Andy McErlean graduated with a BFA in Graphic Design from Auburn University in 2012. Currently, he is a UI / UX (user interface / user experience) designer working in Austin, TX.

Andy 's image, used for the cover, was his response to a class assignment. It is an example of camera-less photography created by layering objects on light sensitive paper and exposing the composition to sunlight.

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About the Editors

Conner Dobson graduated from Auburn in May 2016 with a Bachelor's of Science in Chemical Engineering (specialization in Biomedical Engineering). While at Auburn, Conner worked as an Undergraduate Research Fellow under the guidance of Dr. Robert Arnold in the Harrison School of Pharmacy to develop nanocomposite drug delivery systems for cancer therapy and diagnosis. He is also the founder and president of the Auburn chapter of the Biomedical Engineering Society and co-founder of the Auburn University's 3-Design Lab, which is intended to give Auburn students open acess to 3D printing technology. In his free time, he enjoys cooking, supporting Auburn athletics, traveling, and surfing during the summer. As of Fall 2016, Conner will pursue a PhD in Biological Engineering at the Massachusetts Institute of Technology (MIT) with the support of a graduate research fellowship from the National Science Foundation.

Ellen Rankins is a recent graduate of Auburn University with a Bachelor of Science in Animal Sciences- Equine Science. Her undergradaute research, under the guidance of Dr. Wagner and Dr. Weimar, focused on equine movement. She was an active member of both Ag Ambassadors and Block and Bridle. During her spare time, she can be found volunteering and teaching at Storybook Farm, a therapeutic riding center, where she is dedicated to bringing "Hope On Horseback" to their special riders. She is now pursing a Master of Science in Animal Sciences at the University of Florida.

Hazl Torres is a junior pursuing a Bachelor of Chemical Engineering. She is an Office Assistant for the Office of Undergraduate Research. Hazl's other on-campus involvement includes serving as a facilitator for the Alabama Power Academic Excellence Program and being a member of the American Institue of Chemical Engineers. Hazl is also an undergraduate researcher with the Adamczyk Research Group at Auburn University. In her spare time, Hazl enjoys hiking, working out, attending sporting events, and karaoke. Upon graduation, she plans to pursue a career as a chemical engineer.

Kelleen Legge is a first year graduate student pursing her Doctorate in Audiology. Kelleen graduated from Ohio University with a Bachelor of Science degree in Communication Sciences and Disorders. She is an Office Assistant for the Office of Undergraduate Research. Kelleen's other on-campus involvement includes being a member of the Student Acadamy of Audiology. In her spare time, Kelleen enjoys working out, spending time with family and friends, and traveling.

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Research Highlights

Brief summaries of student engagement in research

Ultrafast Nano-manufacturing of Fullerene-like Metal Chalcogenides

Holland Matthew Bankston

This project focuses on developing a method for synthesizing transition metal chalcogenide nanocomposites using a common kitchen microwave and polypyrrole nano-fibers (PPyNF). Such a nanocomposite would otherwise require a more involved process, such as heating with a blast furnace or chemical vapor deposition. Traditionally used as dry lubricants in high temperature applications, nano-composites are now being studied for capacitance and energy storage. Successful manufacturing of these composites through an affordable method may revolutionize energy storage.

Our recent research has helped to validate the microwave method for creating transition metal chalcogenide nano-composites. For this study, eight different composites were synthesized via microwave synthesis using two different transition metals (molybdenum & tungsten) and four chalcogens (oxygen, sulfur, selenium, and tellurium (polonium was left out because its radioactivity requires a more complex process than desired for the microwave method)). All samples were subjected to a preliminary cyclic voltammetry (CV) test to prove which composites are the most electrochemically reactive. The four most promising nano-composites were selected to be further characterized through energy dispersed spectroscopy (EDS) and scanning electron microscopy (SEM). Previous literature confirmed that the structures predicted by EDS coincided with previous formation of the same composites, lending credence to the microwave nano-manufacturing method.[1]

This research demonstrates that the ultrafast nano-manufacturing of metal chalcogenides is viable for forming nano-composites (Figure 1). We discovered that reducing the amount of polypyrrole (PPy) in each composite mixture generally increased the structures created between the transition metal and the chalcogenide.

This reduction in the composite reagent ratio may reach as low as five milligrams of PPy per 50 milligrams of transition metal and chalcogenide. However, any reduction below five milligrams of PPy usually rendered the composite incapable of reaching the temperatures required for composite formation. Conversely, too much PPy may cause the glass vial to overheat, crack, melt, and in extreme cases, explode.

Electrochemically, the composites are inconclusive, as further testing has not yet yielded many results. Although the composites are semi-conductors with potentially great electrochemical potential, the study could not confirm whether the nano-structures formed are fullerene-like or whether the incorporation of various chalcogenides improves the composites' electrochemical performance. Both attributes require further testing to examine their validity. Without confirmation by a transmission electron microscope (TEM), it is not really possible to determine that the structures are fullerene-like.

Based on the outcomes of this study, future research should focus on obtaining consistent results from electrochemical testing. Additional testing will allow us to continue researching the properties of the nano-composites for energy storage applications. Should their electrochemical properties prove unsuitable, metal chalcogenides have many other applications that would benefit from a cheap, mass production method. Future efforts should also be directed toward optimizing the structure formation. Currently, the only way to control the end structures is through changing the composite reagent ratio and cook time. Optimizing this ratio and time should produce enough structures in the sample to justify a TEM analysis to confirm or deny fullerene-like structure formation.

Statement of Research Advisor

Holland's research seeks to develop a novel approach towards nanomanufacturing of nanocomposites for catalysis applications. His research investigates the mechanism of the chemical reactions and a formulation of the nano-manufacturing technique. He also optimized the related synthetic process. This research will lead to a new methodology for the synthesis and processing of nanomaterials for energy and catalysis applications.

– *Xinyu Zhang, Chemical Engineering*

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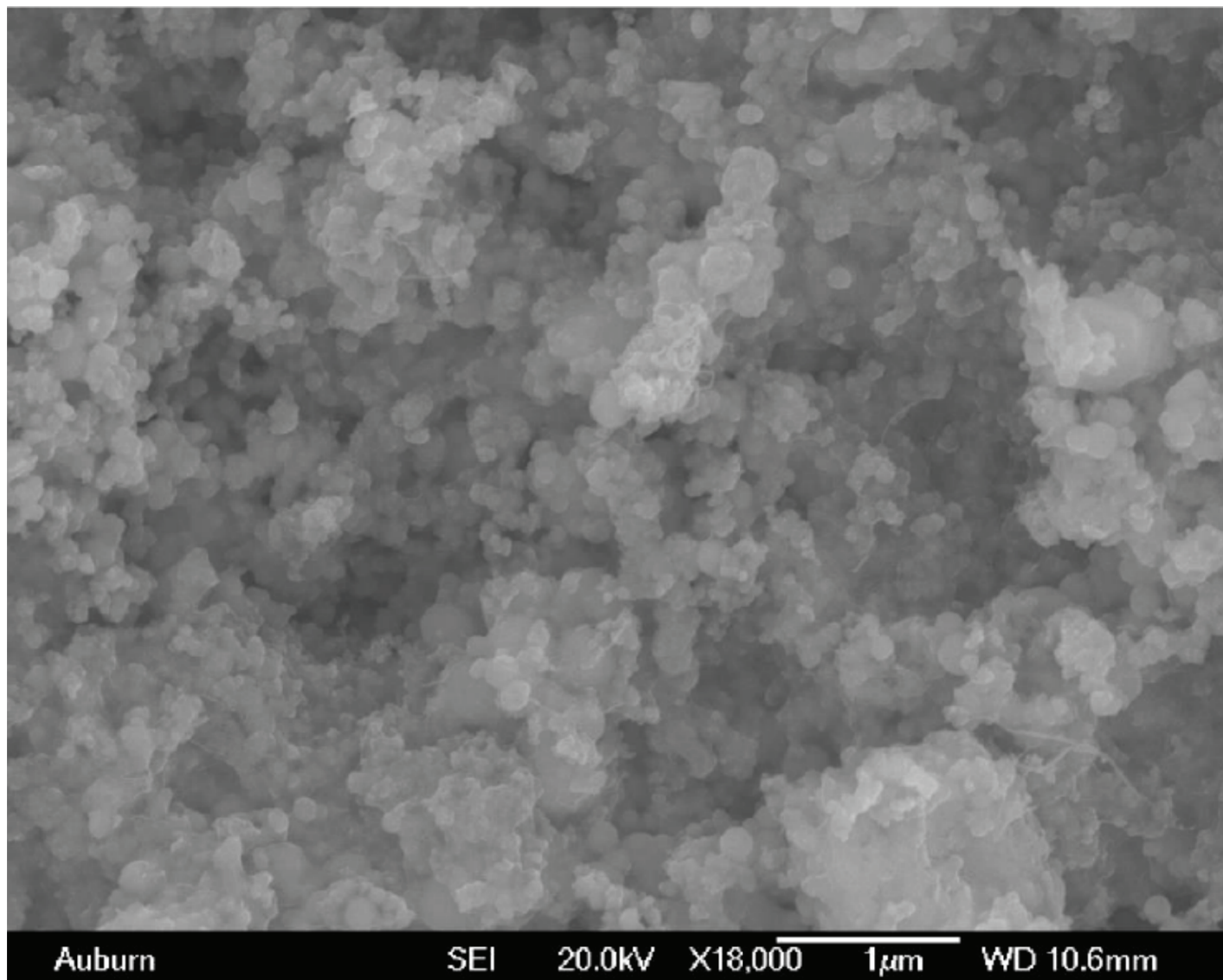
Figure 1. MoSe composite created with 5 mg of PPy

Halloysite-Polymer Composites for Controlled Antibiotic Release

Sean M. Bittner, Lee Robeson, and Edward W. Davis

Effective wound treatment is a prominent issue in medicine. Identifying and treating persistent infections is particularly important, as untreated infections can rapidly escalate. Halloysite, a naturally abundant, nontoxic clay nanotube, can be loaded with 10-30 wt% antibiotic, extending release from minutes to hours or days, and has been shown to improve the drug encapsulation of polymer films when admixed. However, the literature surrounding halloysite is deficient in some areas. Although PVOH and PMMA composites are common, experiments with other biologically relevant polymers are limited. Additionally, the literature primarily consists of experiments using tetracycline, a small, water soluble antibiotic. My project attempts to address these deficits by investigating tetracycline release from PLGA composite films, a polymer widely used in the medical community, as well as the release of novel antibiotic gentamicin sulfate.

To evaluate tetracycline release from composite films, drug-loaded halloysite/PLGA film slices were added to deionized water and held at 37°C in a shaking water bath. Samples were periodically tested using a UV spectrophotometer. Controls were prepared with pure PLGA, unloaded halloysite/PLGA composites, and tetracycline-loaded PLGA.

On release, the "burst" of drug content is significantly reduced and release is prolonged. On comparison of the 5% DLH/PLGA composite and equivalent polymer, an approximate 30% decrease in release rate is observed, indicating considerably better encapsulation. A similar relationship is observed between the 10% DLH/PLGA film and equivalent, yielding ~75% reduction. Drug encapsulation was also demonstrated on comparison of the 5% drug-loaded polymer with the 10% DLH/PLGA film. Despite the composite having twice as much loaded drug, the drug released after five hours is much higher in the 5% pure polymer, again indicating that halloysite incorporation is effective at mitigating antibiotic release.

The tetracycline results matched expectations from previous work and the literature at large. A block ratio comparison study also shed light on how this ratio impacts drug release; it was noted that increasing lactic acid yielded a higher initial burst and overall release rate, indicating some insolubility of tetracycline in lactic acid. However, it was noted that halloysite incorporation into an 85:15 (LA:GL) composite film tailored release between a pure 50:50 film and a 50:50 composite film, which is beneficial in the case that a lactic acid-based polymer is needed for drug delivery.

The results of novel antibiotic trials were inconclusive, owing to unforeseen complications caused by heating composite films. Release profiles suggested significant drug degradation, as the total mass in solution over time appeared to decrease. UV analysis of gentamicin solutions, however, showed that the drug produced consistent absorbance spectra. After verifying that the o-phthaldialdehyde solution components, which are used as a drug marker in UV testing, gentamicin were not degrading as a result of heat treatment, and that halloysite is negligibly impacted below 100°C, it is suspected that the PLGA itself masks the absorbance signature of gentamicin.

Moving forward, several areas should be investigated. The immediate focus should be alternative quantification for gentamicin. Several alternatives are being explored, with High Performance Liquid Chromatography being the most popular. It is also important to measure degradation rates of the composites as a result of halloysite incorporation, as the degradation profile of the chosen material needs to fit the application.

Statement of Research Advisor

The research Sean has conducted demonstrates the ability to utilize halloysite as a drug reservoir in biodegradable polymer systems. His efforts have demonstrated controlled release from these composite materials. His work forms the foundation for understanding of the combined effects of polymer degradation and desorption from the halloysite lumen on release of bioactive molecules from these materials.
– *Edward Davis, Materials Engineering*
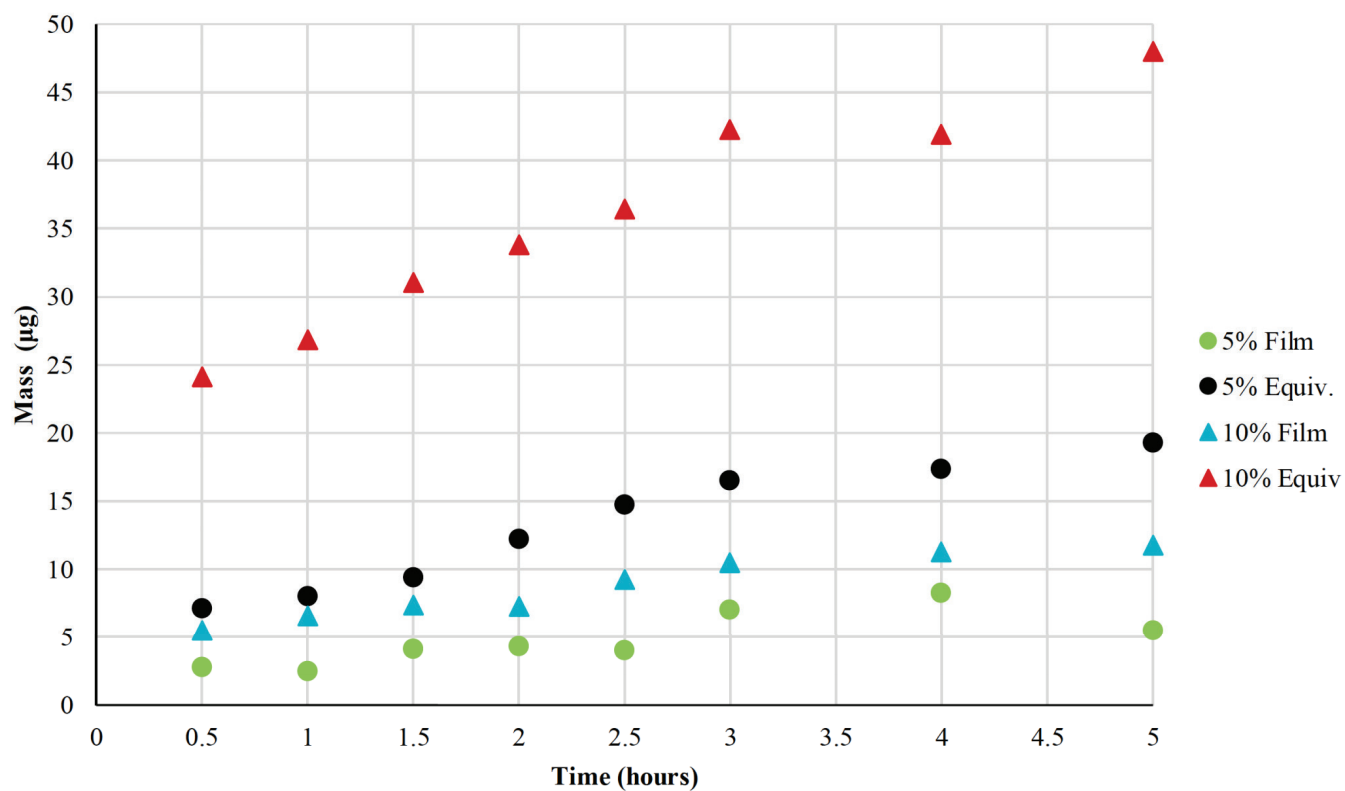
Figure 1. Tetracycline release from DLH/50:50 PLGA using 5 and 10 wt% composite films and equivalent hallyosite-free films.

Expanding the Scope of Gallium-Catalyzed Olefin Epoxidation

Fraser Bronston and Christian R. Goldsmith

Catalysts capable of allowing common synthetic reactions to take place in water instead of the usual organic solvents have long been sought after because of their potential to offset both the cost and the environmental impact of research. The majority of catalysts used in modern synthetic chemistry fall victim to a mixture of unfavorable physical and chemical interactions when exposed to water which render them ineffective. Furthermore, what few compounds that are capable of catalyzing useful reactions in such water often rely on chemical species whose actively catalytic forms are transient and poorly characterized, suffer from inconvenient interactions with certain classes of molecules, or show poor selectivity for their target reaction.

Recent work in the Goldsmith laboratory has shown that two gallium(III)-based complexes, $[Ga(phen)2Cl^2]Cl$ (A) and $[Ga(bispicen)Cl^2]Cl$ (B), are capable of catalyzing the epoxidation of alkenes by peracetic acid in both water and acetonitrile, showing exceptional

selectivity for the epoxide in both environments with no observed side products. Further investigation of the aqueous activity in constant-pH solutions showed that both catalysts are equally effective under both highly acidic and basic conditions, but nearly completely inactive in the near-neutral pH range. Functional group tolerance experiments conducted in acetonitrile suggest that alcohols, ketones, and chlorides are not affected by the presence of the catalysts, but that amines and aldehydes might result in a complex mixture of products or otherwise adversely affect their activity.

Statement of Research Advisor

Fraser has contributed to the discovery of small molecule catalysts for hydrocarbon oxidation and the development of redox-responsive contrast agents for magnetic resonance imaging. He performed all of the catalytic reactions and data analysis and synthesized these two compounds when necessary.
— *Christian R. Goldsmith, Chemistry and Biochemistry*
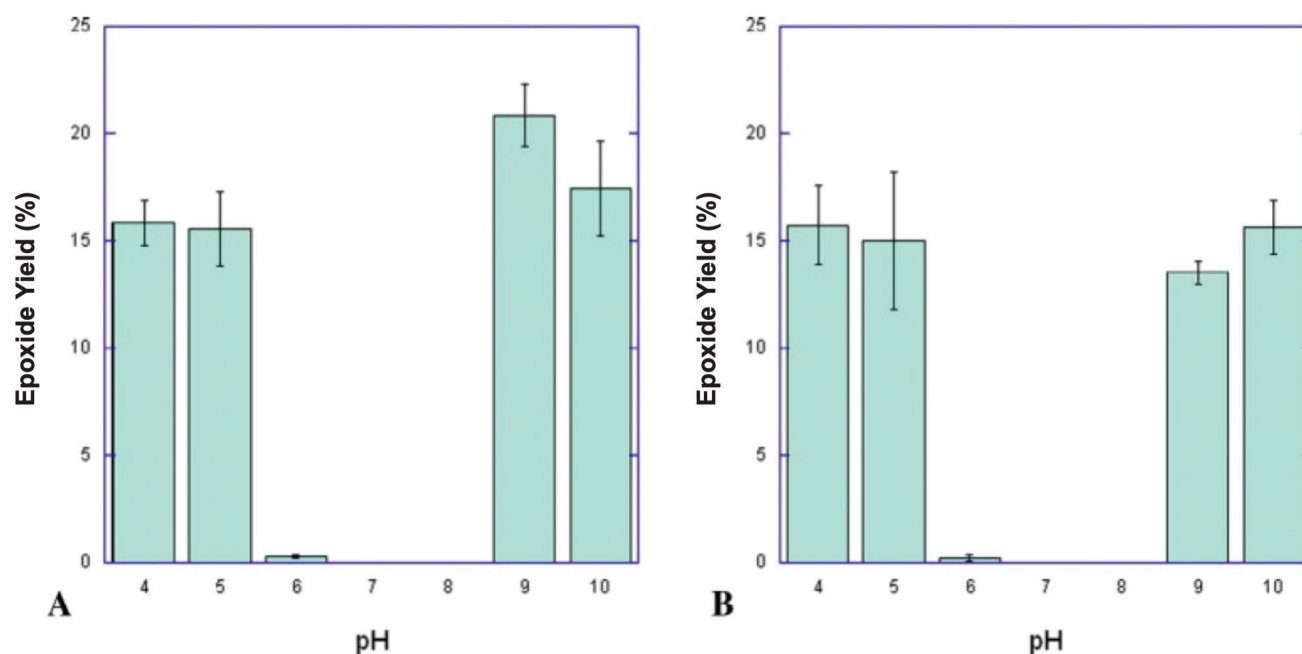
Figure 1. Yields of cyclohexene oxide generated in aqueous solutions at various constant pH values (A) Reaction conditions: $[Ga(phen)2Cl^2]Cl = 0.75$ mM, [alkene] = 75.0 mM, [peracetic acid] = 151 mM. (B) $[Ga(bispicen)Cl^2]Cl$ =0.85 mM, [alkene] = 85 mM, [peracetic acid] = 169 mM. Both series of experiments were performed under air at 25 °C.

Study of Dissociative Electron Attachment to Carbon Tetrafluoride (CF$_4$) Using the Momentum Imaging Method

James Edmond, Dylan Reedy, Allen Landers, and Michael Fogle

Dissociative electron attachment (DEA) is a type of atomic-level process in which a low-energy (sub-ionization energy) electron attaches to a molecule forming an anion. This molecular anion species is transitory in nature and leads to bond relaxation. As the bond is relaxing, it can eject the additional electron and return to the ground state neutral molecule. Otherwise, the bond (or multiple bonds) will break and one fragment of the molecule will carry the negative charge.

We study this process using momentum imaging of the anion fragments. The technique relies on well-collimated beams of target molecules and electrons that are crossed. After the pulsed electrons interact with the molecular beam and a DEA event occurs, we pulse a perpendicular electric field to extract all of the anion fragments formed during DEA. The molecules are randomly oriented, however, we can determine their momentum by measuring their time-of-flight to the detector and their position on the detector. After acquiring many millions of DEA events, the data is post-processed to orient the molecules with respect to the incoming electrons in order to study angular dependences and the energy released during dissociation.

This research provides a benchmark to test theories used to model such interactions and to perhaps use that information to engineer ways to control or enhance bond cleavage for chemical processes. One particular area that is impacted by such is understanding of how low-energy electrons cause bond cleavage in biological effects of radiation. Single and double DNA strand breaks seem to be directly linked to low-energy electron cascades caused by radiation. These electrons are in the range where DEA is a predominant process that can break bonds and lead to radical formation even below ionization energies.

Currently, we are studying the CF$_4$ molecule as one of the many test cases to be benchmarked against theory. In this particular case we are aiming to measure the DEA dynamics related to this molecule as it seems to exhibit some dynamics that are not predictive based on other molecular systems, given the known properties of the molecule. This has been hinted at by the observations of another research group but the results we have obtained so far seem to contradict their results. This illustrates the primary importance to study a wide range of molecular species for benchmarking and ensure reproducibility.

Statement of Research Advisor

Andy's work is an important part of the series of DEA studies we are aiming to complete to better understand the predictive nature of theoretical models. He has learned that such research requires a great deal of effort to overcome the tremendous hurdles that accompany such a complex, custom-made experimental apparatus. We always seem to uncover interesting artifacts in the molecular dynamics wherever we look. Andy's contribution has helped to enable these and future efforts in studying the DEA process.

– Allen Landers, Physics

Exploring the Scope of a New Cascade Reaction

Taylor Farmer, Peter Livant, and Xiaoxun Li

A central challenge to synthetic organic chemists is the problem of how to form a bond between two carbon atoms. The ability to form carbon-carbon bonds allows one to join together, with precise control, two smaller molecules to form a larger, more complex product. This is a core activity of the synthetic organic chemist.

In our laboratory, we had need of compound 2. Our original method of synthesizing 2 involved three separate reactions, starting with compound 1 (i.e., path a in Figure 1). Xiaoxun Li in our group discovered that compound 1 could be converted to compound 2 in one step rather than three by treatment with an excess of sodium hydride (path b in Figure). The reaction is termed a "cascade" reaction because several sequential reactions (in this case three) occur in one reaction vessel.

This new reaction forms a carbon-carbon double bond, highlighted in green in Figure 1. Reactions that form a carbon-carbon double bond by joining together previously separate molecules (rather than converting a single bond to a double bond within a molecule) are a somewhat rare type of reaction and quite important in organic chemistry. Examples of this type of reaction are the olefin forming metathesis reaction, the Wittig reaction, and the McMurry reaction.

Due to the importance of the formation of a carbon-carbon double bond during our reaction, we strove to understand it in more detail. One means of testing how a new reaction functions is by testing its scope. The scope of a reaction is the range of materials that can take part in the reaction successfully. This is a common way to understand new reactions to see what helps or hinders how the reaction works. An example might be adding or taking away a small part of the starting material to see if this helps. At this point only compound **1** had been used to make compound **2**. We chose three new compounds structurally similar to compound **1**.

These are bromo-nitro compounds **4**, **5**, and **6**. Like **1**, all have a bromo (Br) and a nitro (NO_2) group attached to the same carbon in the molecule. After using each of these as the starting material for our "cascade" reaction, the yields of product were found to range from 16-47%. These yields are comparable to those obtained when using compound **1** to give compound **2**.

To make these bromo-nitro compounds, a bromo-nitroso compound must be made first, see compound **3** in which a NO takes place of a nitro group (NO_2). Due to the similarity in structure we proposed that these could be used as starting materials as well.
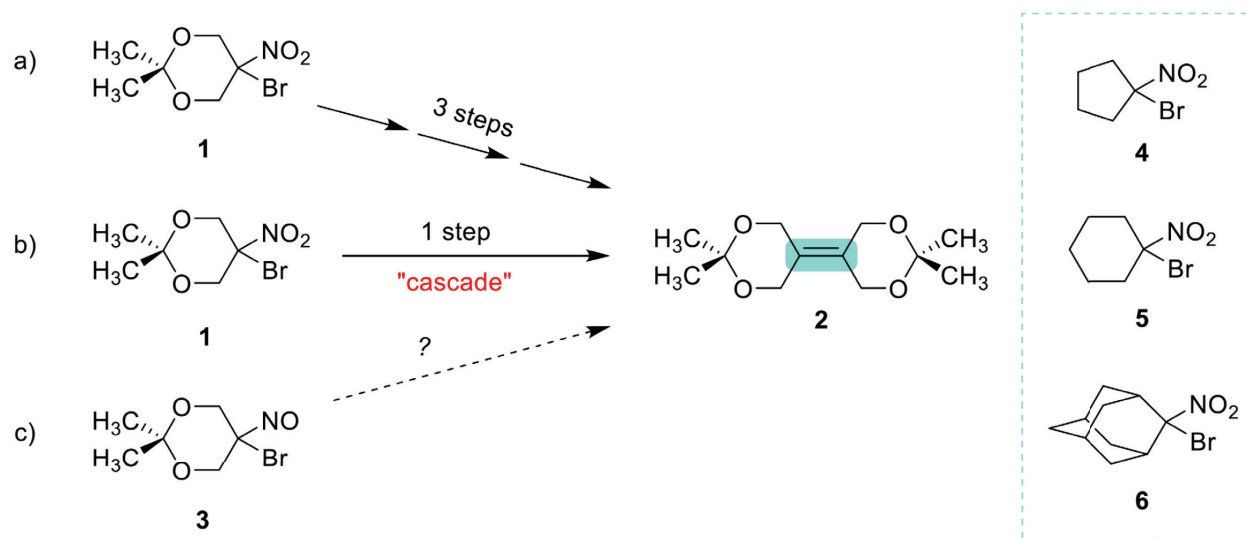
Figure 1. The cascade reaction and bromo-nitro compounds.

While results are preliminary, we have seen in at least one case that the carbon-carbon double bond formed! This means that we discovered a new reaction, which will be studied further.

Statement of Research Advisor

Taylor has provided much needed empirical confirmation that the cascade reaction has broader applicability than the single example that existed before she began. Much of her effort was spent finding and perfecting a general method for synthesis of bromo-nitro compounds. That work led to the idea of trying bromo-nitroso compounds in the cascade reaction, an idea that has yielded positive preliminary results

– *Peter Livant, Chemistry & Biochemistry*

# The Effects of Macronutrients on Inducing Satiety via Peptide YY

Caroline E. Hubbard, Heidi A. Kluess, Leslie E. Neidert, and Elise K. Mann

Several metabolic polypeptides are present in the saliva. These include Peptide YY (PYY), which is a known substrate of the enzyme Dipeptidyl-Peptidase IV (DPP-IV). DPP-IV cleaves PYY into PYY_{3-36}, a form that can bind to the Y_2 receptor in the mouth.[1, 3, 4] The Y_2 receptor is involved in sending signals of satiety to the brain. Although it is suggested that satiety is mediated by a mechanism in the mouth, the physiological mechanism is not well understood. The purpose of this study was to investigate the effects of glucose and whey protein on salivary DPP-IV activity as well as salivary PYY levels and feelings of satiety.

Twelve healthy college-age subjects participated in the study. During each visit, subjects either consumed a whey protein (Optimum Nutrition, Aurora, IL, USA) or glucose (Sierra Mist, PepsiCo., Purchase, NY, USA). During each visit, satiety was measured via a visual analog questionnaire[2] and a saliva and blood sample were taken for biochemistry measurements. All measurements were collected pre-condition and thirty minutes post-condition. A uorometric assay was used to measure DPP-IV activity in the saliva and plasma developed by Scharpe et al. An EIA (PYY3-36 human, Phoenix Pharmaceuticals, Inc., Burlingame, CA), was utilized to determine salivary PYY protein levels. The visual analog scale contained a series of five questions regarding perceived hunger and satiety, and subjects indicated their answers on a 100 mm line below each question. Satiety composite measures were calculated using a verifed mathematical formula from previous literature[2].

The mean saliva DPP-IV activity levels for the carbohydrate condition and the whey protein condition showed no significant change (Figure 1A). There was no significant change found with the plasma DPP-IV for both the carbohydrate and whey protein condition (all:35.7±8.6U/L). The pre-whey protein condition PYY levels were significantly higher than the pre-carbohydrate condition PYY levels (*p<0.05 di erent from Pre-CHO, Figure 1B). This can be attributed to natural variation as the two conditions were counterbalanced. PYY levels did not significantly change from pre to post for either of the two conditions. In the whey protein condition, the satiety composite scores significantly decreased from pre to post (+p<0.05 different from whey pre, a p<0.05 different from post-CHO, Figure 1C). This decrease in composite satiety score indicated the subjects felt more sated after drinking the whey protein shake. There was no significant change in satiety measure seen for the carbohydrate condition.
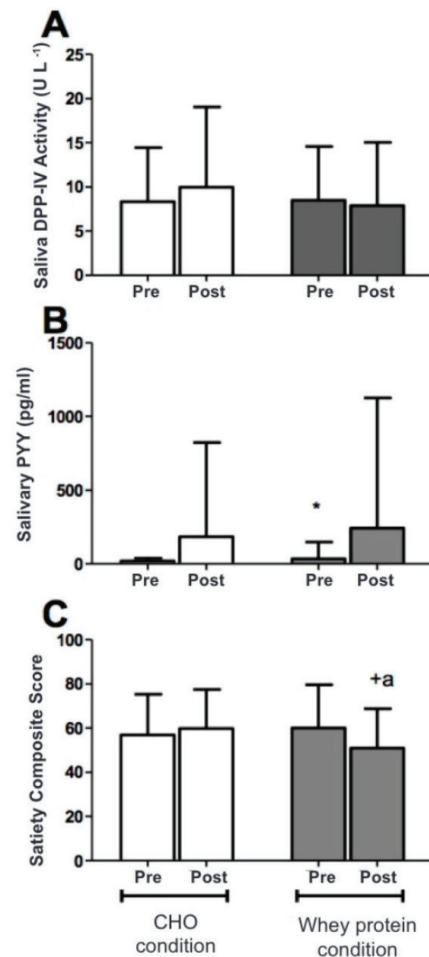
Figure 1. Shows Saliva DPP-IV Activity, Salivary PYY, and Satiety Composite Scores for both CHO and Whey protien pre and post-condition.

These results suggest that macronutrient consumption has a physiological effect in terms of satiety as a significant change was seen in the composite satiety score with the whey protein condition. Although it is suggested that there is a mechanism present in the mouth that mediates this physiological response, we did not find any evidence that PYY and DPP-IV is involved. Further research into satiety should be conducted as understanding the mechanism that mediates this physiological response would allow for better insight into controlling food intake.

Statement of Research Advisor

This project was the second study in a series that the lab performed on mouth based mechanisms. Caroline was integrally involved in the rest study and chose to do this second study as the primary researcher. Caroline wrote and won an Undergraduate Research Fellowship from the College of Education to support this project. Caroline collected the data herself with minimal help and ran all of the assays. Caroline wrote the abstract and presented this work at the Southeast American College of Sports Medicine Annual meeting in February 2016. She was awarded rst place in the undergraduate research competition. Caroline is a COSAM Dean's Medalist and an extremely accomplished student.
– *Heidi Kluess, Kinesiology*

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Variations of Toeplitz' Conjecture

Doyon Kim and Andras Bezdek

Otto Toeplitz in 1911 conjectured the following: Every Jordan curve in the plane contains all four vertices of a square. In mathematics, a curve is called Jordan curve if it is planar (can be drawn on a paper), simple (does not cross itself) and closed (walking along the curve starting at any point of the curve one will come back to the starting point). We say that a polygon P is inscribed in a curve C if all vertices of P are on C. So far Toeplitz' conjecture is solved for curves which are 'smooth enough', but the problem in its full generality is still open. All curves people can draw with a pencil on a piece of paper are smooth, but a closer look at Jordan curves reveals that they can be as complicated as fractals. This is exactly why the problem is extremely difficult in spite of its intuitive nature.

We studied the existing literature and learned about very clever elementary geometric proofs and very deep and hard to understand topological proofs. The general question in this area can be stated in the following form: *Under what condition does a Jordan curve have a specific inscribed polygon?*

We considered the following new variation of the original problem. We said that a polygon P is strongly inscribed in a curve C, if P is inscribed in C and if its interior is contained by the region enclosed by the Jordan curve. We wanted to find a general statement regarding the existence of a polygon P strongly inscribed in a curve C. Even though a lot of research has been done about the original Toeplitz' conjecture, nobody has done a research about the problem with this new condition imposed. This new condition caused a lot of complications, mainly because it prevented us to use a standard "continuity argument", where one continuously changes both the size and the position of a strategically selected square and argues that along this change at least once a desired square must appear.

The following are the theorems we found:

- Theorem 1: For every θ > 45°, there is a Jordan curve that does not have a strongly inscribed triangle whose smallest angle is at least θ.

- Theorem 2: Every Jordan curve has a strongly inscribed triangle.

- Theorem 3: Let C be a Jordan curve and let T be a triangle. Then there exists a triangle T' similar to T such that the interior of T' is contained by the region enclosed by C and two of the vertices of T' belong to C.

- Theorem 4: Let C be a Jordan curve and let D be a quadrilateral. Then there is a quadrilateral similar to D such that the interior of D' is contained by the region enclosed by C and two of the vertices of D' belong to C.

We were able to develop a new geometric method to prove our theorems. Next we will try to generalize Theorem 3 and 4 for all convex polygons. Since we succeeded to prove that any Jordan curve contains at least two vertices of a triangle or a quadrilateral of any shape, we expect to prove the same statement for convex polygons with more than four 4 vertices. We also plan to identify classes of Jordan curves that admit strongly inscribed triangles of any prescribed shape.

Statement of Research Advisor

Discrete geometry is rich in fascinating simple stated problems. Doyon Kim worked on new variants of a beautiful, over 100 year old problem. The questions he was asked to answer gave him an opportunity to show that he is able to do independent research and prove new results. His research will be published in a peer-reviewed math journal.

– Andras Bezdek, Department of Mathematics and Statistics

A Cross Correlation-Based Stock Forecasting Model

Sungil Kim and Michael E. Baginski

Researchers are continuously seeking to develop and improve the current stock forecasting models by analyzing the past value of a company and predicting future performance based on past data trends. Many previous studies of technical analysis of stocks focus heavily on forecasting a single stock price based on its own past data. This type of analysis is susceptible to stock market volatility and not very effective for intraday trading; in addition, it is difficult to apply a method used for a particular stock market sector to other market sectors. In this study, we present a cross-correlation-based forecasting model using sets of closely related stocks to forecast future stock performance.

Cross-correlating two stocks works as follows: When the price of stock A is related to the price of stock B but there is a time delay of K days, predicting stock B's price based on stock A's price will reflect the future performance of stock A, K days earlier. For highly correlated pairs, the two stocks are assumed to exhibit a similar pattern in the short term. For a long-term investment, an algorithm must be run continuously that "buys" stock B whenever stock A shows a marked increase in price if the correlation is strong and delayed by K days. The algorithm will also include a sell price once the order is filled that reflects the expected increase in value of stock B.

The proposed forecasting model discussed generates buy and sell signals along with corresponding trade dates and takes the following inputs: a pair of stocks, range of dates, correlation coefficient ($-1 < \rho < 1$) threshold, and maximum number of tries. The model first retrieves data from two stocks in a specified range of dates. Then, it calculates the cross-correlation and finds (1) whether the two stocks are strongly correlated ($\rho > \rho$-threshold) and (2) whether the time delay (lag) is not zero, meaning a time delay between the two stocks. After these two conditions are met, the forecasting model generates a buy or sell signal depending on the performance of one stock that influences the other stock with the lag. In case either of the two conditions fails, the algorithm either adjusts the range of dates

or changes the pair of stocks when it reaches the maximum number of tries.

The accuracy of the developed model is measured using US stocks from the energy sector, which is more volatile than other indexes (i.e., S&P 500) and the technology sector. We choose the energy sector to measure the resistance to volatility, effectiveness in accuracy, and profit per dollar. In particular, we choose Whiting Petroleum Corporation (WLL) and United States Oil Fund (USO), use data from the previous seven years to compute the cross-correlation, and forecast for 47 days. Results show that the proposed model accurately forecasts the upward trend 15 out of 17 times (88.2%) and the downward trend 26 out of 30 times (86.7%), for a total of 87.2% (see Figure 1). Compared to a previous study[1] that uses a data-mining algorithm with lagged correlation with 67% accuracy, the proposed model is significantly more accurate. Furthermore, the proposed model generates 3.2% profit per dollar over the span of the forecast 47-day interval. This result shows that the developed forecasting model is ideal for high-risk, high-return investments. In addition, the model can be used for intraday trading for a pair of stocks with a lag of less than a day.

This research developed a cross-correlation-based forecasting model and demonstrated that a pair of strongly related stocks shows a similar trend in the near future. The proposed model provides new insight to researchers, investors, and individuals regarding how cross-correlation can improve the accuracy of forecasting highly volatile stocks.

Statement of Research Advisor

During the last year, I have directed Sungil Kim's research in using cross-correlation information for classes of stocks to predict future stock performance. The method he developed does work, and the forecasting technique could easily be applied in other arenas such as weather prediction. He has done an excellent job and we're planning on publishing his results shortly.

– *Michael E. Baginski, Electrical & Computer Engineering*

Lag	Cross-Correlation
0.0	-.10
2.5	.23
5.0	.41
7.5	.49
10.0	.55
12.5	.60
15.0	.66
17.5	.69
20.0	.74
22.5	.67
25.0	.62

Lag = 20 hours (3 days 30 min)

Algorithm generates buy/sell signals (with lag 20 hours)
-> Forecasting USO based on WLL

Lag	Cross-Correlation
0	.87
6	.89
12	.86
18	.82
24	.78
30	.67
36	.46
42	.31
48	.45
54	.54
60	.63

Lag = 6 hours (1 day)

Algorithm generates buy/sell signals (with lag 6 hours)
-> Forecasting WLL based on USO

Forecasting Models	Predicted Up	Actual Up	Buy Signal Accuracy	Predicted Down	Actual Down	Sell Signal Accuracy	Total Accuracy	Profit Per Dollar
Previous [3]	6	5	83.3%	21	20	95.2%	67.0%	<< $1.032
Proposed	17	15	88.2%	30	26	86.7%	87.2%	$1.032

Figure 1. The forecasting model that generates sell signal (top), buy signal (middle), and the summary of result (bottom).

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Detrital Zircon Age Populations From the Lower and Upper Levels of the Moine Supergroup, Scotland, and Their Implications for Tectonic Evolution

Kelly Kindgren and Mark Steltenpohl

During the middle parts of the Paleozoic Era, between ~450 to 400 million years ago (m.y.a), the ancient proto-continents of Laurentia (today North America and Greenland) and Baltica (northwestern Europe) collided to help form the supercontinent Pangaea. The resulting mountain chain that sutured these continental masses is called the Appalachians in eastern North America and the Caledonides in east Greenland, Scotland and Scandinavia.

Structural geologists seek to understand the pre-Pangaea (before ~ 450 m.y.a) arrangement of major continents and how they have since evolved. Northwest Scotland is the focus of this study because of its geologic complexity and location at the center of the Caledonian - Appalachian mountain chain. The Moine Supergroup is a sedimentary rock unit exposed in Scotland that was deposited roughly 1,000 m.y.a. along the eastern margin of Laurentia as the obscure, pre-Pangaean supercontinent of Rodinia began to rift apart and disperse. However, the Moine Supergroup is so complexly dissected by multiple Caledonian-aged (450 m.y.a) thrust faults that its original stratigraphic order and source area is uncertain.

Identifying the source of the rocks of the Moine Supergroup is vital to understanding Scotland's plate tectonic role in the conguration of Earth's continents. Sediments formed from the erosion of mountain systems contain trace amounts of the mineral zircon, a durable mineral that can be isotopically dated. Zircon contains the isotopes U-238 and U-235, which decay into Pb-206 and Pb-207, respectively. Once a zircon crystal is formed within a cooling magma, the ratio of uranium (U) to lead (Pb) is locked into its crystalline structure. By measuring the current ratios of these isotopes, and using their half lives and decay constants, the time of crystallization can be calculated. Zircons obtained from two samples, one from the Loch Eil Group (top of Moine Supergroup) and another from the Morar Group (base of Moine Supergroup), were dated using Laser Ablation Inductively Coupled Mass Spectrometry (LA-ICPMS) (J. Schwartz, personal communication, 10/16/15). Results can be used to correlate the Moine Supergroup to sequences and source areas of the widely dispersed continents.

The purpose of this research is to better understand one of the most tectonically complex areas in the world. Land is the most indispensible element to all of human kind. In the early 1800's, Charles Lyell, a founding father of Geology said, "The past is key to the present." History of Earths land masses and the processes that formed them, therefore, are crucial to understanding how life evolved and valuable clues into how we might sustain it into the future.

Statement of Research Advisor

Kelly's research provides valuable new information on the depositional age, source areas, and pre-Caledonian extent of the Moine Supergroup. Her work suggests that the Moine actually contains two separate units of rocks, rather than one, with one package appearing to be far younger than was previously thought for the Moine.
– Mark Steltenpohl, Geosciences

Ultra High-Field, High-Resolution Neuroimaging in Adolescents

Anna E. Kirkland and Jennifer L. Robinson

There is a gap in the literature regarding ultra high field (>3 Tesla), high resolution (<2mm voxel resolution) functional neuroimaging in adolescents. Ultra high field, high resolution imaging can greatly improve sensitivity (through increases in signal-to-noise-ratio) and image quality, but it is not yet certain how preprocessing steps can alter sub-millimeter data outcomes. This study begins to address the variability in preprocessing pipelines for 7T functional magnetic resonance imaging (fMRI) data collected from adolescents. Common preprocessing pipelines include smoothing, motion correction (MT), and slice time correction (ST). Smoothing reduces the effect of noise and/or artifacts and improves signal to noise ratio.[1] Motion correction uses algorithms to limit the effect of movement during scanning sessions.[2] Slice time correction shifts the collected image slices by a given amount to temporally align the data.[3] Data were collected from 19 adolescent participants during an inhibitory Go/No-Go task in Auburn University's Siemens 7T MAGNETOM scanner (sequences had the following parameters: 37 slices acquired parallel to the AC-PC line, 0.85mmx0.85mmx-1.5mm voxels, TR/TE: 3000/28ms, 70° flip angle, base/phase resolution 234/100, A>P phase-encode direction, iPAT GRAPPA acceleration factor = 3, interleaved acquisition). All data were processed in FMRIB Software Library (FSL). To establish the effects of smoothing, the Gaussian smoothing kernel size was adjusted (0mm, 1mm, 3mm, and 5mm) while all other components were held constant. Then, the effects of motion correction and slice time correction were tested while keeping smoothing at 5mm. The analysis of the data resulted in a notable change in activation patterns as smoothing increased. Similarly, adding motion correction and/or slice time correction to smoothing at 5mm demonstrated the processing steps effect the size, extent, and location of activation across all slices collected. Interestingly, the effects of preprocessing appear to be more pronounced using high-resolution data compared to lower resolution data. Further complicating matters, adolescent populations, such as the participants in this study, are rarely examined using ultra high field means. In this environment even small movements, such as eye movements or breath-

ing, can affect the image outcomes of the data. This adds another layer of complexity when working with adolescents as they tend to move more than adults. In conclusion, the increase in magnetic field strength has allowed for improvements in sensitivity and spatial resolution, but as demonstrated in this study, there is still an underlying uncertainty concerning how to process this type of data.

Statement of Research Advisor

Anna has been a true pleasure, and exemplifies an undergraduate research fellow. Her research has addressed a critical gap in the literature and we look forward to publishing the results in the coming weeks.
– *Jennifer Robinson, Psychology*

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Exploration of Viable Methods to Form 1-thia-3,4-diazolidine-2,5-dione (TDAD)-Based Polymers

Kaylee McCormack and Michael Squillacote

Novel, well-designed photodegradable polymers have the potential to profoundly in influence society due to their wide range of applications. The photochemistry and bisfunctionality of the 1-thia-3,4-diazolidine-2,5-dione (TDAD) structure allows for the development of these unique materials. An area of particular interest with TDAD polymers is that of photoresists. Photoresists are light sensitive polymers used to coat silicon wafers that are etched to create integrated circuits, which are a vital component of modern electronics. Portions of the photoresists are photolyzed, and then a wash is required to remove the remaining organic molecules. Etching the exposed sections of the silicon wafer creates the semiconductor of the integrated circuit. If a photodegradable polymer used in this process photolyzed completely to innocuous gaseous molecules, the wash step to remove the products of the photolytic decomposition could be eliminated (See gure 1). The cost, waste, and time associated with this wash would therefore be unnecessary, which would have a massive impact upon the industry.

Our initial experiments with TDADH utilizing base-catalyzed anion polymerization have shown that with efficient leaving groups, the intermediate TDAD anion can rearrange, leading to a thermal decomposition. Experiments using 1,2-diiodoethane have exhibited this decomposition, which is partially due to the stability of the ethylene decomposition product. I am examining new methods of forming these polymers which will avoid this rearrangement.

For instance, I am using 1,1-disubstituated dihalides instead of 1,2-disubstituted dihalides in the anionic polymerization. Decomposition of the intermediate TDAD anion made from this type of dihalide would afford high-energy carbenes, making this undesirable thermal rearrangement unlikely.

In the latest polymerization effort diiodomethane was used in the alkylation of the TDAD salt, as it is a 1,1-dihalide that would minimize the likelihood of the undesirable rearrangement. Solubility tests indicated that solids produced by this reaction were soluble in dimethyl sulfoxide but insoluble in chloroform. Importantly, some of the solid produced is insoluble in water. The combination of insolubility in less polar organic solvents, coupled with solubility in the very polar DMSO and insolubility in water is positively indicative of the presence of a TDAD polymer or oligomer. The TDAD polymer with just a CH_2 group between the rings may be so polar that it is water soluble which would explain the partial solubility the products show.
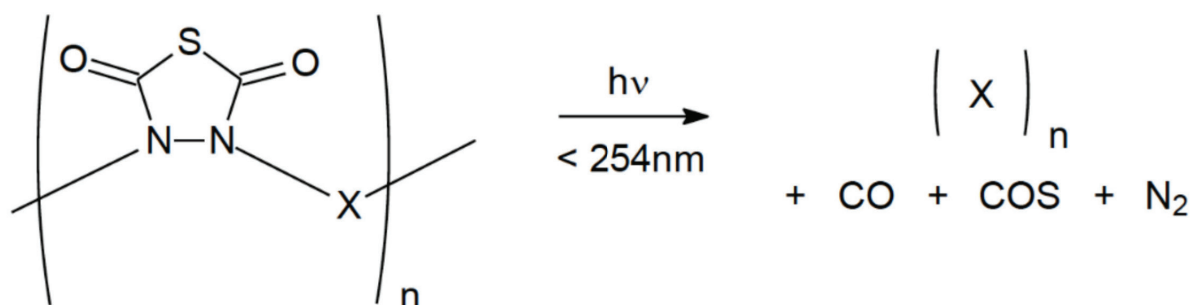
Figure 1. Photolysis of a TDAD polymer to produce small gas molecules.

To eliminate confusion, we have recently synthesized 1,1-dibromoheptane which we will use to create a TDAD polymer with a long organic chain. is nonpolar group will decrease water solubility of the resulting TDAD polymer. The solubility tests would be made clearer and the carbon chain would give the polymer more groups that could be examined spectroscopically. Because TDAD polymers offer the possibility of different connecting groups a variety of syntheses are possible. Besides experimenting with alternative leaving groups and manipulating the alkylation processes as mentioned, I intend to explore the nylon 6 approach, acid-catalysis and ring opening metathesis-type polymerizations to work towards the goal of developing a photodegradable TDAD polymer to be used in photoresists.

Statement of Research Advisor

Kaylee's work represents the beginnings of investi-gations into the usefulness of the 1-thia-3,4-diazo-lidine-2,5-dione moiety in acting as the centerpiece of a whole new type of polymer. When successfully synthesized these polymers have the potential to have a signi cant societal impact.

– *Michael Squillacote, Chemistry & Biochemistry*

Modelling Heat Transfer in the Presence of Acoustic Waves

William C. Moore, Joshua Batterson, and Joseph Majdalani

One repercussion of acoustic instability is increased heat transfer to the combustion chamber itself. This is due in part to unsteady combustion but more so because of unsteady convection. The latter can cause a local buildup of heat that can ultimately produce "hot-spots" within the chamber.[1] Being able to predict the increased heat loads on the chamber walls during instability is therefore essential in our efforts to predict the chamber's safety margins and overall cooling requirements. This is especially true in regions where heat builds up naturally – such as the converging section of a nozzle where both the mean flow and the longitudinal modes can be large.

The problem of acoustic waves evolving in combustion devices is a well-known problem in the propulsion community. Extensive work exists to model these acoustic modes and add special insight into the thermodynamic dependence of the acoustic mode shapes.[2] With this knowledge in hand and the technical tools in place to estimate the location where acoustic modes are most intense, the available unsteady convection/conduction heat transfer models can be used to predict the thermal load on the chamber itself. To address this issue, numerical heat transfer analysis of an arbitrarily-shaped propulsive device will be incorporated into an already well-established vortico-acoustic wave solver.

Since an accurate acoustic mode shape can be calculated, the unsteady heat transfer character can be accurately modeled. Such a thermal analysis can be essential during the developmental design stages of new engines where the stability characteristics are not yet known. By achieving a better prediction of the thermal loads, the design can be adjusted to the extent of improving its safety margin. Furthermore, looking beyond propulsive devices, unsteady heat transfer analysis can be incorporated as part of the design process in industrial applications where tailoring the design to maximize the unsteady heat transfer can substantially increase the thermal effectiveness of the device in question.

In this study, basic models are developed to illustrate the possible increase in heat transfer as a result of instabilities propagating through simple geometries with well-understood mean flows. These models are realized by solving the heat equation for the surface of the geometries.[3] The boundary conditions for the heat equation are determined by simulating heated flow over the surface and imposing a time dependent acoustic wave on the heated flow. Once fluid properties are estimated, the convection coefficient may be determined. Using root finding methods, a heat balance is performed at the surface of the combustion chamber to determine the temperature of the solid boundary (See figure 1). In this process, the temperature throughout the solid is computed using a second order finite difference method to solve the governing heat equation.

Ongoing work entails the application of the solver to increasingly more complex geometric configurations associated with propulsion devices. In this context, the nozzle is of particular interest for capturing longitudinal mode effects. Also, the solver will possibly be applied to industrial devices where increased heat loads can be desirable.

Statement of Research Advisor

Chandler's research seeks to capture the link between traditional acoustic waves and the very elusive problem of heat transfer augmentation in rocket chambers. His work may be viewed as groundbreaking because it opens up a new avenue for research into the direct e ects of acoustic mode shapes on thermal loading of chamber structures, namely, what could be referred to as unsteady uid/structure interactions in large combustors.

*– Joshua Batterson and Joseph Majdalani, Aerospace Engineering*

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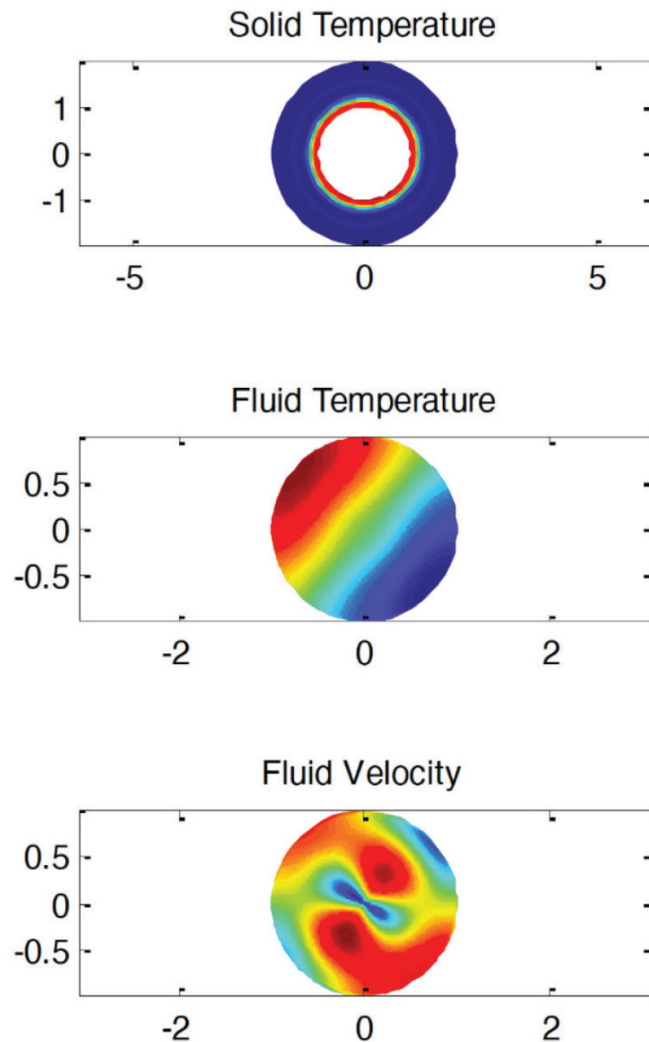
Figure 1. Effects of radial acoustic waves on the fluid and sodium domain.
x-axis: Normalized Position, x/r (-)
y-axis: Normalized Position, y/r (-)

Regioselective Functionalization of [n]*para-terphenylophanes*

Natasha Narayanan and Bradley L. Merner

[n]*para*-terphenylophanes are compounds that contain three benzene rings linked at the para, or most remote, positions (Figure 1). The two outer (terminal) benzene rings are connected by a "tether" consisting of a bridge of atoms, where n refers to the number of atoms in the tether. Due to this tether connecting the two terminal benzene rings, the central benzene ring of the *para*-terphenyl unit is distorted out of planarity. Decreasing the number of atoms in the bridge shortens the tether, which increases the distortion of the central benzene ring and the strain energy of the molecule. Our group has developed a short, efficient synthesis of a series of *para*-terphenylophanes with varying tether lengths. We have recently turned our efforts towards the regioselective functionalization of these compounds for two reasons. First, in order to use these *para*-terphenylophanes as templates in the bottom-up synthesis of carbon nanotubes, functional group handles must be installed on the benzene rings in order to perform reactions necessary for elongation in the vertical direction. Secondly, a bent phenol moiety is present in the structure of a natural product known as haouamine A, which was isolated from a tunicate off the coast of Spain in 2003 and has shown promising anti-cancer activity. We hope to apply the synthetic methodology developed by our group for making bent functionalized arenes to the total synthesis of haouamine A, and in particular to the construction of the macrocyclic core containing the nonplanar phenol.
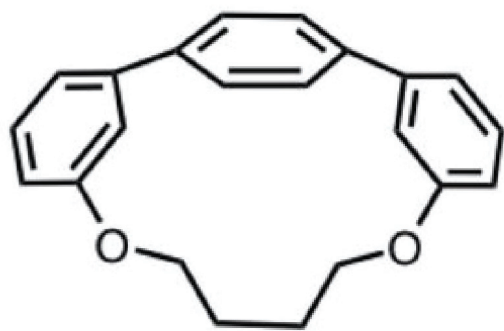

Figure 1. [6]*para*-terphenylophane.

Beginning with a cyclohex-2-ene-1,4-diol, which serves as a bent precursor to the aromatized system in our synthesis of *para*-terphenylophanes, we envisioned that we could obtain the α,β-unsaturated ketone from the oxidation of the cyclohex-2-ene-1,4-diol in a [3.3] sigmatropic rearrangement. The dehydration of this α, β-unsaturated ketone would yield the nonplanar phenol. Various oxidation procedures reported in the literature to achieve tertiary allylic alcohol oxidation in a [3.3] sigmatropic rearrangement were tested, including PCC oxidation, IBX oxidation, and DMP oxidation, with no success. The desired transformation was achieved using a literature procedure that employs a TEMPO tetrafluoroborate salt (Figure 2).[1] Attempts to aromatize the compound by eliminating a molecule of water have so far been unsuccessful. Future work will involve improving the yield of the TEMPO oxidation reaction, finding reaction conditions to aromatize the central benzene ring in order to obtain the nonplanar phenol, and investigating other synthetic routes to bent functionalized aromatic rings.

Figure 2. TEMPO$^+$BF$_4^-$ oxidation.

Recently, some exciting advancements have been made regarding the regioselective functionalization of the two terminal benzene rings of [n]para-terphenylophanes. We predicted that the two tertiary alcohols present in the cyclohex-2-ene-1,4-diol could be used as directing groups to direct the C-H functionalization of the terminal benzene rings. Based on a literature procedure, a tertiary alcohol-directed C-H functionalization reaction was used to successfully install a phenyl ring on one of the terminal benzene rings of a paraterphenylophane (Figure 3).[2]

This regioselective C-H functionalization chemistry can be used as a way to extend para-terphenylophanes into templates of sidewalls of carbon nanotubes.
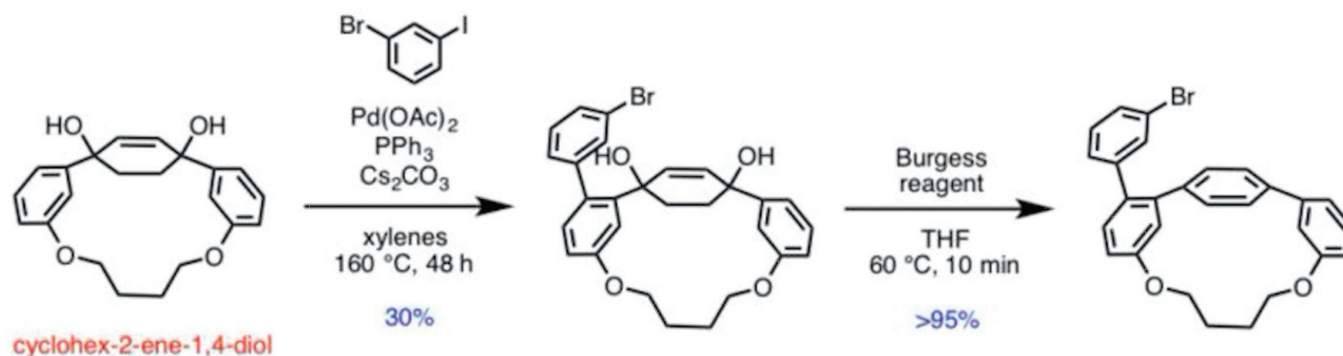

Figure 3. Regioselective C-H functionalization.

Statement of Research Advisor

Natasha has been developing new synthetic strategies for oxidizing macrocyclic cyclohex-2-ene-1,4-diols into strained arene-bridged phenol units. These methods, if successful, will be of great importance in developing a novel class of anti-cancer compounds, and functionalized benzeoind macrocycles that will be employed in the bottom-up chemical synthesis of carbon nanotubes and related substructures. Natasha has single-handedly completed the first step in this challenging process.
— *Bradley Merner, Chemistry and Biochemistry*

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Development and Application of Gold-Lipidic Nanocomposites to Enhance Chemotherapeutic Delivery and Release

Christina M. Pickering, Connor S. Dobson, Peter R. Panizzi, Allan E. David, and Robert D. Arnold

Chemotherapy efficacy is limited by toxicity and tumor drug resistance. Liposomal drug carriers are nano-scale, spherical particles with a phospholipid bilayer surrounding an aqueous core. With increased circulation and improved tumor deposition due to the enhanced permeability and retention effect, liposomes increase treatment efficacy and reduce toxicity. However, the chemistry of many efficacious chemotherapeutics prevents their encapsulation within liposomes and poses a challenge for formulating treatments. Consequently, the development of improved drug delivery technologies is a large area of current drug research. Additionally, drug delivery carriers capable of multi-drug or component delivery are desired because of their flexibility and high applicability.

I hypothesized that composite systems, gold nanoparticles within liposomes, may be used to improve drug delivery of both currently used therapeutics and ones traditionally incompatible with liposomal delivery. I formulated a novel gold-lipidic nanocomposite to capitalize on the drug delivery capabilities of liposomes and the facile conjugation of gold nanoparticles. I proposed new techniques for the formulation of nanocomposites comprised of 2 mm gold clusters capped with glutathione (G-AuNC) or mercaptosuccinic acid (MSA-AuNC) encapsulated within pegylated, long-circulating "stealth" liposomes. The included figure displays the techniques used to formulate the gold-lipidic nanocomposites. Physical characterization was completed using atomic absorption spectroscopy (gold quantification), dynamic light scattering (size distribution), and cell metabolic assays (cytotoxicity). I also studied separation methods for the removal of unencapsulated gold and the strengths and challenges encountered.

These nanocomposites can be produced by a simple, scalable method with narrow size distributions around 100 nm and consistent nanoparticle encapsulation. I tested the resulting encapsulation and proposed alternative separation methods to counteract the problems encountered with the dialysis method. Research in this area is ongoing. Intracellular uptake and *in vivo* biodistribution of the gold-lipidic nanocomposites was compared to the standard liposomes. These data support my hypothesis that gold-lipidic nanocomposites can be prepared and justify preclinical *in vivo* studies in murine models of human tumors to improve cancer treatment.

While there were no differences in intracellular uptake between the standard liposomes and the nanocomposites, we did observe altered tumor deposition relative to tumor volume in nanocomposites compared to traditional liposomes. The initial results were ultimately very favorable and indicate much potential for future work in this area.

Future aims on the project include the co-encapsulation of gold nanoparticles and model chemotherapeutic in liposomes, investigation of the effect of gold nanoparticles on drug encapsulation and release, covalent linkage of paclitaxel to gold to enhance stability and tumor deposition, and exploration of multispectral opto-acoustic tomography (MSOT) to examine the ability of the targeted particles to identify metastasis and improve antitumor activity.

Statement of Research Advisor

Christy's research focused on the development of multifunctional nanomedicines to identify and treat primary cancers and metastatic disease using imaging probes and optimizing drug release. Her research will advance the development of composite nanomedicines that permit multi-modal imaging (e.g., optical, ultrasound and MRI) and can be tailored to improve concomitant delivery of multiple therapeutic agents simultaneously.
– *Robert Arnold, Drug Development and Delivery*
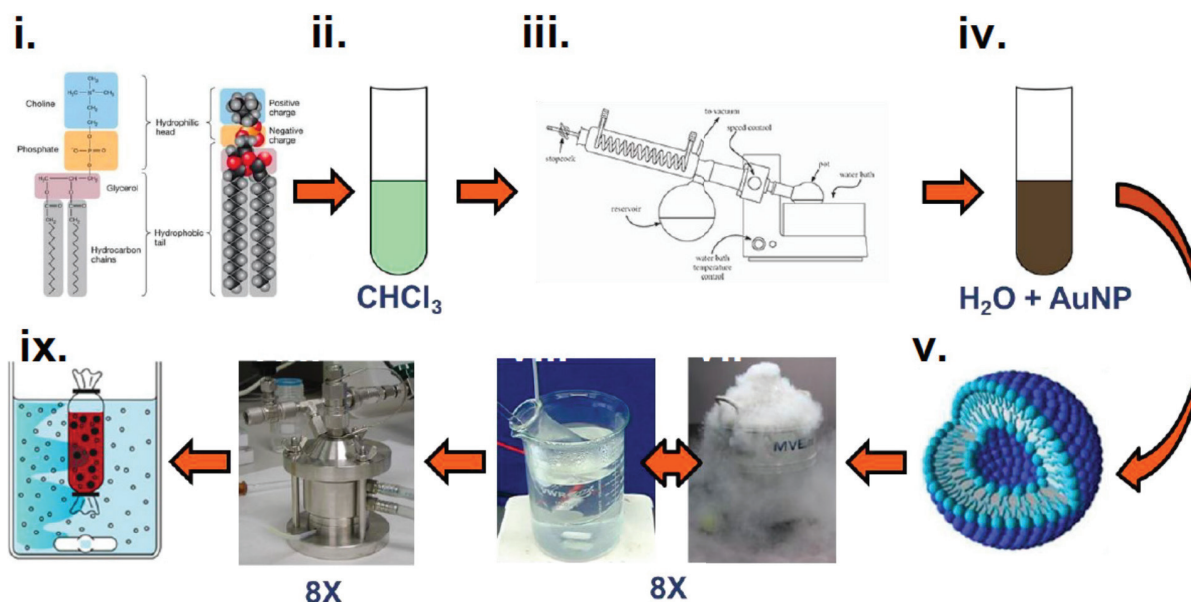
Figure 1. Formulation of gold-lipidic nanocomposites using the standard dry film hydration method with extrusion sizing. The formulation of liposomes is the same except that the hydration in (iv) is only water and (ix) is not included. The lipids (i) are originally dissolved in chloroform (ii). The chloroform is then evaporated using a rotary vacuum evaporation system (iii). The resulting thin film is hydrated with the aqueous gold nanoparticle solution (iv), creating liposomes (v). The liposomes are sized through a liquid nitrogen freezing (vi)/hot water thawing (vii) cycle and then high pressure extrusion (viii). The unencapsulated gold particles are removed through dialysis (ix).

Role of Sugary Water Consumption in Adipose Gene Expression

Jami Reece and Michael W. Greene

Although obesity is not an infectious disease, one could reasonably describe the state of obesity in the US as epidemic due to the relatively high prevalence that transcends age, gender, and socioeconomic groups. Subsequent conditions linked to obesity include but are not limited to type II diabetes, non-alcoholic fatty liver disease, heart disease and stroke, and even some types of cancer. Although obesity is most closely associated with elevated body mass, it is more accurately diagnosed by excess adipose tissue, which can result from diets high in fat and sugar like those common in the US. To better understand the role of sugar in adipose gene expression, transcriptional profiling using RNA seq was performed in adipose tissues of mice fed a control chow diet, a high fat Western diet (HFWD), and a HFWD with 4% sugary water (HFWDS). We observed 548 differentially expressed epididymal white adipose tissue (eWAT) genes greater than 2-fold in mice fed the HFWDS compared to those fed the HFWD. Quantitative reverse transcription-PCR was conducted on retroperitoneal white adipose tissue and inguinal white adipose tissue in addition to eWAT in order to verify the RNAseq results. Our results confirm expression of key up-regulated and down-regulated genes with diets. Further, statistical analysis revealed that the expression of two key genes also correlated with obesity-associated parameters. The expression of Cacna1e, which was demonstrated to be down-regulated in association with HFWDS, exhibited positive correlation with normalized eWAT mass. The expression of Glt6d1, which was instead demonstrated to be up-regulated, exhibited positive correlation with blood glucose levels. Additional studies of these genes and their expression in adipocytes will further elucidate their role in adipose tissues. Our findings may pave the way to uncovering novel mechanisms for pathogenesis within adipose tissue and potential targets for therapeutics to treat obesity-linked conditions.

Statement of Research Advisor

Jami's research focused on validating results from a gene expression discovery experiment to examine the role of sugary water consumption. Our objective was to identify genes that may regulate adipose tissue dysfunction, which is commonly associated with obesity. Jami's results indicate that consumption of sugary water in an animal model of obesity results in differential regulation of specific genes within the adipose tissue. Her results have contributed to our understanding of the role of adipose tissue in the pathophysiology of obesity.

 –*Michael Green, Nutrition*

Physiological and Psychological Effects of Music

Sarah Stevenson, Paula Bobrowski, Ann Knipschild, and Jennifer Robinson

Any listener of music will agree that music can evoke emotions, such as pride, elation, or relaxation. Research suggests that music does more than that for humans: it stimulates various parts of the brain and bodily responses, including the release of stress hormones. The current research project addressed the questions: How do different kinds of music affect the human body physiologically and psychologically? Is the unconscious experience elicited by the autonomic nervous system analogous to what is experienced consciously through emotions?

To attempt to answer these questions, a total of ¬¬¬88 participants over three semesters from a Music and Science course at Auburn University wore a respiration belt, two electrodermal activity electrodes, and two electrocardiogram electrodes and listened to 2-minute audio recordings of Stravinsky's "The Rite of Spring" (song 1) and Satie's "Gymnopédie No. 1" (song 2) as BIOPAC software recorded their responses. After hearing each of the songs, the students completed a paper-and-pencil psychological survey in which they rated emotions elicited by the music clips.

The raw data was then analyzed to obtain various measurements. (See figure 1.) Results over all three semesters were not always consistent or significant ($p<0.05$), most likely because the research protocol was updated and improved after each semester; however, some trends were identified over the course of the study. Measures of sympathetic nervous system activity (event count and sympathetic nerve activity) were higher during song 1, with the exception of skin conductance level. This could mean that song 1 elicited more overall activity, though the electrodermal activity baseline was lower. Measures of parasympathetic nervous system activity (respiratory sinus arrhythmia and vagal nerve activity) were higher during song 2. Beats per minute, an end organ measure (culmination of sympathetic and parasympathetic nervous system activity), indicated that there was more overall activity during song 1. Therefore, we can conclude that song 1, "The Rite of Spring," provoked more sympathetic activity and song 2, "Gymnopédie No. 1," provoked more parasympathetic activity.

The physiological results were analogous to the psychological results from the emotion surveys; participants rated their emotions as alert, attentive, and excited during song 1 and relaxed, calm, and interested during song 2. In conclusion, there was an overall more aroused response in terms of physiological and psychological activity during the more musically complicated song 1 (Stravinsky's "The Rite of Spring").

These results will contribute to the body of knowledge regarding music and science. In future semesters, the project will continue to investigate the relationship between music and the body, examining specific qualities of music that elicit reactions. This information can then be applied to areas such as therapy, education, and healthcare.

Statement of Research Advisor

The result of this research is already making a significant impact on the field of music and science. It is being used in general education courses as a demonstration project to inform students on the interrelatedness of science and music as well as engaging them in their own research projects. It is being presented at multiple national forums and has resulted in additional funding for outreach projects and other NSF grants to conduct future research into the subject matter. I predict the results of this project to reach far into the future and positively impact the quality of life for a wide range of populations.
– *Ann Knipschild, Department of Music*
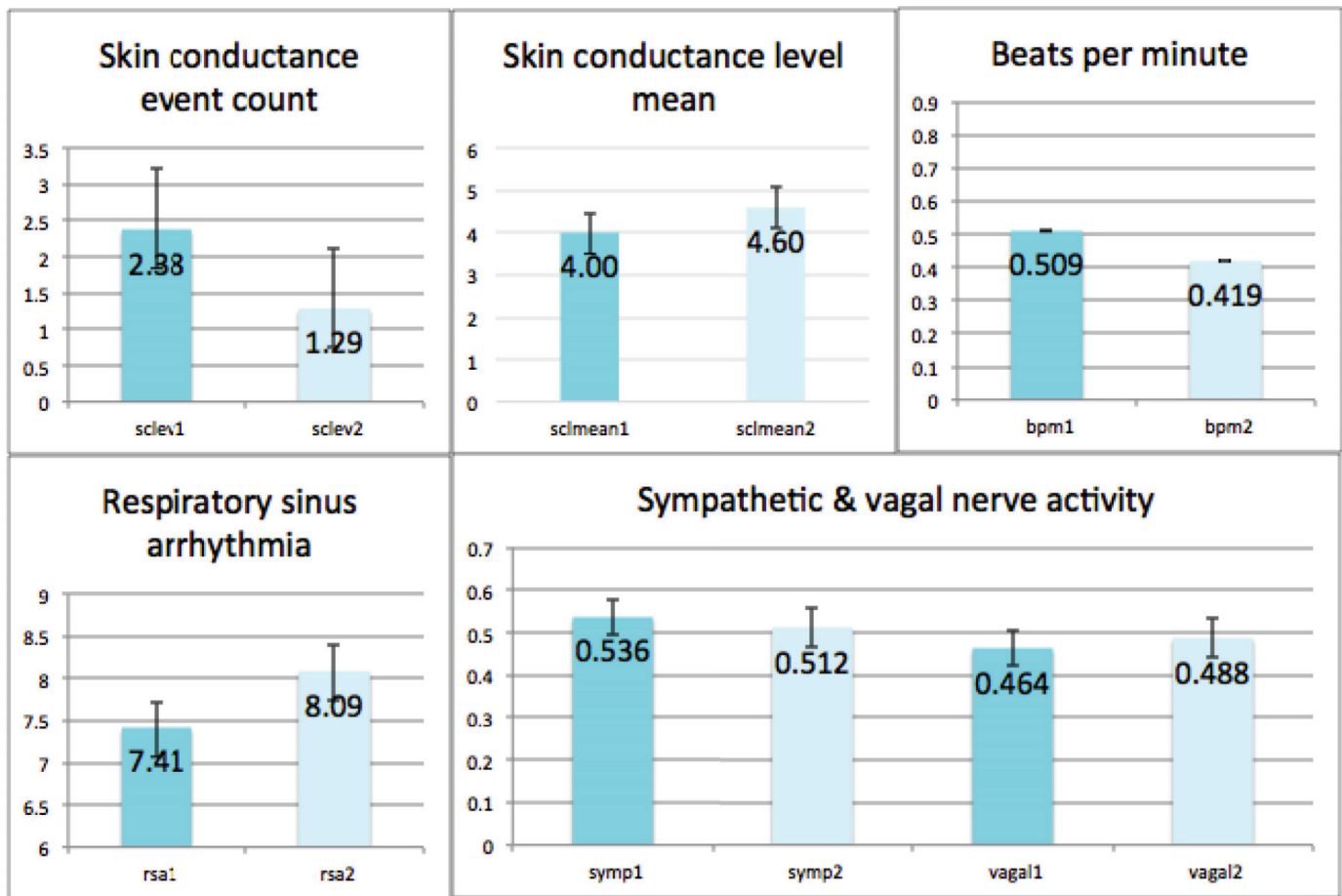
Figure 1. Significant results from the study: skin conductance event count, skin conductance level, and sympathetic nerve activity are all measures of the sympathetic nervous system. Respiratory sinus arrhythmia and vagal nerve activity are measures of the parasympathetic nervous system. Beats per minute is a culmination of both sympathetic and parasympathetic nervous system activity.

Computational Study of Electrostatically Tunable Band Offsets in MoS$_2$ Multilayers

Martin Wang and Marcelo Kuroda

The objective of my research project was to determine the viability of molybdenum disulfide (MoS$_2$) for the purpose of application in low-power electronic devices and flexible optoelectronics. The greatest motivation for this research topic lies in its ramifications for that crucial and ubiquitous electronic component: the transistor. Traditionally, transistors have relied on the physical properties of their bulk materials; however, as modern circuit components continue to scale down, materials with reduced dimensionality have emerged as alternative solutions for optoelectronic applications. This change in paradigm follows the new challenges posed by modern technological applications.

Among this novel class of alternative materials, MoS$_2$ presents remarkable properties for electronic devices: this unique material has several key characteristics which make it an interesting study in the context of transistor technology. First, MoS$_2$ has the property of being a two-dimensional material – it exists naturally in stable, one-molecule-wide layers. The advantages of 2-D materials is twofold: it lacks the unstable hanging bonds which cause the shortcomings traditional materials, and it enables more flexible electronics by allowing different layers to slide by each other. The second interesting property of MoS$_2$ is the existence of two phases of MoS$_2$: the 1T phase and the 2H phase. These two phases of MoS$_2$ use the same atoms in different molecular geometries, producing different electrical properties – the 1T phase is a metallic conductor while the 2H phase is a semiconductor. Thus MoS$_2$ can, by itself, singly form both the transistor contacts and channel. However, this system comes with its own important challenges to overcome: when MoS$_2$ is interfaced with bulk metals, it suffers from Fermi level pinning that results in a large contact resistance.

In order to probe the electronic properties of MoS$_2$, Density Functional Theory (DFT) within the generalized gradient approximation (GGA) using the pseudo-potential method was employed. The calculations modeling various configurations of MoS$_2$ vertical heterostructures were conducted using the computing resources generously provided by the Alabama Su-percomputing Center, as well as Auburn's own CASIC cluster. These calculations aimed at establishing the possibility of circumventing the problem of Fermi level pinning using MoS$_2$ heterostructures.

These calculations began with 'relaxation' calculations which were used to determine the proper lattice constant of the MoS$_2$ crystal models and the relative positions of the MoS$_2$ atoms. The project then proceeded to calculating the electron bands for MoS$_2$ heterostructures ranging from the two layer 1T-2H to the four layer 1T-2H-2H-2H. Finally, the calculations applied field and charge to the models and generated the band structures which could be analyzed to determine the electronic susceptibility. In the end, the analysis of band movement with respect to layer number and con-figuration revealed that MoS$_2$ produced relatively large electronic susceptibility when the 1T phase is config-ured to be above the 2H phases, and that the electron-ic susceptibility increased approximately linearly with additional 2H layers. This property alleviates the Fermi level pinning and offers promising indications for the viability of MoS$_2$ for the stated purposes in low-power electronic devices and flexible optoelectron-ics. Moving forward, more sophisticated and computa-tionally expensive calculations must to be performed to overcome the limitations of DFT and further validate our findings.

Statement of Research Advisor

Martin Wang has performed a large number of first principles calculations and computational tools to analyze the outcomes of those simulations. These encouraging results show that the behavior in MoS$_2$ het-erostructures is remarkably different from those using bulk metals, opening new possibilities for MoS$_2$ -based electronic applications.

– Marcelo Kuroda, Department of Physics

Main Reservoirs of the Bacteria *Aeromonas hydrophila* in Commercial Catfish Raceways and Ponds

Evelyn Willmon, Covadonga Arias, Francisca Burgos-Valverde, and Candis Ray

Aeromonas hydrophila is a gram-negative bacteria that causes Motile Aeromonas Septicemia (MAS) in many fish species. Typically, *A. hydrophila* is considered an opportunistic pathogen but an emergent strain, which is especially deadly to commercially farmed catfish, has become a major concern for the catfish industry since 2009. Alabama is the 2nd leading state for catfish production, and catfish is the top aquacultured species in the United States. The emergent strain of *A. hydrophila* affects larger fish, which means that the fish are lost at market size resulting in enormous financial losses for farmers. The strain is especially prevalent in east Mississippi and west Alabama, which are two of the largest areas for catfish production.

The goal we were looking to accomplish was to determine sampling protocols for monitoring the number of the *Aeromonas* bacteria in production ponds. We wanted to determine if the bacteria had a niche preference within the ponds and to determine that we quantified its numbers in water, sediment, and biofilm. In addition, we wanted to investigate if there was seasonal distribution of this pathogen in aquaculture ponds. We also wanted to determine whether or not the introduction of a probiotic in the diet of the catfish would significantly change the amount of *Aeromonas* species (spp.) present in the environment.

Sampling started in late July and was done monthly until mid-October, as well as during any disease outbreaks caused by *Aeromonas spp*. Samples were obtained from the same three ponds from a commercial catfish farm located in west Alabama. Serial dilutions were made from the samples and were then filtered, then placed on both a general growth media and a media selective for *Aeromonas spp*. After being incubated 24hrs, plate counts were done to determine the number of bacteria. This process was done after every sampling event.

While statistical analysis of the data is still in progress, preliminary results indicate that biofilm and sediment appear to be the main reservoirs of *Aeromonas spp*. in particular. It also indicates that as the water cooled off in October (water temperatures in the October sampling were around 20-22°C compared to 30-33°C during the summer months), the amount of *Aeromonas spp*. present in the water decreased but the amount present in the sediment increased. This aligned with our hypothesis that the *Aeromonas* might use the sediment as a refuge during cooler weather.

The next step for this project is to finish the statistical analysis of the data. We are also in the process of completing DNA extractions from the samples in order to determine if the *Aeromonas spp*. that were present in the samples were of the virulent strain, as it is impossible to determine without genetic analysis.

By identifying the main reservoirs of pathogen, farmers can take steps to limit the amount of it present. This will help decrease disease outbreaks and minimize the financial losses these farmers suffer from this bacteria.

Statement of Research Advisor

Evelyn has done an excellent job at organizing collection events, getting samples from a remote location, and processed them in the lab. Her work is the first one to prove that the presence of *Aeromonas* in commercial catfish ponds is surprisingly high in all samples tested and that sediments and fouling of equipment favors the persistence of this pathogen in the farm environment. Her work will set the basis for further studies aimed at improving farm management strategies to reduce disease impact in aquaculture.
– Covadonga Arias, School of Fisheries, Aquaculture and Aquatic Sciences

Uncertainty Calculations for Theoretical Atomic Data Toward the Applications of Astrophysical Spectroscopy

Zechun "Ken" Yang, Stuart Loch, and Hans-Werner van Wyk

Most of our knowledge about our universe comes from observing the photons (light) that the atoms in astrophysical objects emit. Using theoretical models, such observations can return a wealth of information on temperatures, densities, velocities, and plasma composition. However, there is usually not any estimate of the uncertainty on the theoretical calculations, and as a consequence we often do not have a meaningful range of values for the diagnosed parameters. In this work, we develop methods to assign uncertainties to atomic data and carry such uncertainties through to diagnosed plasma parameters.

The difficulty in assigning uncertainties to theoretical atomic data lies in the complexity of the Schrödinger equation. This second order partial differential equation,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{r},t) + V_0(\boldsymbol{r},t)\Psi(\boldsymbol{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t),$$

where $-\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator and $V_0(\boldsymbol{r},t)$ is the potential energy, is challenging to solve and does not propagate uncertainties on the wavefunctions linearly. The solution may be very sensitive to the initial conditions.

In this project Helium like oxygen (O^{6+}) was considered. This two electron system is an important temperature diagnostic in X-ray emitting plasmas. The atomic data for O^{6+} was calculated (excitation, ionization, and recombination), and uncertainties were assigned to the data. A Monte-Carlo method, with randomized input values within our uncertainty range, was used to compute the diagnostic line ratios. One million Monte-Carlo iterations were sufficient to cover the parameter space, and standard statistical methods were employed to analyze the data. A spectral line ratio as a function of plasma electron temperature was generated along with an uncertainty estimate on the line ratio. This will allow astrophysicists to assign a meaningful temperature range to their plasmas.

The project led to a new avenue for study, to look at correlation effects in the atomic data. Small changes were made to the orbital wavefunctions that were used in the atomic structure code,[1] and the effects were carried through to spontaneous emission and electron-impact excitation rate coefficients. A case study on a controversial line ratio of Fe^{16+} was also investigated, and it was found that a counter-correlation (see Figure 1) may be help to explain much of the discrepancies in the literature.[2]
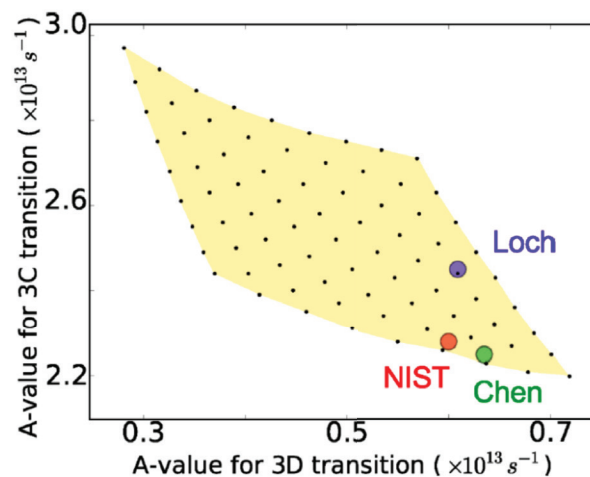
Figure 1. A-values for the 3C and 3D transitions for Fe^{16+}. The negative slope shows the counter-correlation in the values.

Statement of Research Advisor

I guided the overall project direction and taught Mr. Yang how to run the large computer codes, with the exception for the ionization balance codes which Mr. Yang wrote by himself.
– Stuart Loch, Physics

References

[1] Badnell et al., Astronomy and Astrophysics, **406**, 1151 (2003)

[2] S. Bernitt et al., Nature, **492**, 7428 (2012)

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