and selectivity of bio-oil products from catalytic pyrolysis of biomass using HZSM-5

Authors: Gregory Zakem, Brendon Shea, Dr. Charles Coe, Dr. Justinus Satrio
Advisor: Dr. Justinus Satrio

Lignocellulosic biomass is a promising feedstock for the production of chemicals and fuels. One promising approach that has gained interest for processing lignocellulosic biomass to produce chemicals and fuels is fast pyrolysis. Fast pyrolysis is a thermochemical conversion process in which biomass is decomposed to produce a liquid (bio-oil), a solid (bio-char), and a non-condensable gas mixture (syngas) by exposing biomass to high temperatures, typically between 400 and 600oC, in the absence of oxygen. The yields and selectivity of the products are highly dependent on pyrolysis process conditions and physicochemical properties of the feedstock. The chemical groups contained in bio-

oil primarily include carboxylic acids, aldehydes, furans, anhydrosugars, ketones and phenols. The presence of the wide variety of chemicals, specifically oxygenated chemicals, makes the utilization of bio-oil as intermediate feedstock for producing end products difficult. The oxygenated compounds, primarily acids, aldehydes and ketones, render bio-oil to become unstable and highly acidic. One approach for producing bio-oil with lower amounts of oxygenated compounds is using HZSM-5, an aluminosilicate zeolite. The solid acid catalyst functions to promote the production of aromatics while reducing selectivities towards oxygenated compounds. In this work, catalytic pyrolysis studies by using 4 different biomass feedstock, i.e. pinewood, switchgrass, phragmites, and manure-containing bedding material from a horse farm have been conducted. Results indicate that pinewood produces the largest total amount of aromatics per unit mass of biomass pyrolyzed. Switchgrass produced the largest fraction of aromatics within the bio-oil. Pyrolysis of pinewood produced the greatest amount of CO and pyrolysis of phragmites produced the greatest amount of CO2.

D53 – Microbial fuel cell - in-silico model

Author: Nicholas Ribaudo
Advisor: Dr. Zuyi Huang

Our society's diminishing energy supply, and the rapidly accelerating energy demand, generates a need for new energy solutions. Microbial fuel cells (MFCs) provide a source of renewable energy through bacterial metabolism using inexpensive hydrocarbon based fuel and a bacterial microbe catalyst. Little work has been done in developing realistic and practical in-silico models for MFCs. The principal aim of this research is to develop the first 3-dimensional in-silico model of a MFC, which can be used to perform parameter optimization and overall scale-up. SolidWorks was used to generate a representative geometry of the fuel cell, which was then implemented into ANSYS Workbench for meshing and Computational Fluid Dynamics (CFD) simulations. The ANSYS Fluent model development included multiphase, species transport, viscous fluid dynamics, and energy models as the basis of computation. Primarily focusing on the fluid dynamics and multiphase aspects of the model, simulation results for the flow patterns inside both the anode compartment and cathode compartment were successfully obtained. These flow patterns included the inlet and outlet of acetate solution in the anode compartment, and the inlet sparges of oxygen gas into the cathode compartment. Obtaining appropriate velocity contours for fluid flow throughout the entire system is essential to species transport and biochemical reactions that will take place. Currently, the implementation of specific mixture solutions, reactions, and user-defined functions is being worked on. Once this aspect of the model is completed, the program results will be compared and fit to experimental data in order to validate the model. Future work includes this model validation, as well as elucidating optimal scale-up conditions and parameters. Due to a MFC's renewable energy production and its economic advantages, improving capabilities and optimizing performance will be essential in streamlining the technology.

D54 – Design of inexpensive phase change material blends for use in thermal barriers to improve building

Authors: Michael Morabito, Dr. Aaron Wemhoff
Advisor: Dr. Aaron Wemhoff

The International Energy Agency stated in 2011 that 53% of energy consumption in buildings is due to heating, ventilating, and air conditioning (HVAC). In residential buildings, considerable energy is expended in the summer due to heat flow from the attic space or under-roof airspace to the living space. Phase change materials (PCMs) can act as an excellent insulator between the non-inhabitable heated attic space and the cooled living space below. Commercial PCM insulating technology currently uses expensive pure PCMs, which are not suitable for large-scale use due to cost. Past research (e.g., Humphries, Report NASA TN D-7690, 1974) has shown that the blending of pure PCMs can tailor the melting point, so this project investigates the viability of blending inexpensive bulk waxes with small amounts of relatively expensive pure PCMs to create a blend with a desired melting point for large-scale residential insulating applications. Soy wax and candle wax serve as the bulk inexpensive base waxes, and pure paraffins and unsaturated acids act as the pure additives. Inexpensive PCM blends (IPCMBs) are investigated using differential scanning calorimetry (DSC) to ascertain the melting point and latent energy associated with the solid-liquid phase change. Multiphysics simulations are then applied to model a heated non-inhabitable attic space and a cooled living space below to determine the efficiency of the IPCMB by assessing the thermal energy barrier. This work represents the first effort to provide accurate models for IPCMBs useful in a multiscale modeling framework.

D55 – Development of an ultra-stable blood substitute: enhancing the stability of earthworm and human hemoglobin

Author: Payal Shah
Advisor: Dr. Jacob Elmer

Although transfusing donated blood is primarily safe and effective, there are certain drawbacks that could be eliminated by creating a blood substitute. Developing an ultra-stable blood substitute could eliminate the need for refrigeration and would have a longer shelf-life. Many people have attempted to use mammalian hemoglobin in the development of a blood substitute, but have not had much success. This is because mammalian hemoglobin proteins are housed in protective red blood cells, so when they are taken out of the red blood cell there are several negative impacts. When released freely into the vasculature, mammalian hemoglobin quickly reacts with nitric oxide to cause vasoconstriction which rapidly increases blood pressure which can lead to heart attack or stroke. Also, free mammalian hemoglobin in the bloodstream has fast heme oxidation rates where iron oxidizes from Fe2+ to Fe3+ which then causes the hemoglobin to lose its ability to transport oxygen throughout the body. Ultimately, mammalian hemoglobin poses these drawbacks because it is not adapted to being outside the RBC, so an extracellular hemoglobin should be the next blood substitute target. Earthworm

hemoglobin, an extracellular hemoglobin, is the basis for the ultra-stable blood substitute in development in Dr. Elmer's lab. The goal is to enhance the stability of the earthworm hemoglobin protein, LtEc. This is done by running a thermal shift assay from 30°C-90°C and testing various buffers, salt concentrations, and reducing agents to see which conditions allow for increased stability of the LtEc.

D56 – Cold atmospheric plasma: an inside look through optical diagnostics
Authors: Liesl Krause, Dr. Prasoon K. Diwakar, A. Hassanien
Advisor: Dr. Prasoon Diwakar

A new technology used in emerging medical applications is cold atmospheric plasma (CAP). This is generated using a "pen" that emits plasma at room temperature, using various gasses to generate and carry the plasma effluents and species. Recently, success has been shown when cold atmospheric plasma is applied to oncology treatments (including apoptosis), accelerated wound healing, pathogen disinfection, and various material-changing surface effects. However, the mechanisms behind these effects are still speculative and not well understood. The goal of this study is to use multiple diagnostic techniques including fast photography, two color emission spectroscopy and optical emission spectroscopy to better characterize the plasma properties and eventually correlate this information to further test the plasma's interaction with biological samples. The plume dynamics are observed using fast photography methods with an ICCD. This allows determining visible intensity, plume length, and peak intensity, especially as gas flow rates are varied as well as the type of gas mixture used. A two color emission spectroscopy approach is used for determination of plume temperature. Plume images are recorded using narrow band optical filters at 480 nm and 510 nm. A ratio of intensities is determined and used to predict the temperature. A novel image processing code is used to automate the process of estimating the ratio of intensities from filtered images on a pixel-by-pixel basis. Additionally, optical emission spectroscopy is used to determine the chemical species, electron density, and rotational temperature at various spatial locations in the plasma plume. Detailed characterization of plasma along with the role of various gas mixtures on plasma properties provides new insight into why the plasma interaction on biological samples causes positive health effects. Further mechanisms on the plasma interaction with cancer cells as well as human pathogens will be discussed.

D57 – A green remediation strategy for contaminated soils and sediments
Author: Cory Byrnes
Advisor: Dr. Wenqing Xu

TNT has been a wildly used explosive material for the past century. It has been so readily used, that by 1992, the U.S. alone, had released over 313 million kg of TNT to the environment. However, while TNT is an extremely useful explosive, it is also a highly toxic compound with fairly hydrophobic properties. The lethal dosage for fifty percent of tested lab mice has been calculated to be about six

hundred and sixty mg TNT/kg body mass and it is currently on the EPA's Contaminant Candidate List 3, classified as a class C possible human carcinogen. Therefore, given its abundant usage and prevalence in those areas of use, it poses very serious threats to ecological and human life that may reside in or around those locations. To address this issue and to further understand the capabilities of carbon and activated carbon, a series of tests have been performed to better understand how carbon can decompose TNT, and potentially other similar compounds, through a surface hydrolysis reaction. Through these experiments a multitude of very promising results regarding the hydrolytic capabilities of carbon have been firmly established. Along with these affirmations has come the identification of an intermediate compound in the decomposition of TNT, giving further insight into the complex mechanisms of this process. To the understanding of the Environmental Engineering Department, this research is the only one of its kind and could potentially open the door to many new avenues for soil remediation.

English

D58 – Theology, Morality and the Dystopian Craze: How Dante informs Divergent
Author: Francesca Cocchi
Advisor: Dr. Michael Tomko

This paper considers the moral, ethical, and theological implications of Veronica Roth's contemporary dystopian trilogy, Divergent. Recent scholarship attributes the hype of young adult dystopian fiction to the appealing calls for individualism, freedom, and authenticity apparent in best sellers like The Hunger Games and The Giver. Though comparable in popularity among readers, Divergent attracts less scholarly attention and critical acclaim. Using Dante's Divine Comedy as an interpretive framework, this piece deconstructs the complex tension between virtue and vice that exists within each of the five factions and concludes that the dystopian elements of Beatrice Prior's world hinge on its social system's dearth of prudence, love, and true communities. Roth delivers the action, violence, and romance that young adult dystopian fans expect, but she ultimately elevates a holistic theory of virtue and Christian morality.

D59 – Not Wholly Communion: Skepticism and the Instrumentalization of Religion in Stoker's Dracula
Author: Stephen Purcell
Advisor: Dr. Gregory Hoskins

Critics often treat the protagonists of Stoker's Dracula as representative either of Christianity overall or of a specific branch of Christianity. However, despite presenting themselves as devout Christians, Stoker's protagonists demonstrate almost no religious faith. Instead, the protagonists believe only what they can empirically prove. Rather than adopting Christianity as a belief system, the protagonists

instrumentalize Christianity to facilitate and justify their hunt for vampires. Just as the protagonists use Christian items like crucifixes and communion wafers as weapons, they use Christian theology, terminology, and imagery to obscure the immorality of their motives and methods.

Environmental Science

D60 – Global warming affecting the adaptation of methanotrophs in wetland ecosystems
Author: Mary Rose Makoski
Advisor: Dr. Nathaniel Weston

Over time, methane has become the second most important greenhouse gas contributing to climate change. It is responsible for twenty percent of global warming and will continue to increase surpassing carbon dioxide over time. Wetlands are a major natural methane source contributing to about fifty percent of the global methane budget. Wetlands produce methane through a process called methanogenesis. Prokaryotic bacteria called methanotrophs act as a "biofilter" for the oxidation of methane. Methanotrophs are very important for the wetland environments because they limit the flux of methane into the atmosphere and also consume atmospheric methane. With the constant increase of anthropogenic emissions polluting our environment, scientists are unclear whether methanotrophs will adapt or die from certain pollutants and sea level rise. An experiment was conducted comparing wetlands in Plum Island, Massachusetts and wetlands along the Delaware River in New Jersey. Sediment cores were taken and were put into conditions where salinity, nitrate, and ammonium were increased to see if methanotrophs would adapt. For the Massachusetts samples methanotrophs adapted to the conditions by methane decreasing over time. However, the Delaware River samples did not adapt to conditions since methane increased over time. Overall, if methanotrophs cannot adapt to anthropogenic environments, wetlands will release majority of its methane into the atmosphere. This will increase greenhouse gases which will accelerate global warming. However, through education and future land-use and environmental policies, society can stop this phenomenon from occurring.

E61 – Sediment import/export analysis of Shad Creek, Plum Island, MA
Author: Kevin Corbusier
Advisor: Dr. Nathaniel Weston

Salt marshes are one of the most productive ecosystems on the Earth. Created in part from the flooding and draining of water and materials brought in by the tides, salt marshes are crucial for the cycling of nutrients and sediments in the coastal zone. Sediment transported from watersheds down rivers and into estuaries provides material for marsh accretion, and salt marshes can grow vertically in accordance with the rate of relative sea level given sufficient sediment supply. However, recent evidence suggests that the rate of relative sea level has increased at the same time that marshes have

experienced declines in sediment supply, which has dire implications for salt marshes. The import of water and sediment on flood tides and the export on ebb tides was analyzed for Shad Creek, a tidal creek in the salt-marsh complex of the Parker River National Wildlife Refuge in Plum Island, MA. Import/export analyses were performed for one full tidal cycle (~24 hr) on a neap tide (June 24, 2015) and a spring tide (July 7, 2015) to obtain an accurate representation of sediment transport for Shad Creek at various flooding regimes. By examining the import and export of sediment on tides, we will more accurately determine whether the Shad Creek is accreting or losing sediment. Sediment loss or retention will suggest whether Shad Creek is in danger of permanent submergence with increased rates of sea level rise. In addition to sediment, DIC (dissolved inorganic carbon) and phosphate concentrations were examined. DIC will allow us to evaluate metabolic processes during flood/ebb tides, and phosphate import/export will suggest whether the marsh at Shad Creek is a sink or source of nutrients to Plum Island Sound. The analysis of sediment import/export along with concentrations of DIC and phosphate in Shad Creek will help us better determine the overall health of the salt marshes in this system and evaluate the ecosystem services they provide. It will also help scientists more accurately predict whether certain salt marsh land will be submerged in the near future with rising sea levels.

E62 – Evaluating the magnitude and chemistry of suspended sediments in the ephemeral streams of Taylor Valley, Antarctica

Authors: Kate Henderson, Dr. Steven Goldsmith, Julie Sheets, Susan Welch
Advisor: Dr. Steven Goldsmith

The McMurdo Dry Valleys are a polar desert and form the largest ice-free region of Antarctica. Ice-covered closed-basin lakes are found throughout the valleys, fed by glacial meltwater streams during the austral summer. Taylor Valley, one of the more well-studied valleys, contains numerous ephemeral streams which carry water from the glaciers to the lakes for four to ten weeks annually. While a substantial amount of research has been conducted on the aqueous geochemistry of the streams and lakes as well as the soil chemistry of Taylor Valley, a knowledge gap exists with regards to the quantity and quality of suspended sediments transported by these ephemeral streams. This study focused on Andersen Creek, a small stream draining the western side of Canada Glacier, with the following goals: 1) to quantify the suspended sediment loads of these streams, and 2) to determine the mineralogical composition, relative weathering state, and potential sources of the suspended sediments. Daily suspended sediment samples collected throughout the 2014-2015 melt season were supplemented with diurnal sampling events to build a robust sediment rating curve. Substitution of 15 minute interval discharge values into the resulting equation revealed a seasonal sediment flux of approximately 4 tons a-1. This rating curve was then used to back-calculate seasonal sediment fluxes from 1993 to 2015, with values ranging from 1 to 54 tons a-1. The flux calculation for the 1997-1998 melt season was twice as high as a previous estimate based on a few data points. Relatively consistent mineral compositions of sediments observed both over the course of a day as well as the austral summer suggests that wind is an important amalgamating factor in Taylor Valley. Relatively weathered volcanic

ash material was also present in larger quantities than previously thought, indicating that it may be an important source of both silica and trace elements to the streams and lakes of Taylor Valley. Collectively, these revised flux estimates coupled with this relative abundance of volcanic ash indicates that leaching from suspended sediments may play a greater role in the geochemistry of Dry Valley streams and lakes than previously assumed.

E63 – An examination of fracking and other determinants of water quality in freshwater streams in Bradford County, PA
Author: Danielle Radomile
Advisor: Dr. Nathaniel Weston

As the human population continues to grow, energy consumption is expected to increase. In order to meet demand, alternative fossil fuel extraction methods are being pursued. One emerging method, known as hydraulic-fracturing, maximizes natural gas extraction through horizontal drilling. The environmental consequences of this new drilling method are not well understood. The purpose of this study was to identify determinants of water quality of streams in Bradford County, PA. Water and sediment samples were collected from 11 streams in Bradford County in July 2015. Samples were tested for TSS, radium, and heavy metal contamination. Stream health was then correlated to surrounding land-use practices, well-pad density, pipeline density, and road density. GIS data on pipeline width was acquired through the County of Bradford and supplemented with widths measured in the field via GPS. One goal of this is to estimate the loss of carbon-storage resulting from biomass removal— land is clear-cut of preexisting biomass so construction of well-pads and pipelines can proceed. Quadrats measuring 10inx10in were used to collect current biomass samples above pipeline right-of-ways. These samples were then used to calculate carbon-storage loss or gain as a result of pipeline and well-pad construction. Further analysis will include both Susquehanna County and Wyoming County.

E64 – Microbial iron reduction rates along a salinity gradient in wetland ecosystems in the Gulf Coast, Mid-Atlantic, and Northeast United States
Author: Brian Donnelly
Advisor: Dr. Nathaniel Weston

Coastal wetland ecosystems provide many valuable services to a variety of species on the planet, including humans. However, these wetlands are disappearing at an alarming rate and with that loss, their ecosystem services go with them. Iron reduction by anaerobic microbes in marsh soils is an important respiration pathway that may be influenced by salinity, and about which we know relatively little. By examining rates of iron reduction and the effects of salinity, depth, and below ground biomass in marsh soils, we can better predict future impacts of losing wetlands. In this study, we examined iron reduction rates along a salinity gradient of coastal wetlands in Barataria Bay, LA, Plum Island,

MA, and the Delaware River, NJ. We concluded iron reduction declined with both increased salinity and depth. Iron reduction rates were also controlled heavily by soil characteristics such as water content, organic carbon content, and reduced iron concentrations. Surprisingly, there was no statistically significant link between iron reduction rates and below ground biomass. If freshwater wetlands salinized due to salt water intrusion as well as sea level rise, iron reduction rates will decline, contributing to reduced wetland health. River diversions to combat both land loss and salt water intrusion could preserve wetlands as a large influx of fresh water would counteract the increase in salinity while the sediment deposits could help rebuild these wetland ecosystems.

E65 – Heavy metal concentrations in Corbicula fluminea: an investigation into accumulation factors and the effects of urbanization on waterways in Southeastern Pennsylvania.
Author: Cara Mathers
Advisor: Dr. Stephen Levas

In the past decade, clams have gained popularity as bioindicators of heavy metal contamination in waterways that have been polluted due to the biogeochemical impacts of urbanization. However, there is limited research assessing precisely the effects of different environmental agents upon the accumulation of heavy metals in the organic tissue and shells of bivalves. This experiment sets to establish whether filtration or feeding has the greater effect upon the accumulation of lead in an invasive species of clam, Corbicula fluminea, and also compares heavy metal concentrations in clams collected from various point sources of pollution in Southeastern Pennsylvania: quarries, dams, concrete production sites, wastewater treatment plants, and agricultural plots. The experiment began with sixty acclimatized clams, split evenly into six test groups: two filtration groups, two feeding groups, and two control groups. Every three days, twenty clams were exposed to lead nitrate at a concentration of .1mg/L, and another twenty clams to a 40ml suspension of phytoplankton inoculated with lead at a concentration of 1mg/L. After thirty days, half of the clams were collected and frozen at -80°C while the rest were collected ten days later to determine depuration of lead. Using inductively coupled mass spectrometry (ICP-MS), we determined average lead concentrations in each test group as well as Cr, Mn, Fe, Co, Ni, Cu, Zn, Ba, As, Se, Mo, Ag, Cd, Al in clams collected in situ. Lead concentrations were statistically compared between treatment type and length of depuration while clams collected from point sources were statistically compared to other locations, water concentrations, and sediment concentrations.

Environmental Studies

E66 – Exploring potential impacts of hydraulic fracturing on Pennsylvania's surfacewaters using trace elemental concentrations of streambed sediments
Authors: Meghan Walsh, Dr. Steven Goldsmith, Dr. Nathaniel Weston
Advisor: Dr. Steven Goldsmith

Unconventional gas extraction, particularly in the Marcellus Shale, has transformed our energy supply; yet this transformative process is not without controversy. To date, a limited number of studies in the scientific literature have documented localized stream and well water contamination due to improper disposal and/or leakage of flowback and produced waters from drilled wells. However, discerning impacts of hydraulic fracturing activities at a regional level has been hindered by the lack of baseline data, the lack of regional sampling networks, and prohibitive costs of scaling up studies. Here we attempt to address these knowledge gaps by testing the use of streambed sediments as an integrator of contaminants within a watershed. Streambed sediments were collected from 24 small (<10mi2) watersheds in northeastern Pennsylvania in in June 2015. Sediments were sieved to <63 μm (silt and clay) and processed through a partial acid digestion in order to recover the acid soluble fraction. The samples were subsequently analyzed using inductively coupled mass spectrometry (ICP-MS) for the presence of Ba, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Mo, Ag, Cd, and Pb. Sample concentrations were statistically compared to a variety of factors for each watershed, including relative land use patterns, number of hydraulic fracturing well pads, spud dates, and number of drilling related violations. Statistically significant correlations were observed between elements Zn, Cu, and Ag, and varying intensities of developed land. Statistically significant correlations were also observed between elements Rb, Sr, Se, Pb, and Cd, and total well violations with in the last three years. These findings suggest streambed sediments have potential as an indicator of historical streamwater contamination in areas affected by hydraulic fracturing activities.

Humanities

E67 – From Memorial Altars to Altered Memory: Memorializing the Collective Trauma of Zanzibar's Slave Trade
Author: Katrina Marks
Advisor: Dr. Gordon Coonfield

The Zanzibar slave trade began under Portuguese rule in 1698 and continued under Omani Arab rule until its abolition in 1873. The Mkunazini Slave Market in Stone Town, Zanzibar, active 1804-1873, was both the pivotal market for wholesale slave trading between Africa and various Middle Eastern nations and the last to be closed. After abolition, Mkunazini Market was promptly converted from 1873-1880 into an Anglican cathedral, Christ Church Cathedral of Zanzibar. This site and the history of its alterations serve as a tangible artifact of shifts in collective memory and trauma relating to the

slave trade. Through rhetorical analysis and observational field research, this research project explores the behavioral and material rhetorical dimensions of collective trauma.

Institute for Global Interdisciplinary Studies

E68 – Patrick Modiano's Memory: Reading Postmemory into Suspended Sentences
Author: Matthew Zarenkiewicz
Advisor: Dr. Gordon Coonfield

Broadly, postmemory names the connection descendants of Holocaust survivors feel towards their ancestors' memories and stories of survival. Defining and naming a latent period as a postmemorial one presents us with a way to read and understand art effectively. An example of a postmemorial artist is the French author Patrick Modiano. Critically acclaimed in France, Modiano has begun to gain attention in the English speaking world since winning the Nobel Prize in 2014. To read postmemory into Modiano, I will consider the most recent translated collection titled Suspended Sentences. In this paper I will argue, each novel in Suspended Sentences reveals a trope of postmemory, which represents a larger movement in post-Holocaust artistic representation. Reading post-memory into these novels demonstrates the work of appropriation common to post-Holocaust art as well as allows for an analysis of the, at times indistinguishable, narrator(s) of the novels.

Mathematical Sciences

E69 – Modeling the 2014-2015 Ebola outbreak in West Africa using differential equations of SIR form and Markov matrix manipulation
Author: Ronald Berna, Dr. William Fleischman
Advisor: Dr. William Fleischman

The 2014-2015 Ebola outbreak in West Africa has been unprecedented in both epidemic size and geographic area affected. Since December 2013, over 27,000 individuals have been infected, primarily in Sierra Leone, Guinea, and Liberia6. In response to the outbreak, first Doctors without Borders and then the World Health Organization implemented containment efforts in the affected areas. However, political instability16, a lack of medical infrastructure6, public mistrust of health officials12, and movement16 have made containment more difficult and presumably increased the size of the epidemic. The nature of the outbreak and the variety of responses to it have led to many modeling approaches hoping to identify key factors in the spread of the disease and the most effective containment measures. Similar to many of these approaches, we used an SIR model of time-dependent differential equations to model the spread of the current outbreak. Moreover, a hybrid model incorporating Markov matrix manipulation was utilized to mimic more reasonable, isolated population movement. With data from the current epidemic, these models were used to examine the implementation of proper burial practices, the effect of earlier or later intervention, and the optimal

quarantine practices in order to assist present efforts and guide public health efforts in future outbreaks.

Nursing

E70 – Aggression and risky behaviors in high school students: an examination of traditional bullying versus cyberbullying
Author: Meghan Long
Advisor: Dr. Elizabeth B. Dowdell

Aggression has been identified as a growing and pervasive problem among children and adolescents, often taking various forms of physical (e.g., hitting), verbal (e.g., name-calling), relational (e.g., social isolation), and now on the Internet as electronic (e.g. cyberbullying). The literature suggests that there may be a relationship among physical aggression and electronic aggression. The purpose of this study was to examine the Internet behaviors of traditional bullies (those who bully in person) compared to their traditional victims, and the internet behaviors of cyberbullies (those who bully using the Internet) compared to their cyber victims.

Philosophy

E71 – Poetry and Painting: Reinterpreting Sartre's Theory of Political Commitment
Author: Abram Capone
Advisor: Dr. Gabriel Rockhill

Sartre's theory of political commitment hypothesizes that any work of literature is committed to a political cause by virtue of the method and style with which it reveals society to its readers. Important to Sartre's original theory, but less central to later interpretations, is the representative aspect of language as literature uses it. In What is Literature? Sartre actively rails against those who want to "commit painting too" and suggests that only representational language is capable of true commitment. In later works, such as Black Orpheus, Sartre suggests that poetry (an art form he strongly compares to painting) is also capable of commitment. Poetry, he argues, demonstrates the same revelatory properties of literature. Taking Sartre's theory on prose and poetry, it seems only natural to extend the theory to visual art. Given the parallels already drawn between poetry and painting, and Sartre's own application of his theory to poetry, painting appears the next most likely candidate for political commitment. Furthermore, a denial of committed painting runs the risk of denying revelatory capacity to painting.

Physics

E72– Structural, morphological and micromagnetic characterization of $MnFe_2O_4$ nanostructures obtained through mechanochemical synthesis
Authors: Karim Boyd, Arthur Viescas, Dr. Georgia Papaefthymiou
Advisor: Dr. Georgia Papaefthymiou

Ferrites are oxidized compounds, containing transition metals, of general composition MFe_2O_4 (where M = Co, Ni, Mn, Mg, etc.) with unique electrical and magnetic properties. Their crystallographic structure is depicted by (A)[B]2O4 in which (A) and [B] correspond to tetrahedral and octahedral cation sites, respectively, and O indicates the oxygen anion site. $MnFe_2O_4$ is a soft magnetic material with low coercivity, which exhibits excellent chemical stability and mechanical hardness making it a good contender for the application as a low-loss material at high frequencies, such as microwave devices. Also, $MnFe_2O_4$ nanoparticles have been recently recognized for potential use in nanomedicine, referring to the introduction of these superparamagnetic particles into the tumor tissue for magnetic hyperthermia cancer therapy.

Iron oxide in the hematite form (α-Fe_2O_3) and manganese (II) oxide (MnO) were used as precursors to synthesize $MnFe_2O_4$ through mechano-chemical synthesis using a SPEX Sample Prep 8000M high-energy ball miller with zirconia jar and balls. The process was performed under argon to ensure that the sample did not absorb oxygen during the milling process, as MnO is known to be unstable towards oxidation in air. The milling process took a total of 6 hours. X-ray diffraction scans were performed to confirm the completion of the reaction ($Fe_2O_3 + MnO \rightarrow MnFe_2O_4$) and the purity of the nano-sized $MnFe_2O_3$ obtained. Mössbauer spectra were collected at room temperature in order to analyze their micromagnetic properties as reflected in the degree of inversion of (A) vs. [B] cation site occupation by Mn^{2+} or Fe^{3+}. The sample was also viewed under a transmission electron microscope for morphological characterization and particle size distribution analysis. The sample was dispersed in a liquid solution with oleic acid acting as a surfactant. This solution was placed onto a copper grid coated with a layer of formvar for optimum resolution. The end product was confirmed to be a spinel super-paramagnet.

E73 – Structural and magnetic phase coexistence in oxygen deficient perovskites $(Sr,Ca)FeO_{2.5+d}$
Authors: Michael Evans, Jamie Alexander Anczarski, Jimmin Ock, Joseph Pollichemi
Advisor: Dr. Jeremy P. Carlo

A wide variety of compounds crystallize into perovskite and similar structures, making them versatile laboratories for a variety of phenomena and applications, including colossal magnetoresistance, multiferroicity, superconductivity, and photovoltaic devices. Oxygen-deficient perovskites ABO_x, where $x<3$ represents oxygen deficiency, have attracted interest for use in fuel cells and related applications due to high oxygen mobility, as well as the possibility of charge disproportionation. In addition to the usual structural flexibility of perovskites obtained through reductions in lattice

symmetry and rotations/distortions of the BO6 octahedra, oxygen-deficient perovskites exhibit further structural versatility owing to ordering of oxygen vacancies.

We have synthesized and studied oxygen-deficient perovskites based on (Sr,Ca)FeO2.5+d using x-ray diffraction and Mossbauer spectroscopy, permitting study of both structural and magnetic behavior. While the ideal perovskite has d=0.5, in the present case that requires oxidizing Fe to the 4+ state, which requires very high oxygen partial pressure, or strongly oxidizing environments. When grown in air, Fe prefers the 3+ state, resulting in d values near zero. While SrFeO2.5+d exhibits cubic perovskite Pm3m symmetry (a = 3.87164 Angstroms), CaFeO2.5+d has a more distorted structure (orthorhombic space group Pnma with a rotated unit cell having a = 5.42112 A, b = 14.79082 A, c = 5.59115 A; this is known as the brownmillerite structure, exhibiting alternating tetrahedra and octahedral of oxygen-coordinated iron). In the intermediate doped compounds (Ca,Sr)FeO2.5+d we find the existence of phase separation over a wide range of (Ca,Sr) substitution. In particular, compositions ranging between about 30% and 80% calcium content are associated with the coexistence of significant quantities of both the cubic and orthorhombic phase, with some evidence of (Ca,Sr) mixing on the A sites in each phase.

Although no significant lattice parameter changes are observed in the cubic phase, the lattice parameters of the orthorhombic phase do exhibit evolution. As expected, the orthorhombic unit cell volume increases with increasing Sr content, although this is driven almost entirely by expansion of the b lattice parameter. However, there is a small but significant evolution of the ratio c/a; both this evolution and the composition dependence of the b lattice parameter are consistent with rotation/distortion of the FeOx units, driven by the radius mismatch of Ca and Sr. Mossbauer spectra of the (Sr,Ca)FeO2.5+d samples allow for the tracking of magnetic behavior. The undoped parent compounds SrFeO2.5+d and CaFeO2.5+d are paramagnetic and magnetic at room temperature, respectively. Intermediate doped compounds exhibit coexistence of paramagnetic and ordered phases, and more detailed analysis of the Mossbauer spectra permits determination of the magnetic behavior at Fe nuclear sites.

E74 – Synthesis and structural characterization of geometrically frustrated double perovskites Ba2YMoO6 and La2LiMoO6

Authors: Jimmin Ock, Jamie Alexander Anczarski, Michael Evans
Advisor: Dr. Jeremy P. Carlo

Geometric frustration occurs when magnetic ions in a material are spatially arranged in a way which inhibits the development of magnetic order. This is most commonly associated with antiferromagnetically correlated moments (that is, favoring antiparallel alignment) on triangles or tetrahedra, and manifests in a wide array of materials, including spinels, pyrochlores, and Kagome lattices. Frustrated materials exhibit rich phase diagrams with a wide variety of magnetic ground states, driven by exotic physics and high sensitivity to external parameters, because of the cancellation of normally dominant interactions. As such, frustrated materials have been a topic of intense research in recent years, and dedicated searches for and careful characterization of frustrated systems is critical

to understanding their underlying physics. Double perovskites A2BB'O6, with "rock-salt" arrangement of magnetic B' cations, exhibit frustration, and the chemical versatility of the perovskite structure enables the synthesis of a variety of materials with varying magnetic properties, making them ideal laboratories for studies of frustration physics.

We report our attempts to synthesize two double perovskites, Ba2YMoO6 and La2LiMoO6, using solid-state techniques. In both, magnetism is driven by the 4d1 Mo5+ magnetic cation, and may also be affected by the relativistic spin-orbit coupling expected in heavy ions. We also report the results of preliminary structural characterization using x-ray diffraction. Ba2YMoO6 has previously been reported to crystallize in the ideal cubic double perovskite structure, with strong antiferromagnetism and a gapped singlet ground state; magnetic order is suppressed entirely by exquisite cancellation of magnetic interactions. In contrast, La2LiMoO6 crystallizes in a distorted monoclinic structure, and previous reports have suggested short-range magnetic order. However, further attempts to refine the synthesis, and follow-up measurements using techniques such as neutron scattering, will be vital to understanding the behavior of this material.

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