

**2009**  
*Summer Undergraduate  
Research  
Symposium*

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Biology : Thurs., July 23  
Mathematics : Fri., July 24  
Mats. Sci. & Chemistry: Thurs. and Fri, July 30 and 31

On the campus of James Madison University  
Harrisonburg, VA

Supported by  
the National Science Foundation REU Program  
&  
the U.S. Department of Defense ASSURE Program



## Colleges and Universities From Which REU Students Have Come to JMU Since 2001

- Allegheny College
- Benedictine College
- Bethany College
- Bethel College
- Blue Ridge Community College
- Bridgewater College
- Boston College
- California State—Long Beach
- Central State University
- College of William and Mary
- Clemson University
- Davidson College
- Drake University
- Eastern Mennonite University
- East Tennessee State University
- Edgewood College
- Elizabeth City State University
- Elon University
- Fairfield University
- Florida Atlantic University
- Framingham State University
- Gallaudet University
- Grove City College
- Hampden-Sydney College
- Harvey Mudd College
- High Point University
- Hood College
- Illinois Wesleyan University
- Ithaca College
- James Madison University
- Longwood College
- Lynchburg College
- Mary Baldwin College
- Merrimack College
- Miami University
- Millersville University
- Mississippi State University
- Montana Tech
- Mount Holyoke College
- Mount Union College
- Niagara University
- Norfolk State University
- Northern Virginia Community College
- Paul Quinn College
- Piedmont Virginia Community College
- Pomona College
- Pontifical Catholic University of Puerto Rico
- Princeton University
- Providence College
- Queen's University, Belfast
- Radford University
- Randolph College
- Rochester Institute of Technology
- Rutgers University
- St. John Fisher College
- Saint Joseph's College
- St. Olaf College
- Southern Illinois University
- Stevenson University
- Sweet Briar College
- SUNY-New Paltz
- Technical University of Denmark
- Towson University
- University College, Galway
- University of Alabama
- University of Belgrade
- University of Dayton
- University of Evansville
- University of Mary Washington
- University of Maryland, Baltimore Co.
- University of Maryland, College Park
- University of Missouri—Rolla
- University of North Carolina—Asheville
- University of North Carolina—Wilmington
- University of Rochester
- University of San Diego
- University of Virginia
- Villanova University
- Virginia Union University
- Washington & Lee University
- Wheaton College
- Western Carolina University
- Willamette University
- Winona State University

*Note : Throughout this program, the underlined names are those of the presenting authors. The names with stars beside them are the faculty mentors.*

**Breakfast Meeting**  
**Thursday, July 23**  
**8:30 - 9:30 AM**  
**Burruss Hall 238**

Mandatory for all Biology NSF REU students (discussion to include information on how to be reimbursed for travel and other final program details)

**Biology – Poster Session I**  
**Thursday, July 23**  
**9:45 AM – 10:45 AM**  
**Burruss Hall, Second Floor**

1-A. **The Hunt for Cytotoxic Genes in Mycobacteriophage Maury.**

Chelsea L. White, Nishal C. Patel, \*Steven Cresawn

Dept. of Biology, James Madison University

Bacteriophages are viruses that infect bacteria. Mycobacteriophages specifically infect mycobacteria, such as the bacteria responsible for causing Tuberculosis, Leprosy, and Buruli Ulcer. A new mycobacteriophage, Maury, was discovered in Harrisonburg during the summer of 2008 and we have subsequently sequenced its genome. Many bacteriophages have multiple genes that encode cytotoxic proteins. Therefore, it is likely that Maury also encodes various proteins that are cytotoxic to its host. The host used for lab studies is a fast growing soil bacterium known as *Mycobacterium smegmatis*, strain mc<sup>2</sup>155. Methods have included isolating pure samples of phage by lysate harvest, purifying Maury DNA, using PCR to amplify the predicted Maury lysin and holin genes as positive controls for cytotoxicity, and testing colonies of *M. smegmatis* that could possibly be Maury lysogens. Many rounds of DNA agarose gel electrophoresis have also been used to analyze the Maury DNA samples and PCR products. The future goal is to shear the genome (which is 75.6 Kb in length) into pieces that are between one and three kilobases in length and then clone those pieces into a plasmid vector. Methods will include nebulization, electroporation, and possibly sonication if necessary. Any genes found to be cytotoxic in *M. smegmatis* will be tested in *Mycobacterium ulcerans*, the causative agent of Buruli Ulcer.

Funding sources: NSF REU Grant # 0649045, Department of Biology

1-B. **Analyzing the Effect of Stage Specific RhoA Depletion during the *Drosophila* Life Cycle.**

Maureen Filak and \*Susan R. Halsell

Dept. of Biology, James Madison University

Human birth defects often arise from morphogenetic mistakes. Morphogenesis is comprised of organized cellular processes that determine an organism's structure. Since morphogenetic errors lead severe consequences, understanding these cellular morphogenetic mechanisms requires *in vivo* analysis. The RhoA signal transduction pathway critically induces changes in morphogenetic cell shape change; therefore we investigate RhoA function using the *Drosophila* model. Complete loss of function *RhoA* mutations are embryonic lethal, resulting in dorsal anterior holes in the cuticle. To better understand the morphogenetic defect causing this embryonic lethality, time-lapse confocal microscopy of wild type embryos bearing a GFP-moesin fusion protein are underway. These studies focus on the embryonic process of head involution. Subsequently, confocal analysis will be performed on *RhoA* mutant embryos. In order to study post-embryonic RhoA requirements, experimental depletion of RhoA will utilize a heat inducible wild type *RhoA* transgene introduced into the genome. Seven individual transgenic lines have been established. Segregation analysis is underway to finalize the location of the final three insertions. Currently, a *RhoA*<sup>+</sup> transgene insertion located on the X-chromosome is being crossed into *RhoA* mutant strains; this is the final step in building the stocks for use in the depletion studies. These studies complement RhoA analyses in vertebrates.

Funding sources: NSF REU Grant # 0649045,

1-C. **Expression and Purification of Three *Arabidopsis*  $\beta$ -amylase (BAM) Proteins in *E. Coli*.**

Kevin Fedkenheuer and \*Jon Monroe

Dept. of Biology, James Madison University

In *Arabidopsis* and other plants,  $\beta$ -amylase proteins are involved in starch degradation. During the day, starch accumulates in chloroplasts by photosynthesis, and it is degraded in the absence of light to provide energy for cell respiration. To better understand the function of BAMs in starch degradation, BAMs 3, 8, and 9 were expressed in *E. coli*, strain BL21, and purified using metal-affinity chromatography. The catalytic domain of BAM 8 was expressed and purified as well. The function of these BAMs will be assessed by various biochemical assays. The techniques used in this process were aimed at optimizing expression, keeping expressed protein soluble, and maintaining protein functionality. Growing conditions and concentrations of IPTG were manipulated to optimize soluble protein yield. Since the functions of  $\beta$ -amylases 8 and 9 are unknown, the activity of catalytically active  $\beta$ -amylase 3 was measured in a starch assay to find conditions that optimize protein functionality. Purification of these proteins will help us further understand starch degradation in plants. We have shown that BAMs 8 and 9 lack catalytic activities against starch, and this information allows for new hypotheses as to what role the proteins play in the process of starch degradation.

1-D. **Anti-oxidants and stress responses in *Arabidopsis*.**

Jie Ren<sup>1</sup> and \*Steve Cessna<sup>2</sup>

<sup>1</sup>Dept. of Biology, J. Sargeant Reynolds Community College, <sup>2</sup>Dept. of Biology, Eastern Mennonite University

Plants synthesize hormone abscisic acid (ABA) to induce closing of stomatal pores to limit the water loss under drought condition. Guard cells, which modulate stomatal aperture, are located surrounding stomatal pores. ABA-induced stomatal closure is mediated by H<sub>2</sub>O<sub>2</sub>, which has been identified as one of key components of the complex guard cell signaling network. Ced-9 plants are stably transformed with a gene from the worm *C. elegans* which regulates programmed cell death (apoptosis). However, Ced-9 transformed plants appear to be more susceptible to drought. Both mitochondria and chloroplasts are sites of H<sub>2</sub>O<sub>2</sub> production, and thus, Ced-9 expression might alter H<sub>2</sub>O<sub>2</sub>, and thereby reduce stomata sensitivity to ABA, and thereby alter drought response. To better understand the relationship among guard cell responsiveness, Ced-9 plants, as well as ABA and H<sub>2</sub>O<sub>2</sub> signaling, the stomatal apertures of tobacco wild type (WAQ) and transformed Ced 9 were measured. Fluorescence microscopy indicated that Ced-9 plants do indeed produce less H<sub>2</sub>O<sub>2</sub> in response to ABA treatment, and here we show that their stomata do not close to the same degree in response to ABA. In contrast, they close equally as well in response to direct H<sub>2</sub>O<sub>2</sub> treatment, implying that the Ced-9 protein reduces H<sub>2</sub>O<sub>2</sub> and thereby reduces stomatal sensitivity to ABA.

Funding sources: NSF REU Grant, USDA #2007-35100-18267

1-E. **The Role of Repeat Sequences in Regulation of the Polyhydroxybutyrate Depolymerase Gene of *Streptomyces sp. 5A*.**

Shivani M. Dudhia<sup>1</sup>, Nicole M. Hannum<sup>2</sup>, and \*Stephen F. Baron<sup>3</sup>

<sup>1</sup>Dept. of Biology, Allegheny College, <sup>2</sup>Dept. of Biology, Niagara University, <sup>3</sup>Dept. of Biology, Bridgewater College

Polyhydroxybutyrate (PHB) is a biodegradable, plastic-like polymer produced by bacteria. The actinomycete, *Streptomyces sp. 5A*, degrades PHB, using an extracellular PHB depolymerase. Enzyme synthesis is induced by growth on PHB but repressed by glucose, suggesting transcriptional regulation of its corresponding gene (*phaZ*).

The promoter region of *phaZ* contains direct and inverted repeats which may be binding sites for transcriptional regulators. To study the function of these repeats in *phaZ* regulation, directed mutations were introduced into these sequences using a PCR procedure, which retained the putative *phaZ* promoter sequence. The PCR constructs were introduced upstream from the promoterless *xylE* reporter gene of plasmid pJJ4083. To determine the effects of the mutations on *phaZ* regulation, the resulting recombinant plasmids will be introduced into *Streptomyces sp. 5A* cells by protoplast transformation, and *xylE* expression observed in cells grown with PHB and/or glucose.

Due to poor reproducibility of the protoplast transformation method, we studied the effects of various conditions on transformation efficiency. Optimal results were obtained with early stationary phase cells grown in tryptic soy broth containing 0.5% glycine. The moisture content of the protoplast regeneration plating medium is also known to affect transformation efficiency in other *Streptomyces* species, and is currently being investigated.

Funding sources: NSF REU Grant # 0649045; Grant #J-713 from the Thomas F. and Kate Miller Jeffress Memorial Trust.

1-F. **Examination of largest coding regions in *Bordetella avium* holds bright future for research in Bordetellosis.**

Tiffany Cummings<sup>1</sup>, \* Dr. Louise Temple<sup>2</sup>

<sup>1</sup>Dept. of Biology, Central State University, <sup>2</sup>Dept. of Biology, James Madison University

*Bordetella avium* is a pathogenic bacterium that causes turkey coryza (Bordetellosis) by adhering to the tracheal cells of turkeys. Symptoms of this disease are as follows: coughing, tracheal lesions, and nasal discharge. Prior to my work in this project, the entire *B. avium* chromosome was sequenced and the genes were identified. The two largest coding regions of the chromosome are BAV 1944 and BAV 1945. This region is flanked by a type I secretion system. This coding region is believed to be of major importance to the virulence of this chromosome due to the fact that, the proteins coded for by BAV 1944 and BAV 1945 are possibly secreted out of the cell making it likely that their presence is necessary for the bacterium's adherence. The antigenic regions of BAV 1945 were cloned and purified. Such processes involved locating the antigenic region using bioinformatic analysis, expressing a peptide containing the antigenic region, and splicing by overlap extension PCR. We have yet to clone and purify the antigenic regions of BAV 1944. By performing the above processes should be able to eventually explain how the presences of BAV 1944 and BAV 1945 affect the virulence in *Bordetella avium*. Antibodies against these purified products will be produced and used in future research in hopes of making an effective vaccine against bordetellosis in turkeys, and could also be helpful in making vaccines in for *Bordetella pertussis* also known as whooping cough in humans.

1-G. **The Effects and Localization Patterns of LET-60 and ICD-1 in Developmental Apoptosis in *C. (Caenorhabditis) elegans*.**

Michele Fiori, Rachel Comer, Tim Bloss

James Madison University

Apoptosis is a regulated process of cell death necessary for survival, and many human diseases are associated its misregulation. Because apoptosis is highly conserved, knowledge gained through its study in the genetic model *C. elegans* can be applied to human apoptosis, ideally to develop diagnostics and treatments for apoptotic-related diseases. We study apoptosis in *C. elegans* to quantify and characterize the putative effect of the Ras homologue LET-60 on apoptotic control. We counted apoptotic events during development in *let-60* loss of function (*lf*) mutants versus wild type embryos and found a 30% increase in apoptosis in the *let-60* mutants (8.8 +/- 2.0 vs. 5.6 +/- 2.2 respectively), indicating that LET-60 represses apoptosis. To characterize this putative role of LET-60 repressing apoptosis, we are determining the localization of LET-60 in wild-type and mutant embryos in the presence and absence of a known apoptotic inhibitor ICD-1 (inhibitor of cell death). Because previous studies indicate that ICD-1 and LET-60 physically associate, our hypothesis is that ICD-1 inhibits apoptosis through control of LET-60 localization, and that mislocalization of LET-60 results in an increase in apoptosis. Preliminary results show an increase in apoptosis in *let-60 (lf)* mutants, but no noticeable change in localization. We are currently determining if the increase in apoptosis observed with the removal of ICD-1 correlates with a change in LET-60 localization. Ultimately, we want to characterize the putative role for LET-60 in control of apoptosis in hopes that this will provide insights into a role for Ras in control of human apoptosis.

Funding sources: NSF REU Grant # 0649045

**Biology – Keynote Address**

**11:00 AM – 12:00 PM**

**Burruss Hall 238**

**Themis Is a Member of a New Metazoan Gene Family  
and is Required for Thymocyte Development**

Dr. Andy Johnson

NIH / Oxford Biomedical Research Scholar

**Biology – Lunch  
Thursday, July 23  
12:15 PM – 1:15 PM  
Circle in front of Burruss Hall**

**Biology – Poster Session II  
Thursday, July 23  
1:30 – 2:30 PM  
Burruss Hall, Second Floor**

**2-A. Potential dimerization of BAM8 in the presence of maltose or DTT.**

Katie Weihbrecht<sup>1</sup>, Kevin Fedkenheuer<sup>2</sup>, \*Jonathan Monroe<sup>2</sup>

<sup>1</sup>Dept. of Biology, University of Evansville, <sup>2</sup>Dept. of Biology, James Madison University

In *Arabidopsis thaliana*, nine putative  $\beta$ -amylase (BAM) genes have been identified. While BAM enzymes are known for their role in the degradation of starch in the chloroplast, surprisingly, BAM8 is localized to the nucleus. BAM8 contains sequence coding for a DNA-binding basic helix-loop-helix (bHLH) motif and is known to act as a transcription factor. Many transcription factors (TF) are known to function as dimers, including the bHLH TF family, thus BAM8 may function as a dimer. The presence or absence of specific substrates and/or redox reagents often cause the TF to dimerize, creating a sequence of events that leads to changes in gene expression. Whether or not BAM8 dimerizes and under which conditions it dimerizes is not yet known. Starch is synthesized in chloroplasts during the day and is broken down into maltose at night, resulting in high maltose levels at night and low maltose levels during the day. Moreover, plant cells use sunlight to create reducing conditions during the day. In this study, we used gel filtration chromatography for size determination to determine whether or not BAM8 dimerizes in the presence of maltose or reducing agents. Early findings indicate that BAM8 dimerizes in the presence of maltose.

**2-B. Cloning of the Upstream Region of the Polyhydroxybutyrate Depolymerase Gene of *Streptomyces* sp. 5A.**

Nicole Hannum<sup>1</sup>, Shivani Dudhia<sup>2</sup>, and \*Stephen F. Baron<sup>3</sup>

<sup>1</sup>Dept. of Biology, Niagara University, <sup>2</sup>Dept. of Biology, Allegheny College, <sup>3</sup>Dept. of Biology, Bridgewater College

Polyhydroxybutyrate (PHB) is a biodegradable, plastic-like polymer produced by soil bacteria. The actinomycete, *Streptomyces* sp. 5A, degrades PHB, using an extracellular PHB depolymerase. Synthesis of the enzyme is induced by growth on PHB but repressed by glucose, suggesting transcriptional regulation of its associated gene (*phaZ*). The promoter region of *phaZ* contains direct and inverted repeats which may be binding sites for transcriptional regulators of *phaZ*. We hypothesized that genes for such regulators may be located just upstream from the promoter region.

In order to locate potential regulatory genes upstream from *phaZ*, we used three PCR-based gene walking techniques with *phaZ*-specific primers. These included single specific primer PCR (SSP-PCR), ligation anchored PCR, and inverse PCR. Selected PCR products (inserts) were ligated together with plasmid vectors and introduced into *Escherichia coli* by transformation. Plasmid DNA from selected clones was extracted and the inserts sequenced. The insert sequence from one SSP-PCR clone showed significant homology to two-component system response regulators; however no overlap with known sequence from the *phaZ* promoter region was found, suggesting that the insert had resulted from non-specific priming in the PCR. We are currently optimizing PCR conditions to improve specificity, using different primer pairs, denaturation temperatures, and annealing temperatures.

Funding sources: NSF REU Grant # 0649045; Grant #J-713 from the Thomas F. and Kate Miller Jeffress Memorial Trust.

**2-C. The Role of Interleukin 3 (IL-3) in the Immune Response of BALB/c Mice to Cutaneous Leishmaniasis.**

Leonid Zlotcavitch<sup>1</sup>, \*Dr Kenneth Roth<sup>2</sup>, Chris Lantz<sup>2</sup>, Bryan Saunders<sup>2</sup>,

<sup>1</sup>Dept. of Biology, Harriet Wilkes Honors College, Florida Atlantic University, <sup>2</sup>Dept. of Biology, James Madison University

Cutaneous leishmaniasis is an infection caused by the protozoan parasite of the genus *Leishmania*. The disease currently affects 10 million people in 82 countries around the world. *L. major*, one of the two species that causes the disease, is transmitted to humans and mammals when they are bitten by infected sandflies. The clinical course of the disease involves the development of lesions that heal and resolve without intervention after months to years, often leaving permanent scarring. Moreover, bacterial infections are common with cutaneous leishmaniasis. A genetic predisposition for susceptibility or resistance to *L. major* infection in mice correlates with the dominance of a T-Helper 2 response that is not protective, and a T-Helper 1 response that promotes healing and resistance. We hypothesize that IL-3 driven cellular response contributes to the establishment of an unproductive immune response against *L. major* in susceptible BALB/c mice. In this research we were trying to assess the role of IL-3 in the immune response to the infection and to what degree *L. major* infection elevates IL-3 production in BALB/c mice.

Funding source: NSF REU Grant #0649045

**2-D. Involvement of the Raphe Pallidus in Cardiovascular Responses to Stress**

Ashley Wright<sup>1</sup>, Nhut Le<sup>2</sup>, and \*Justin W. Brown<sup>2</sup>

<sup>1</sup>Dept. of Biology, Bridgewater College, <sup>2</sup>Dept. of Biology, James Madison University

The brainstem mediates cardiovascular responses to stress by influencing the autonomic nervous system. The precise mechanism by which this occurs is still uncertain. The raphe pallidus (RaPa), a brainstem locale rich in serotonin, likely influences the cardiovascular responses to stress by modification of heart rate (HR) and blood pressure (BP). By altering neurotransmission in the RaPa, this project investigated its role in the cardiovascular responses to stress. Five male Sprague-Dawley rats were instrumented with radiotelemetry probes that measured HR and BP. Each rat was also instrumented with an indwelling brain cannula to permit microinjection of 300nL of ACSF (control), lidocaine (inhibition of neuron firing), muscimol (GABA agonist), or 8-OH-DPAT (serotonin 1A receptor agonist) at the RaPa. Immediately after microinjection, the rats were stressed either by startle or handling. Early results show a partially attenuated heart rate response following microinjection with lidocaine (+69 bpm N=1 vs +82 bpm (control) N=4), muscimol (+14 bpm N=2), or 8-OH-DPAT (+15 bpm N=1). BP responses to stress with ACSF, lidocaine, and 8-OH-DPAT injection were relatively consistent, muscimol was not. These data suggest that serotonin 1A receptors in the RaPa may be involved in regulation of HR responses to stress. Such information could improve understanding of the etiology of SIDS and facilitate development of preventative treatments. Funding sources: NSF REU Grant # 0649045

2-E. **Anti-oxidants and stress responses in Arabidopsis.**

Andrew Kirk and \*Steve Cessna

Dept. of Biology, Eastern Mennonite University

Recognition of nutritional value in antioxidants has caused quite a stir in the media and popular culture in recent years. As consumers seek to increase their intake of antioxidants, food producers look to science for methods to increase antioxidant their products antioxidant yields. This study evaluates the mechanisms of antioxidant production in plants and examines several potential agricultural practices aimed at increasing the nutritional value of food sold to consumers. Literature suggests that three simple approaches (application of external fatty acids, day time vs. night time harvesting, and temperature stress) could have potential to increase antioxidant harvest. Unfortunately, these methods demonstrated little effect when tested in the lab setting.

2-F. **Co-Culture in Rabbit Cornea Stromal Cell Protein Expression.**

Tina Safavie and \*Marta Bechtel

Dept. of Biology, James Madison University

The cornea is made up of three cell layers: the endothelial, epithelial, and stromal layer, with the stromal layer comprising ~90% of the cornea tissue and containing keratocytes. If the cornea is wounded or grown in-vitro, the keratocytes differentiate into the repair fibroblast phenotype and up-regulate  $\alpha$ -smooth muscle actin ( $\alpha$ -SMA) expression. The purpose of this study was to grow endothelial cells in co-culture with fibroblasts to investigate the effect of co-culture on the fibroblast wound healing phenotype and expression of  $\alpha$ -SMA. Stromal fibroblasts (FB) and endothelial cells (EN) were isolated from whole rabbit corneas. FBs were seeded in twenty-four well plates on glass cover slips. EN cells were seeded on trans-well inserts containing 3  $\mu$ m semi-permeable membrane (50 cells/mm<sup>2</sup>). Co-culture samples were fed with 1/2 EN and 1/2 FB media (SMEM) with 2% FBS. Control FBs in monoculture were fed SMEM, SM with 2% FBS and SM with 10% FBS. Our preliminary results indicate in vitro culture of FB cornea cells in the presence of FBS increase expression of a-SMA expression, with a greater increase of a-SMA levels seen with 10% FBS. Co-culture of FB with EN cells results in a decrease in a-SMA expression. Future studies will include further quantification of  $\alpha$ -SMA expression in FB through Western-Blot Analysis

**Biology – Ice Cream Cake Finale**

**Thursday, July 23**

**2:30 PM – 3:00 PM**

**Burruss 238**

Mathematics – Oral Presentations

Friday, July 24

11:00 AM – 1:30 PM

Roop 103

**11:00 What Moves You: Using Legs for Vehicular Transportation.**

Jonathan Graf<sup>1</sup>, Olga Stolov<sup>2</sup>, and \*Jim Sochacki<sup>3</sup>

<sup>1</sup>Towson University, <sup>2</sup>SUNY New Paltz, <sup>3</sup>James Madison University

Most vehicles are transported by the rotation of wheels. The Department of Mathematics and Statistics and Department of Engineering are interested in developing vehicles that will be driven by the motion of legs rather than wheels. In this talk we discuss the motion of five different legs: first, we derive the equations of motion for each leg; second, we calculate the equations for velocity, acceleration, energy and power; third, we optimize the motion by minimizing energies and forces. In order to obtain these results, we developed a differential equation, solved it using the Parker-Sochacki Method and reached the optimal solution using Maple's minimization package.

**11:30 Diversions: Sudoku, Shidoku, and ... Grobner Bases? An Algebraic & Computer Systems Approach to Counting Boards.**

Katharina Carella<sup>1</sup>, Matt Menickelly<sup>2</sup>, \*Beth Arnold<sup>3</sup>

<sup>1</sup>Ithaca College, <sup>2</sup>Miami University, <sup>3</sup>James Madison University

We investigate various counting proofs for Shidoku boards and related variants, such as the number of possible solution boards from incomplete puzzles. We also look into the algebraic group derived from symmetries of Shidoku boards. We use these group isomorphisms to classify all possible numbers of solutions from incomplete puzzles. We use Grobner Basis representations of Shidoku and Sudoku to obtain these results. We provide a complete classification of all the possible number of solutions that can result from incomplete Shidoku puzzles.

**12:00 Bayesian Approach to Estimating Binomial Parameters.**

Dallas Joder, Christina Ludlow, and \*Ling Xu

James Madison University

Accurately estimating proportions can be difficult. Frequentist confidence interval methods frequently suffer from volatile coverage. This problem can occur in Bayesian credible intervals, but there is a lack of information on the effects of various informative and noninformative priors. We compare the performances for multiple Bayesian priors for one binomial proportion and the difference of two proportions using randomized simulations. We make a series of recommendations of preferred priors for different situations.

**12:30 Improved One-Sample Confidence Interval and Multiple Comparisons of Binomial Proportions.**

Kristin Haldeman<sup>1</sup>, Christopher Tait<sup>2</sup>, and \*Kane Nashimoto<sup>3</sup>

<sup>1</sup>Cal State–Long Beach, <sup>2</sup>Hampden-Sydney College, <sup>3</sup>James Madison University

We study confidence intervals and tests of hypotheses involving binomial proportions. In the first part of the study, we examine one-sample confidence intervals. The commonly used Wald interval suffers severe undercoverage. The Score interval performs more favorably. The Agresti and Coull interval (1998), which uses the "add 2 method", shows overcoverage. We propose a modification of Agresti and Coull that has more uniform coverage probabilities over a wide range of true proportions. In the second part of the study, we consider comparisons of  $k$ -independent proportions. In this context, Agresti et al. (2008) show that pairwise comparisons using the Studentized range distribution work better than the comparisons using the Wald or Score methods with Bonferroni adjustments. We propose a new 2-stage method of multiple comparisons (global test followed by pairwise comparisons). Simulation results show that our method is more powerful than most of the existing methods and that it keeps the familywise error rate near the nominal level.

**1:00 Distance Functions and Attribute Weighting in a k-Nearest Neighbors Classifier with an Ecological Application.**

Alyssa Frazee<sup>1</sup>, Matthew Hathcock<sup>2</sup>, and \*Sam Prins<sup>3</sup>

<sup>1</sup>St. Olaf College, <sup>2</sup>Winona State University, <sup>3</sup>James Madison University

To assess environmental health of a stream, field, or other ecological "object," characteristics of that object should be compared to a set of reference objects known to be healthy. Using streams as "objects," we propose a k-nearest neighbors algorithm (Bates Prins and Smith, 2006) to find the appropriate set of reference streams to use as a comparison set for any given test stream. Previously, investigations of the k-nearest neighbors algorithm have utilized a variety of distance functions, the best of which has been the Interpolated Value Difference Metric (IVDM), proposed by Wilson and Martinez (1997). We propose two alternatives to the IVDM: Wilson and Martinez's Windowed Value Difference Metric (WVDM) and the Density-Based Value Difference Metric (DBVDM), developed by Wojna (2005). We extend the WVDM and DBVDM to handle continuous response variables and compare these distance measures to the IVDM within the ecological k-nearest neighbors context. Additionally, we compared two existing attribute weighting schemes (Wojna 2005) when applied to the IVDM, WVDM, and DBVDM, and we propose a new attribute weighting method for use with these distance functions as well. In assessing environmental impairment, the WVDM and DBVDM were slight improvements over the IVDM. Attribute weighting also increased the effectiveness of the k-nearest neighbors algorithm in this ecological setting.

## Chem/Mats - Session I - Oral Presentations

Thursday, July 30

9:30 AM - 10:30 AM

ISAT/CS 159

Dr. Brian Utter, Presiding

## 9:30 Dehydrogenation of 2-propanol and zinc based compounds.

Brandy Schell<sup>1</sup> and \*Thomas C. DeVore<sup>2</sup><sup>1</sup>Bridgewater College, <sup>2</sup>James Madison University

Fuel cells and hydrogen fueled vehicles need a convenient source of hydrogen to be commercially viable. One possible source of hydrogen is from the catalytic oxidation of alcohols. This reaction can follow two possible pathways: oxidative dehydrogenation to produce hydrogen and a carbonyl and dehydration to produce the alkene. The reactions of 2-propanol using several zinc catalysts were investigated under vacuum at temperatures between 180°C and 400°C. The oxidation of 2-propanol over zinc borate, zinc oxide, and zinc sulfide follows the oxidative pathway to produce hydrogen and acetone with over 95% efficiency. The kinetics of this process was investigated using isothermal flow kinetics. The amount of conversion was found to depend on the temperature and the initial flow rate of the 2-propanol. The reaction followed the Langmuir mechanism over all catalysts tested. The apparent activation energy was approximately 70 kJ/mol for all catalysts.

9:45 Cloning and expression of 5-enolpyruvylshikimate-3-phosphate synthase from *Thermus thermophilus* HB27 and *Colwellia psycherythaea* 34H.Jaleal Sanjak, Robert East, Tiffany Shellie, and \*Victoria Mariani

James Madison University

The *aroA* gene encodes for the expression of 5-Enolpyruvylshikimate-3-phosphate (EPSP) synthase which catalyzes the reversible reaction forming EPSP from shikimate-3-phosphate (S3P) and phosphoenolpyruvate (PEP) in the sixth step of the shikimate pathway. The shikimate pathway, which links the metabolism of carbohydrates to aromatic amino acid biosynthesis, is found in plants, fungi, and bacteria. Because of this aforementioned exclusivity, EPSP synthase is a promising target for antibiotic, antiparasitic, and herbicide development. Through structural characterization of thermophilic, mesophilic, and psychrophilic EPSP synthases, we also hope to elucidate which particular moieties outside of the active site are pivotal to function. Here we report successful amplification of the *aroA* gene from cDNA libraries of *Thermus thermophilus*, *Colwellia psycherythaea* and *Escherichia coli* via a high fidelity polymerase chain reaction. Restriction enzyme digestion of *aroA* as well as the expression vectors pET-31b and pET19b are being attempted so as to enable a subsequential ligation of the *aroA* gene into the vectors. Upon successful ligation, the recombinant plasmids will be transformed into *E. coli* JM109 strain which will amplify the recombinant plasmid so that it may be extracted and sequenced. The clone will then be transformed into *E. coli* BL21 pLysS strain which will express the EPSP synthase. All actions proceed towards the ultimate goal of performing structural and kinetic analysis on the various EPSP synthases.

10:00 Characterization of the *Escherichia coli* RecA Protein Utilizing Various Techniques.Brittany Danzig

James Madison University

The *Escherichia coli* protein RecA repairs DNA by homologous recombination. RecA cleaves the protein LexA and catalyzes the exchange of single stranded DNA with complementary regions of double stranded DNA. The process of strand exchange is coupled to the hydrolysis of ATP. Previous experiments in our lab have studied the thermally induced unfolding of RecA in different salts. High salt concentrations are known to activate RecA ATP hydrolysis in the absence of DNA. The current studies followed RecA unfolding in the presence of single stranded DNA and a variety of salts. Additional fluorescence experiments were conducted to study the binding of a fluorescent nucleotide analogue to RecA in the same salt solutions that were utilized in the previous CD studies. CD studies showed that the presence of single stranded DNA did not significantly influence the melting temperature of RecA. Fluorescence experiments showed that the nucleotide binding was temperature and salt dependent.

## 10:15 Characterization of a Planar Granular Shear Flow

Richard Knoche and \*Brian Utter

James Madison University

We present results on a 2D photoelastic shearing experiment consisting of photoelastic grains between two belts moving opposite each other, such that the central region approximates planar shear. The granular medium lies horizontally between the belts such that the packing density is unaffected by gravity and can be controlled independently. We measure properties of the flow with particle tracking techniques to characterize velocity fields, vorticities, and plastic rearrangements. We find that, unlike solids or liquids, there are significant elastic, plastic, and correlated motions controlled by local shear rate.

## Chem/Mats - Session II - Oral Presentations

Thursday, July 30

11:00 AM - 12:00 PM

ISAT/CS 159

Dr. Gina MacDonald, Presiding

## 11:00 Device Fabrication and Torsional Characterization of Carbon Nanotubes.

Jake Carey<sup>1</sup>, Lok-kun Tsui<sup>1</sup>, Joe Hardcastle<sup>1</sup>, Chris Flint<sup>1</sup>, Smai Fullerton<sup>2</sup><sup>1</sup>James Madison University, <sup>2</sup>American University

Carbon nanotubes have some very interesting properties which we are studying by constructing unique electro-mechanical devices that allow us to work with these atomic-scale structures. Fabrication of these devices utilizes atomic force microscopy (AFM) and electron beam lithography (EBL) to design patterns and place paddles specific to each sample to measure the torsional properties of an individual CNT. Once a device has finished EBL, hydrofluoric and phosphoric acid etches are done to make the CNT free-standing. Critical point drying (CPD) is necessary to dry the sample off after the phosphoric etch due to the forces that occur during phase transitions. Using transmission electron micros-

copy (TEM) at UNC this summer, we proved our devices could withstand the rigorous fabrication process. We hope to begin torsional testing of the free-standing shortly after the summer.

**11:15 The design and development of a flow loop for the qualitative and quantitative characterization of vortex ring formation past prosthetic heart valves.**

Ann Bailey<sup>1</sup>, Michelle Beatty<sup>2</sup>, and \*Olga Pierrakos<sup>2</sup>

<sup>1</sup>University of Virginia, <sup>2</sup>James Madison University

Every year approximately 200,000 human heart valves are replaced worldwide. Although prosthetic heart valves are widely accepted, their performance is far from ideal, especially when compared to natural and healthy heart valves. There is a need to develop more accurate methods of characterizing the performance and efficiency of prosthetic heart valves. Currently, though, heart valves are evaluated based on trans-valvular pressure characteristics and left ventricular ejection fraction. These current assessment methods overlook the complex flow field downstream of these valves and inside the left ventricle which if understood can provide valuable insight on valvular and cardiac performance. Thus, our research focuses on flow characterization past heart valves. Namely, we are interested in characterizing vortex ring formation, resulting from the roll-up of the shear layers shedding past heart valves. The ultimate goals of this project were to (1) design a flow loop to enable the visualization of vortex ring formation past various mechanical and biological prosthetic heart valves, and (2) to use a computational fluid dynamics software to quantify vortex ring formation past prosthetic heart valves. In the future, this data could be used to compare with data acquired from clinical imaging techniques (Echo Ultrasound and MRI) in patients with healthy, diseased, and replaced heart valves. Furthermore, this data could be used to determine the effectiveness of new heart valve designs.

**11:30 Yeast estrogen screen for endocrine disruptors along the Shenandoah River.**

Nicole Mueller<sup>1</sup>, \*Peter Ruiz-Haas<sup>2</sup>, and \*Tammy Stone<sup>1</sup>

<sup>1</sup>Spotswood High School, <sup>2</sup>Mary Baldwin College

The Yeast Estrogen Screening (Y.E.S.) was used to determine the presence of endocrine disrupting chemicals (EDCs) along the Shenandoah River and its tributaries. The goal is to establish whether EDCs are a contributing factor to the fish kills and the intersex fish. Testing along streams and waste water effluents were done to see whether there is an impact from agriculture and/or human waste products. The Y.E.S. Bioassay involved using genetically modified yeast cells (*Saccharomyces cerevisiae*) that had the human estrogen receptor (hER) incorporated. When exposed to EDCs, the cells produce  $\beta$ -galactosidase. The amount of EDCs in the sample is proportional to the amount of  $\beta$ -galactosidase secreted and thus is a measure of the potency or quantity of endocrine disrupting chemicals. The amount of  $\beta$ -galactosidase is measured by a reaction with ortho-Nitrophenyl- $\beta$ -galactoside (ONPG) that produces a yellow compound. The endpoint optical density was measured to see the variation of the yellow color. The hER reference for this experiment was 17 $\beta$ -estradiol (E2), the most potent EDC. To measure the  $\beta$ -galactosidase secreted by the receptor and thus a measure of the endocrine disrupting chemicals. The amount of  $\beta$ -galactosidase is measured using optical density to see the variation of the yellow color. The hER control for this experiment was 17 $\beta$ -estradiol (E2). The main purpose is to generate a reproducible method that can be used to monitor the endocrine disruptors in the valley for years to come and determine a baseline of endocrine disrupting chemicals in the Shenandoah River watershed. The areas of research consisted of Shenandoah River in Elkton, McGhaysville, Timberville, New Market, and the Woodstock wastewater treatment plant. Samples were taken up river and down river of the water treatment plant to determine if there was a significant contribution to EDCs by the plant effluent. Also, samples were taken at Cub Run, Smith Creek, and Stoney Run on Massanutten Mountain to determine the effect of agriculture.

**11:45 SHMS Hodoscope**

Nathan Holcomb, Kevin Nash, Emmett Randel, \*Ioana Niculescu, and \*Gabriel Niculescu

James Madison University

The Thomas Jefferson National Accelerator Facility (in Newport News, VA) is upgrading the energy of its accelerator to 12 GeV. The current detectors installed in the experimental halls will not be able to detect the higher energy particles and more sophisticated detectors will be needed. Because of this, in experimental Hall C work has begun on constructing a new Super-High-Momentum Spectrometer (SHMS). The group at JMU is working on assembling the paddles for the scintillator hodoscope part of the SHMS. This detector needs to withstand high radiation, have particle detection efficiency higher than 99% and the ability to handle rates in excess of 1 MHz/paddle. This requires a data acquisition system for testing photomultiplier tubes (PMTs), attaching the tested PMTs to the scintillator paddles, and safely storing and transporting them to Jefferson Lab for installation. The scintillator hodoscope will play a key role in the SHMS, providing the main trigger for the data acquisition system and also helping with particle identification.

**Chem/Mats - Session III - Oral Presentations**

**Thursday, July 30**

**1:30 PM - 3:00 PM**

**ISAT/CS 159**

**Dr. Kevin Caran, Presiding**

**1:30 Study of the effect of lead chloride on the aggregation and unfolding of RecA.**

Sonali Patel<sup>1</sup> and \*Gina MacDonald<sup>2</sup>

<sup>1</sup>Gallaudet University, <sup>2</sup>James Madison University

RecA is a 352-residue polypeptide with a molecular weight of 38 kD. RecA is known to be a multifunctional protein as it has many biochemical roles. RecA facilitates the DNA exchange reaction used to repair double strand breaks in DNA and to perform genetic recombination. Previous studies have shown that numerous salts can influence the activity, structure, aggregation and unfolding of RecA. The goal of our experiments was to study how the lead chloride affects the RecA protein aggregation and unfolding. Circular dichroism (CD) was used to monitor RecA unfolding in the presence of lead chloride for comparison to previous studies that used other chloride and sulfate salts. UV/Vis Spectroscopy was used to study how different concentrations of lead chloride changed the aggregation rate at room temperature by monitoring the increase in absorbance at 350 nm. We found that the presence of lead chloride causes RecA to aggregate and precipitate at room temperature at even lower concentrations than those required for the chloride salts to promote aggregation.

**1:45 Behavior of granular slopes under vertical vibration.**Nora Swisher and \*Brian Utter

James Madison University

We study the behavior of a 2D pile of photoelastic grains in a circular drum while varying the amplitude of vertical vibration. We characterize the slope's angle, curvature, and surface roughness by extracting an outline of the pile and fitting curves to the surface. The drum is either rotated at a constant velocity or held stationary. In a rotating pile, we correlate surface roughness and curvature with the angle during the avalanche process. In a stationary pile, we measure the angle, density of packing, and force network with different amplitudes of vibration. We find that the curvature of the slope is consistently negative in the absence of rotation while in a rotated pile the magnitude and sign of the curvature vary with the vibration amplitude.

**2:00 Elemental Analysis by Solution Mode Laser Ablation ICP-MS.**Jacob Smith and \*Daniel Downey

James Madison University

Inductively coupled plasma mass spectroscopy (ICP-MS) is a tool for elemental analysis of liquid or gaseous samples with sensitivity in the ppb to ppt range. Solution mode ICP-MS allows for effective sample introduction but is not time efficient. The program developed in our lab for solution analysis by ICP-MS requires a sample uptake time of 30 seconds and stabilization time of 300 seconds prior to a 2-second analysis. Laser ablation has been used to aerosolize samples from solids for analysis by ICP-MS. Our research has focused on the use of laser ablation to vaporize liquid samples for introduction into the ICP-MS. LA-ICP-MS does not require the uptake or stabilization periods needed in solution mode ICP-MS. Two methods of containing samples for ablation have been explored: wells in a plate and capillary tubes. Standard solutions containing between 0.5 and 2 ppm Mg, Mn, and Ca were produced with 1.0 ppm Ba as an internal standard. Isotopes monitored by ICP-MS included Mg-24, Ca-44, Ca-43, Mn-44, and Ba-137. Inconsistent ablation rates led to a signal for each isotope that varied over time. Isotopic ratios remained steady and quantitative analysis was possible by ratioing the analyte signals to the Ba-137 signal. Ablation from wells yielded a signal that, while lower than that obtained in solution mode, suggested that much lower concentrations could be analyzed. However, significant splattering occurred that led to cross-contamination between the wells. The signal obtained to date from solution contained in capillary tubes has been low. Future research will focus on laser ablation of fish tissue samples utilizing similar isotopic ratioing techniques.

**2:15 Electrical Characterization of Carbon Nanotubes with an Applied Torque.**Christopher Flint<sup>1</sup>, \*Scott Paulson<sup>1</sup>, Smai Fullerton<sup>2</sup>, Joe Hardcastle<sup>1</sup>, Jake Carey<sup>1</sup>, Lok-Kun Tsui<sup>1</sup><sup>1</sup>James Madison University, <sup>2</sup>American University

When measuring the electrical characterization for a certain substance, automation is nearly essential, especially with a large number of samples. A program has been created to automate an electrical characterization of carbon nanotubes (CNT's) and to automate a sweep of these devices over a temperature range and a field effect (gate) voltage range in a synchronous manner. The electrical characterization of CNT's at various gate voltages and temperatures reveals whether CNT's can replace common field effect transistors (FET's) and serves as a control group for viewing changes to a CNT's electrical characterization when a torque is applied to the CNT. A stand was built to pass an electrical current into a scanning electron microscope (SEM) in order to produce a magnetic field which applies a torque to a paddle attached to the CNT.

**2:30 Progress towards the Synthesis of Perylene-tripod Compounds for Single Molecule Studies of Interfacial Electron Transfer.**Lidia Vargas-Claros<sup>1</sup>, Evan Baugh<sup>2</sup>, and \*Debbie L. Mohler<sup>3</sup><sup>1</sup>University of Mary Washington, <sup>2</sup>Johns Hopkins University, <sup>3</sup>James Madison University

The synthesis of the macromolecule, Pe-tripod, is completed to transfer electrons to a TiO<sub>2</sub> nanoparticles. This heterogeneous electron transfer (HET) is a general phenomenon in catalytic reactions, in electrochemistry, and in photoelectrochemistry<sup>1</sup>. After a series of reactions, the molecule 1-(Trimethylsilylethynylphenyl)-3,5,7-tris(4-carboxyphenyl) adamantane has been synthesized so far in the progress to obtain the target molecule.

**2:45 Catalytic Oxidation of *p*-Cresol on Aluminum Oxide-Supported Cobalt Catalysts.**Samuel A. Moore and \*Kathryn Layman

James Madison University

*p*-Hydroxybenzaldehyde (PHBA) is an important starting material and intermediate for the synthesis of many polymers, pharmaceuticals, fragrances, and flavoring agents. *p*-Cresol oxidation may reduce the cost, simplify synthesis, and decrease the environmental hazards associated with the current industrial processes used to synthesize PHBA. Metal oxide catalysts have been demonstrated to oxidize *p*-cresol to PHBA in the presence of NaOH, gaseous O<sub>2</sub> and solvent methanol. Cobalt aluminate (CoAl<sub>2</sub>O<sub>4</sub>) supported on Al<sub>2</sub>O<sub>3</sub>, prepared using a 30 wt% Co loading and calcined at 900 °C for 3 hours, yielded 95.7% conversion of *p*-cresol and 92.4% selectivity to PHBA. Recently, %conversion and %selectivity calculations have yielded irreproducible and unrealistic values, indicating that the current calibration procedure is unsatisfactory. Sad *et al.* recently reported that methanol reacts with phenol, the internal standard, further indicating the need to develop a new calibration methodology. To this end, this summer's research has focused on creating calibration plots based on the ratio of PHBA to *p*-cresol. Future efforts will resume our survey of the catalytic activity of untested weight percent series of Al<sub>2</sub>O<sub>3</sub>-supported Co catalysts using XRD, IR, and HPLC-based periodic measurements of catalytic activity.

**Chem/Mats - Poster Session**  
**Thursday, July 30**  
**3:30 PM - 4:30 PM**  
**ISAT/CS 259 (NTelos Room)**

*Students presenting even numbered posters are asked to be near their posters during the first half hour (3:30-4:00) to answer questions.*  
*Students presenting odd numbered posters are asked to be near their posters during the second half hour (4:00-4:30)*

- 1 **Determining the activity of RecA through the direct examination of ATP hydrolysis and measuring the hydrophobicity of denatured RecA.**  
Deryck Araujo<sup>1</sup>, \*Martin Brakke<sup>1</sup>, \*Gina MacDonald<sup>2</sup>  
<sup>1</sup>Towson High School, <sup>2</sup>James Madison University  
 RecA is a multifunctional enzyme that plays an important role in the DNA strand exchange reaction. Previous research supports a link between protein conformational changes in the presence of the salts MgSO<sub>4</sub>, MgCl<sub>2</sub>, NaCl, NaSO<sub>4</sub>, and CaCl<sub>2</sub> in varying concentrations. In order to further support these findings contact angle measurements and direct ATPase activity assays were performed under various salt concentrations. Contact angle measurements were used to measure the hydrophobicity of denatured RecA. When unfolded, each salt should alter the hydrophobic properties of the RecA protein and cause a change in the liquid/vapor to protein surface contact angle. However, the production of uniform RecA monolayers proved to be difficult by traditional means. Direct ATPase activity assays, as opposed to coupled enzyme activity assays, allow for the measurement of RecA in high salt concentrations while avoiding spectral interference. A Biomol Green kit was used to bind free phosphate released during ATP hydrolysis resulting in the appearance of a visible green color which could be observed quantitatively through UV-VIS spectral absorbance. Although promising, supportive results have been inconsistent and methods should continue to be optimized.
  
- 2 **Jamming In a 2D Granular Silo.**  
Jerod Baker, \*Brian Utter, and \*Roddy Amenta  
 James Madison University  
 In this experiment, we are studying jamming in a 2D gravity-driven flow. We use photoelastic grains in a 2D box with a narrow opening at the base through which the grains can drain. We have set the distance of the opening so that the probability of jamming occurring is approximately equal to the probability of the grains flowing out completely. We place the experiment between crossed polarizers and use a high speed camera to capture images of the flow of the grains. This allows us to observe to force chains created when jamming bridges are formed. We find that jamming occurs when a stable force chain bridges the gap. We also study temporal correlations and observe a force shock rising through the grains above the opening. In a related project, we developed a MatLab program which displays a 2D slice through a simulated crystalline microstructure. The crystals were grown in a voxel (or cell units) represented as pixels in a 2D display.
  
- 3 **Estimation of nutrient and sediment loading in Lake Shenandoah, Rockingham County, Virginia: A continuation of a 1996-97 study.**  
Anne C. Battaglia and \*Daniel M. Downey  
 James Madison University  
 Lake Shenandoah, a recreational reservoir that supports a sport fishery for warm water fish species, is located in Rockingham County, Virginia near the city of Harrisonburg. The lake experiences chronic fishery and aesthetic management problems due to macrophyte growth, sedimentation and eutrophication. In 1996-97, a study was conducted that measured nutrient loading and found that sedimentation and eutrophication problem had occurred due to agricultural practices and recent land development in the watershed. The purpose of this study was to determine if sediment and nutrient loading have changed since the watershed land use has changed from agriculture to suburban development in the last ten years. Water quality parameters include pH, ANC, Ca<sup>2+</sup>, Mg<sup>2+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Cl<sup>-</sup>, NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, ammonia (NH<sub>3</sub>/NH<sub>4</sub><sup>+</sup>), turbidity, conductivity and total phosphorus were determined for each of the two streams entering the reservoir. The average values for nutrient and turbidity (sediment) loading from Massanetta Spring Run were 0.31 ppm PT, 3.43 ppm NO<sub>3</sub>-N, 0.20 ppm NH<sub>3</sub>/NH<sub>4</sub><sup>+</sup>-N and 14.25 NTU. The average values for nutrient and turbidity (sediment) loading from Congers Creek were 0.25 ppm PT, 9.49 ppm NO<sub>3</sub>-N, 0.10 ppm NH<sub>3</sub>/NH<sub>4</sub><sup>+</sup>-N and 12.73 NTU. Further research will be done to investigate runoff during episodic monitoring periods and lake sediment nutrient cycling. These data should provide information useful for management directives for mitigation and restoration of Lake Shenandoah.
  
- 4 **Analysis of the time evolution of structures in POSS-MA thin films deposited by spin casting.**  
Matt Bradley; \*Brian Augustine, and \*Chris Hughes  
 James Madison University  
 Poly(methacrylisobutyl POSS-co-methylmethacrylate) (POSS-MA) is a nanocomposite polymer that can exhibit properties of both the organic polymers and nanometer scale SiO<sub>2</sub>-like glass. POSS-MA may be easily deposited as a thin film by spin casting from a solution in chloroform or other standard solvents. AFM analysis of these cast films show dendritic structures forming on 30% POSS-MA thin films approximately 10 hours after deposition at room temperature. Real time observations were made using AFM and analysis work was also done to attempt to measure the expansion of the structures as a function of time. The growth rate was also measured at varying temperatures and in different environments. It was shown quantitatively that heat increases the rate of growth. It was also shown that regardless of initial surface features, the structures still formed in a similar fashion.
  
- 5 **Comparison of analytical methods for fluoride determination: ion chromatography, ion selective electrode, and spectrophotometry.**  
Robert J. Bradley<sup>1</sup>; \*Stephanie L. Hall<sup>2</sup>, and \*Daniel M. Downey<sup>2</sup>  
<sup>1</sup>Virginia School for the Deaf and the Blind, <sup>2</sup>James Madison University  
 Compounds containing fluorine are added to drinking water supplies throughout the United States to produce fluoride, which helps prevent tooth decay. For this project, water samples were collected from various locations and fluoride concentrations were determined by three different methods: ion selective electrode (ISE), ion chromatography (IC), and spectrophotometry were used to measure fluoride in the same water samples and then compared. The IC method involves minimal sample preparation, is accurate and precise, but time consuming. The ISE method employs a short chemical treatment prior to fluoride determination and is accurate, precise and quick. However, the spectrophotometric method was found to be inaccurate. The sample preparation was time consuming, involving distillation of samples prior to analysis. Concentrations of fluoride in natural waters were found between 0.069 and 0.13 ppm, 0.33 and 0.98 ppm, and 0.0839 and 0.171 ppm for the ISE, spectrophotometric (prior to distillation), and IC methods, respectively. Concentrations of fluoride in tap water were found between

0.74 and 1.2 ppm, 0.024 and 1.3 ppm, and 1.02 and 1.13 ppm for the ISE, spectrophotometric (prior to distillation), and IC methods, respectively. Following distillation for the spectrophotometric method, fluoride concentrations were inconclusive in the majority of the samples.

## 6 Cloning and Expression of Inosine 5-Monophosphate Dehydrogenase from Extremophiles

Courtney Braxton, Jillian Stanton, and \*Victoria Mariani

James Madison University

Inosine 5-monophosphate dehydrogenase (IMPDH) is a critical enzyme in the synthesis of DNA nucleotide purines, adenine and guanine. IMPDH catalyzes the oxidation of xanthosine monophosphate (XMP) which is a precursor for guanosine monophosphate (GMP). GMP, which is readily converted to guanosine-5'-triphosphate (GTP) and guanosine 5'-diphosphate (GDP), is a necessary cofactor for the synthesis of adenosine monophosphate (AMP). An isoform of IMPDH, type II IMPDH, is linked to both cancer and RNA viruses. DNA encoding for IMPDH from extremophilic bacteria *Colwellia pyscherythaea* 34H and *Thermus thermophilus* HB27 was successfully isolated via a high fidelity polymerase chain reaction (PCR). This PCR product, along with expression vector, pET-19b, will be restriction digested in preparation for a ligation reaction to create a means to purify the corresponding recombinant IMPDH enzymes. These enzymes will be compared to their mesophilic counterpart from *Escherichia coli* K12, in which we hope to determine which second tier amino acids are pivotal in the structure and function of the IMPDH.

## 7 Blasts and quakes: Analysis of earth vibrations.

Tim Brooks and \*Anna M. Courtier

James Madison University

This study examines the relationship between three very different sources of seismic energy: earthquakes, nuclear detonations, and rock quarry blasts. Analysis of these earth vibrations will help explain the effect of rock composition and structure on the frequency content and attenuation of seismic energy. The earthquake and nuclear data for this study were gathered from seismic databases (IRIS, NEIC, VTSO), and rock quarry blast data were provided by Luck Stone Corporation. Data from all sources were pre-processed with the same methods; primarily, filtering and deconvolution techniques were used to reduce unwanted noise and to remove instrument biases. All data were initially in seismogram form (amplitude vs time), and Fourier transforms were applied to isolate the dominant frequencies. Changes in amplitude and frequency of the seismic data relate the rate of attenuation to the propagation distance and local rock type. Quarry sites yield the most systematic results, due to the proximity of blasts to seismic monitoring instruments. Data from earthquakes (Virginia) and a nuclear detonation (North Korea) yield information about regional structures.

## 8 Using difference infrared spectroscopy to investigate the effects of pH on PGK-substrate complexes.

Adam E. Colbert, \*Gina MacDonald

Yeast phosphoglycerate kinase catalyzes the reversible phosphate transfer in the reaction: ADP + 1,3-bis-phosphoglycerate /EQUILIBRIUM ARROW/ ATP + 3-phosphoglycerate. Prior research indicates a hinge-bending mechanism occurs during catalysis to bring the substrates into closer proximity. Domain closure is only initiated in ternary complexes, in which both substrates are simultaneously bound to the enzyme. The activity and conformation of PGK is directly influenced by substrate and salt concentrations as well as pH. For example, activity assays confirm that PGK activity increases from pH 6.5 to 7.5. To determine the effects of pH on the conformational changes of PGK, we used difference Fourier transform infrared spectroscopy (FTIR) in conjunction with caged nucleotides. Difference infrared data associated with nucleotide (ATP or ADP) binding to PGK or PGK-3PG complexes was compared at pH 5.5, 6.5 and 7.5. Circular dichroism was also used to study PGK secondary structure at the aforementioned pH conditions. Comparison of the difference FTIR data allowed the isolation of pH dependent vibrations that arise from protein conformational changes induced by substrate binding. We have identified multiple vibrations that are associated with the PGK ternary complex and are influenced by pH. Difference FTIR studies resulted in the identification of specific changes within amino acid side chains and protein secondary structures that are altered by pH and associated with ternary complex formation.

## 9 Monohydride and Dihydride Ruthenium Complexes of Bis(diphenylphosphine) Ligands.

Alexa DeLuca, \*Donna S. Amenta, and \*John W. Gilje

James Madison University

Transition metal complexes of bis phosphinomonoxide ligands ( $R_2P(CH_2)_nP(O)R_2$ ) play important roles in catalytic reactions. We are interested in synthesizing Ru (II) hydride complexes of  $Ph_2P(CH_2)_nP(O)Ph_2$ . The reaction of  $RuHCl(CO)(PPh_3)_3$  with  $Ph_2PCH_2P(O)Ph_2$  in THF produces  $RuHCl(CO)(PPh_3)(PPh_2CH_2P(O)Ph_2)$ . This compound has been characterized by  $^1H$  NMR,  $^{31}P$  NMR, and IR Spectroscopy. The two  $PPh_3$  ligands that are removed in the reaction were *cis* to each other and *trans* to the hydride and carbonyl ligands respectively. The  $Ph_2PCH_2P(O)Ph_2$  ligand chelates to the ruthenium through the phosphorus and oxygen of the ligand and the  $PPh_2$  group is *trans* to the  $PPh_3$  ligand that remains on the compound. In solution  $RuHCl(CO)(PPh_3)(PPh_2CH_2P(O)Ph_2)$  slowly isomerizes to two new compounds. While these two compounds have not yet been completely identified, one has two *trans* phosphino phosphorus atoms and one phosphoryl phosphorus that is *cis* to the other two. The reaction of  $RuH_2(CO)(PPh_3)_3$  with  $Ph_2PCH_2P(O)Ph_2$  in THF produces  $RuH_2(CO)(PPh_3)(PPh_2CH_2P(O)Ph_2)$ . This compound has also been characterized by  $^1H$  NMR,  $^{31}P$  NMR, and IR Spectroscopy. After the two  $PPh_3$  ligands are removed the  $Ph_2PCH_2P(O)Ph_2$  ligand chelates to the ruthenium through both phosphorus and oxygen. The  $PPh_2$  is *trans* to the  $PPh_3$  ligand that remains on the compound and the two hydride ligands which were *cis* to each other in  $RuH_2(CO)(PPh_3)_3$ , have moved to a *trans* conformation. .

## 10 The Synthesis of a Chlorotricarbonylrhenium I Complex of [4, 4'- bis(aminomethyl)-2,2'-bipyridine] .

Seth Ensign, Puja Moody, Amanda Hoffman, and \*Debra L. Mohler

James Madison University

To better understand the influence of anchoring groups on the rate of interfacial electron transfer, chlorotricarbonylrhenium complexes of bipyridines with varying anchoring groups were synthesized and bonded to the rhenium complex. The specific goal of this work is to create a chlorotricarbonylrhenium (I) complex of [4,4'-bis(aminomethyl)-2,2'-bipyridine] for later study by femtosecond IR spectroscopy.

## 11 Determination of grain sizes by best fit ellipsoids in computer generated microstructures.

Douglas Fordham, and \*Roddy Amenta

James Madison University

The crystal size distribution (CSD) in an industrial crystallization vat, that is predominantly liquid, is a result of controlled nucleation and growth rates of the crystals. However, in completely crystallized systems, such as an igneous rock, the grain sizes (and shapes) are modified by the surrounding in microstructure. It is of geological interest to determine the paleo-crystallization rates of rocks but we need to know how the modified crystal sizes affect the CSD. We are attempting to do this in computer simulated microstructures by finding the best fit ellipsoids for each of the crystals using a robust matrix method, singular value decomposition. The intent is to apply this method to 3D data on real grain sizes obtained from computer X-ray tomography.

**12 Electrical characterization of carbon nanotubes and their chemical stability during the wet etch process.**Smai Fullerton<sup>1</sup>, Lok-kun Tsui<sup>2</sup>, Joe Hardcastle<sup>2</sup>, Jake Carey<sup>2</sup>, Chris Flint<sup>2</sup>, \*Scott Paulson<sup>2</sup><sup>1</sup>American University, <sup>2</sup>James Madison University

Carbon nanotubes (CNT) are commonly studied because of their unusual and useful electrical properties. Depending on their structure, they act as conductors or semiconductors. In order to measure the resistance of a nanotube in varying low-temperature environments, we created transistors using e-beam lithography and metal deposition. These devices were pumped into a refrigerator that achieves temperatures as low as 5°K and connected to a voltage source. A student-written LabView program then produced the IV curves that allowed us to characterize the samples. We found that the resistance of semiconducting nanotubes decreased as the temperature rose. In a separate ongoing experiment that measures the torsional properties of carbon nanotubes, the substrate beneath the nanotube is eliminated by a hydrofluoric and a phosphoric acid etch to leave it suspended freely. With the aim of confirming that the nanotube's electrical properties are not altered during this etch, we used the transistor devices to compare the resistance of the nanotube before and after the process. The resistance appeared to remain unchanged within a factor of 10% and thus we concluded that the acid etch is reliable.

**13 Use of the yeast estrogen screen to determine endocrine disrupting chemicals in and around the Shenandoah River.**Katie-Jo Galayda<sup>1</sup>, Nicole Mueller<sup>2</sup>, \*Tammy Stone<sup>2</sup>, \*Peter Ruiz-Haas<sup>1</sup><sup>1</sup>Mary Baldwin College, <sup>2</sup>Spotswood High School

In the past few years, fish kills and observations of fish with deformities in the Shenandoah River and surrounding areas have caused concerns. The causes of these problems are still unknown, but one hypothesis is that presence of endocrine disrupting compounds (EDCs) in the waters may cause some of the effects observed in fish. EDCs can interfere with hormone signals and cause feminization of fish at concentrations as low as 0.5-1 ng/L. To test for presence of EDCs in the waters, the Yeast Estrogen Screen (YES) was used. The YES procedure is a bioassay involving yeast cells (*Saccharomyces cerevisiae*) genetically modified to incorporate the human estrogen receptor (hER). When exposed to EDCs, the cells produce beta-galactosidase, and the amount of beta-galactosidase produced is proportional to the activity of EDCs in the sample. The amount of beta-galactosidase is determined by reaction with o-nitrophenyl-beta-galactopyranoside (ONPG), which is measured in a plate reader. Water samples were collected in the Shenandoah River and tributaries in Elkton, McGayesville, Timberville, New Market, and the Woodstock wastewater treatment plant. After sampling, 1 L of water sample was extracted using C-18 solid phase extraction to increase the concentration of analyte. Each sample showed definite EDC activity although further testing will be required to get more reproducible results.

**14 A Study of Torsional properties of Carbon Nanotubes.**Joseph Hardcastle<sup>1</sup>, \*Scott Paulson<sup>1</sup>, Lok-kun Tsui<sup>1</sup>, Jake Carey<sup>1</sup>, Chris Flint<sup>1</sup>, Samantha Fullerton<sup>2</sup><sup>1</sup>James Madison University, <sup>2</sup>American University

Single and multiwalled carbon nanotubes have shown different properties as they are rotated about their axis. These differences are not well understood and are theorized to be due to interactions between the lattices. Traditional techniques for imaging at the nano scale provide no information about this interface, meaning a new method is required to study such phenomena. In our research we use transmission electron microscopy and electron diffraction to characterize multiwalled nanotubes and study their alterations due to torsional movement. This method allows us to profile the lattice of our nanotube before and after a torsional force, and discover whether the modification of the lattice interface is responsible for rotational friction. Our experiment will allow for a detailed study of the friction between the atomic surfaces of multiwalled nanotubes and will give experiment data about the interactions of nanotube lattices.

**15 Quantitating neurotransmitter levels in blood.**

Beth Kimmitt and \*Gina MacDonald

James Madison University

Studies linking animal behavior with biochemical composition have recently become more abundant. Numerous studies have shown links between increased aggression and differing levels of neurotransmitters/hormones in bodily fluids. Although much information is known about the levels of these neurotransmitters in cerebral spinal fluid few studies have looked for a correlation between the neurotransmitter levels in cerebral spinal fluid and the blood of the same animal. Our studies are focused on using ELISA kits and mass spectrometry to study the correlation between CSF and blood neurotransmitter levels. We obtained samples of rats' cerebral spinal fluid, blood, and brain tissue and have measured serotonin levels for comparison. Here we present the initial data that does not yet allow us to decipher a correlation between the different bodily fluids. However, we have successfully devised a protocol for collecting, preparing, and running samples that will allow for multiple studies in the future.

**16 Infrared Studies of the Effects of High Salt Concentrations and Varying Temperatures on RecA Unfolding.**

Tiffanie King and \*Gina MacDonald

James Madison University

The *Escherichia coli* protein RecA performs the process of DNA repair and recombination. When a "distress" signal is sent, the RecA protein is activated and begins the process of replacing damaged single-stranded DNA, or ssDNA, with new ssDNA. When RecA is activated the structure is altered and RecA adopts an elongated protein filament. Previous studies observed that DNA and ATP must be present in order for RecA to transition to the activated complex. However, in the presence of high salt and the absence of DNA, RecA adopts a similar elongated, activated state. Previous studies have shown that the presence of different salts alter the unfolding of RecA. Our studies have used infrared spectroscopy to compliment previous studies that used circular dichroism (CD) to follow RecA unfolding. Here we present infrared data that shows how the RecA backbone structure is altered at different temperatures in the presence of high salt concentrations.

**17 CO Adsorption on Hydrated Ruthenium Catalysts.**Hollins L. Kitts<sup>1</sup>, Diana Gottschalk<sup>1</sup>, Erin A. Hinson<sup>2</sup>, Adam S. Baird<sup>1</sup>, and \*Kathryn A. Layman<sup>1</sup><sup>1</sup>James Madison University, <sup>2</sup>Western Carolina University

The adsorption of CO on Ru single crystals and supported Ru has been studied extensively in the absence of water. However, water is known to affect both the selectivity and activity of heterogeneous catalysts. Water vapor plays an important role in controlling the surface properties of metal oxides by influencing (1) the extent of surface hydroxylation, (2) the ratio of Brønsted/Lewis surface sites, and (3) the surface metal oxide structure via surface reconstruction. To better understand the influence of water on CO adsorption, we have been investigating CO adsorption on hydrated alumina-supported ruthenium (Ru) catalysts using attenuated reflection Fourier transform infrared (ATR-FTIR) spectroscopy. In these studies, water is readily removed from the surface by flowing dry gas over the sample. Since these gases are used to de-gas and pretreat the samples prior to CO adsorption and since CO adsorption is influenced by the amount of co-adsorbed water, this summer's research has focused on determining the rate of water removal in the presence of H<sub>2</sub>, O<sub>2</sub>, He, and Ar. The influence of the support, sample preparation, and pretreatment gas on the co-adsorption of water and CO were also investigated.

19 **Recognition of Fingerspelled Words.**Laura Morgan, Sabrina Cox, and \*Brenda Seal

James Madison University

As sign language interpreter trainees for the REU 2009 chemistry program, we were expected to observe the professional interpreters, show improvement in voice-to-sign and sign-to-voice interpreting, and conduct research relevant to interpreting. Our interpreting progress was measured with self, mentor, and consumer evaluations at several intervals throughout the summer. Our research question addressed whether or not rehearsing fingerspelled words enhances receptive or decoding abilities. We studied this using two different experiments. For the first experiment, we taught 10 commonly used chemistry words such as "fluid" to 8 hearing chemistry students with no prior fingerspelling experience. Instruction focused on correct formation and production of the letters for each word, smooth transition from one letter to another, and rate in fingerspelling and saying the word simultaneously. At the end of six weeks, each student was administered a video test that included the 10 words familiar words and 10 new words matched for length and difficulty. The students were then scored on their ability to fingerspell or encode all 20 words. The second experiment involved ourselves, interpreter trainees, as subjects to see if similar fingerspelling rehearsal of complex chemistry words resulted in improved decoding or receptive abilities. We rehearsed 20 longer, less common words until we were proficient enough to fingerspell and speak the words at the same rate. We then took a test with the 20 words that we rehearsed and 20 unfamiliar but matched words. Scores on both experiments revealed and support the need for encoding or expressive rehearsal in improving decoding or receptive fingerspelling skills.

20 **Development of pH and Structural Reporter Molecules for Photoacoustic Imaging.**Kathryn M Nesbitt<sup>1</sup> and \*Kevin W. Davies<sup>2</sup><sup>1</sup>St. John Fisher College, <sup>2</sup>James Madison University

The photoacoustic effect is currently used by bio-medical researchers to image living tissues and organs as well as by photo-chemists as a way to study photo-physical properties of molecules. In this research we begin to identify molecules with photo-physical properties that might be useful to selectively image biological features and measure chemical properties (e.g. pH) in humans. Nitrazine yellow (NY), a well-known acid-base indicator, has been shown to localize in the lymphatic system and may allow for photoacoustic imaging to selectively image lymph nodes noninvasively. In this research we have investigated the photo-physical properties of NY and found that it is highly efficient in the conversion of light into acoustic waves in both its acidic and basic forms. Our preliminary research shows that NY should be well-suited to image the lymphatic system selectively while simultaneously measuring the pH.

21 **Success of liming a "sinking" stream versus a perennial surface stream.**Jennifer Phillips, Holly M. Tuck, Carla R. Landes, and \*Daniel M. Downey

James Madison University

Mountain Run is located in the Massanutten Mountain Range of Virginia which is part of the George Washington National Forest. Brook trout and other species in this stream have suffered severe losses due to the decrease in pH caused by atmospheric acid injection (acid rain). To restore water quality, Mountain Run was treated with limestone from 1993 up to 2008. Initial treatments in 1993 and 1997 were done at a location in a lower reach that flows perennially and later (1999, 2002, 2005, and 2008) in an upper reach that experiences several sinks into the soil. Water quality parameters (WQP) were analyzed and fish inventories were taken from 1992 to present. Key WQP values were as follows for four locations: upstream of the perennial site, 1.25 km downstream of the perennial site, upstream of the sinking site and 1.25 km downstream of the sinking site. Average values found were pH = 4.64, 5.73, 4.59, 5.05; ANC = -22.2, 20.1, -28.2, -6.9 ( $\mu\text{eq/L}$ ); Ca:H = 1.3, 265.1, 0.87, 9.0; Al = 303, 108, 409, 184 (ppb). The only location that accommodates trout is the area 1.25 km downstream of the lower reach with a perennial flow. This study compares the effectiveness of liming Mountain Run in the two locations, and how the response from the upper reach is less efficient due to the sinks in the stream and the acidic nature of the soil.

22 **2D Jamming in a Particle-fluid Suspension.**Ibraheem Rasoul, \*Roddy Amenta, and \*Brian Utter

James Madison University

There are a number of systems designed for observing jamming in dry granular materials. We focus on particle-fluid systems where interstitial fluid is important. Compared to dry systems, the presence of the fluid both alters friction between the contacts and couples with particle motion. The current setup consists of two sheets of acrylic with a pulley system connected by belts to drive the flow. We study shear in this system by measuring the particle positions and forces using the photoelastic response of the grains. Compared to a similar experiment with dry grains, we observe that the force chains are less branched and appear to last longer due to slipping between the particles and belts. Overall, particle flow is similar to the dry system with a motion confined closer to the shearing surface.

23 **Cloning and expression of 5-Enolpyruvylshikimate-3-Phosphate Synthase from *Escherichia coli* K12 for comparison to its extremophilic counterparts.**Tiffany Shellie, Jaleal Sanjak, Robert East, and \*Victoria Mariani

James Madison University

The *aroA* gene encodes for the expression of 5-Enolpyruvylshikimate-3-phosphate (EPSP) synthase which catalyzes the reversible reaction forming EPSP from shikimate-3-phosphate (S3P) and phosphoenolpyruvate (PEP) in the sixth step of the shikimate pathway. The shikimate pathway, which links the metabolism of carbohydrates to aromatic amino acid biosynthesis, is found in plants, fungi, and bacteria. Because of this aforementioned exclusivity, EPSP synthase is a promising target for antibiotic, antiparasitic, and herbicide development. Through structural characterization of thermophilic, mesophilic, and psychrophilic EPSP synthases, we also hope to elucidate which particular moieties outside of the active site are pivotal to function. Here we report successful extraction of the *Escherichia coli* genome followed by complete amplification of the *aroA* gene from this DNA via a high fidelity polymerase chain reaction. Restriction enzyme digestion and a ligation of *aroA* DNA and pET19b expression vector are being attempted to yield a clone for mass purification of enzyme. In addition, EPSP synthase has been extracted from *Escherichia coli* via an ammonium sulfate precipitation followed by column chromatography. All actions proceed towards the ultimate goal of performing structural and kinetic analysis on EPSP synthase to compare to its extremophilic counterparts.

24 **Dimeric Propargylic Alcohols .**Michael A. Salim<sup>1</sup>, Yanita W. Boayue<sup>2</sup>, Paris L. Hamilton<sup>1</sup>, Lin Pu<sup>3</sup>, Michal Sabat<sup>3</sup>, and Kevin L. Caran<sup>1</sup><sup>1</sup>James Madison University, <sup>2</sup>Stevenson University, <sup>3</sup>University of Virginia

Our group has previously studied a family of novel low molecular weight organogelators based on a racemic propargylic alcohol (*Langmuir*, 2008, **24**, 7421). These compounds each have a pentafluoroarene group (connected to the alcohol carbon) and a second non-fluorinated arene (connected via an alkyne). Through extensive hydrogen bonding and  $\pi$ - $\pi$  stacking, the compounds self-assemble in a highly organized fashion to gel nonpolar liquids. We report the synthesis and preliminary study of a series of dimeric derivatives, in which two of the propargylic

alcohols are joined by a linear hydrocarbon chain (six, ten, or twelve carbons long) on the nonfluorinated aromatic ring. The bis-propargylic alcohols were prepared in reasonable yield in four steps from commercially available compounds. Because of their resemblance to molecules that assemble into supramolecular polymers, we hypothesize that the bis-propargylic alcohols will form materials of greater strength than the previously studied gels. Self-assembling behavior will be studied with the neat compounds and in various liquids. Preliminary studies including solubility testing, infrared (IR) spectroscopy, x-ray diffraction (XRD), and scanning electron microscopy (SEM) imaging are underway.

## 25 Preliminary Petrologic and Geochemical Studies of a Sapphire-bearing Rock from Cascade Canyon, California.

Hannah V. Shepherd<sup>1</sup>, \*Elizabeth A. Johnson<sup>1</sup>, M. Amelia V. Logan<sup>2</sup>

<sup>1</sup>James Madison University, <sup>2</sup>Smithsonian Institution

Preliminary petrologic and geochemical studies were performed on a sapphire-bearing (corundum, Al<sub>2</sub>O<sub>3</sub>) rock from Cascade Canyon, California. Corundum crystals are pink-purple in color and up to 5mm in length. The mineralogy of the rock was examined in thin section using the Scanning Electron Microscope (SEM) facilities at JMU and the Smithsonian Institution. The matrix is comprised of sodium and potassium feldspar ((Na,K)AlSi<sub>3</sub>O<sub>8</sub>). Other minor minerals include muscovite mica, monazite, and rutile (TiO<sub>2</sub>). In order to learn about the petrogenesis of this rock, a closer look into the sapphire was taken. The sapphire is home to many tiny inclusions of other minerals. Theories suggest that the reason these inclusions exist is because the sapphire grew around them; implying they were among the first minerals to form in the rock. Rutile (TiO<sub>2</sub>) is one type of mineral not only located in the matrix, but the sapphire as well. A Zr-in-TiO<sub>2</sub> geothermometer (Watson, 2006 and 2007) was used to estimate the temperature at which the rutile crystallized. Zr<sup>4+</sup> and Ti<sup>4+</sup> are similar in size, and the amount of Zr<sup>4+</sup> substituting into the structure is dependent on temperature. Chemical analyses were performed on the electron microprobe at the Smithsonian Institution. Results indicate a crystallization temperature of about 800 °C.

## 26 Synthesis of Stable RNA Analogs.

Cameron D. Straughn and \*Debra L. Mohler

James Madison University

The synthesis of stable RNA analogs that can effectively bind via base pairing and can polymerize in a single concerted reaction is a necessary step in therapeutic treatments using siRNA. Therefore the discussion focuses on recent synthetic advances towards producing stable analogs via ring opening metathesis polymerization using synthetic monomers.

## 27 The Synthesis of Nitrogen- and Sulfur-Containing Heterocycles from Cyclopropanol Fragmentation.

Georgia T. Stoyanov, Kelly L. George, and \*Kevin P.C. Minbirole

James Madison University

The prevalence of heterocycles as the backbone of common pharmaceutical entities has created a demand for simple reactions to prepare them. Our research aimed to create six- and seven-membered heterocycles containing both a carbonyl group and either sulfur or nitrogen in the ring. A cyclopropanol fragmentation approach to the formation of oxepanes was developed in the Minbirole lab's previous work. Using a similar approach, our current endeavor is to synthesize nitrogenous heterocycles, particularly piperidines and azepines, as well as sulfur-containing thiepanes. The nitrogenous approach begins with either N-benzyl-protected  $\alpha$ - or  $\beta$ -amino acid ethyl esters which were transformed to cyclopropanols via the Kulinkovich reaction. The resulting  $\alpha$ - and  $\beta$ - amino cyclopropanols were then reacted with various aldehydes to form an aminal. Subsequently, various Lewis acids were used to promote the rearrangement of the aminal into piperidine or azepine formation. This rearrangement is still under investigation. Analogously, a seven-membered sulfur-containing heterocycle was formed by sequential addition of aluminum (III) triflate and bismuth (III) triflate as Lewis acids to a mercaptocyclopropanol/benzaldehyde mixture, though heterocycle was only produced in low yields (<20%).

## 28 Sample Fabrication for the Study of Carbon Nanotubes.

Lok-Kun Tsui<sup>1</sup>, Chris Flint<sup>1</sup>, Samantha Fullerton<sup>2</sup>, Joe Hardcastle<sup>1</sup>, Jake Carey<sup>1</sup>, \*Scott Paulson<sup>1</sup>

<sup>1</sup>James Madison University, <sup>2</sup>American University

The devices needed to conduct the electrical and mechanical study of Carbon Nanotubes require sophisticated fabrication. Our work has concentrated on developing processes to create samples needed for the study of these properties. The mechanical study samples require a suspended CNT with a paddle to apply a torsional force as well as take TEM imaging and diffraction. The membrane preparation, Atomic Force Microscopy, and Electron Beam Lithography patterning with sub-micron accuracy are well refined, and we have confidence that we have gotten these steps to work consistently. We have gone through the final stage of the sample fabrication process, the phosphoric acid etching of the membranes on which our contacts are grown. To prevent the surface tension forces in this stage from damaging our samples, we worked with our colleagues at UNC Chapel Hill to use a critical point drying procedure that allowed our samples to survive the etching process. TEM imaging confirms that we were able to successfully produce a suspended nanotube sample.

## 29 Synthesis and characterization of the products from the reaction of RuCl<sub>3</sub>NO(PPh<sub>3</sub>)<sub>2</sub> with Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub> and Ph<sub>2</sub>P(CH<sub>2</sub>)<sub>2</sub>P(O)Ph<sub>2</sub>.

Lindsay Walton, \*Donna Amenta, and \*John Gilje

James Madison University

RuCl<sub>3</sub>NO(PPh<sub>3</sub>)<sub>2</sub> reacts with Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub> (dppmO) or Ph<sub>2</sub>P(CH<sub>2</sub>)<sub>2</sub>P(O)Ph<sub>2</sub> (dppeO) to form either RuCl<sub>3</sub>NO[Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub> or RuCl<sub>3</sub>NO[Ph<sub>2</sub>P(CH<sub>2</sub>)<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub>. RuCl<sub>3</sub>NO[Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub> is a light orange solid, which was characterized by IR and NMR spectroscopy, along with X-ray crystallography. The compound is octahedral with the two dppmO ligands *trans* to each other. With RuCl<sub>3</sub>NO[Ph<sub>2</sub>P(CH<sub>2</sub>)<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub>, another light orange product was observed and characterized through use of IR and NMR spectroscopy. The IR spectrum indicates the presence of a coordinated NO group, and the <sup>31</sup>P NMR spectrum indicates an AA'XX' spin system with coupling constants characteristic of phosphine ligands coordinated to ruthenium in a *trans* fashion, as expected for a structure analogous to that of RuCl<sub>3</sub>NO[Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub>. Preliminary data indicates that at least one chloride can be removed from RuCl<sub>3</sub>NO[Ph<sub>2</sub>PCH<sub>2</sub>P(O)Ph<sub>2</sub>]<sub>2</sub> by reaction with AgPF<sub>6</sub>.

## 30 Bicephalic (double-headed) amphiphiles.

David Warnock, Kaitlin Simmons, and \*Kevin Caran

James Madison University

A series of bicephalic (double-headed) biscationic amphiphiles with two trimethylammonium heads, an aromatic spacer, and a single 14 carbon hydrophobic tail were synthesized. The orientation of the hydrocarbon tail relative to the normal of the interface was altered by changing the location of the head groups on the aromatic ring. The head groups were located in the 2,3-, 2,4-, 2,6-, 3,4-, and 3,5- positions. The Krafft temperatures (T<sub>k</sub>) of the 2,3- derivative was determined using conductivity and differential scanning calorimetry (DSC). The critical micelle concentration (CMC) was determined using conductivity and proton nuclear magnetic resonance spectroscopy (<sup>1</sup>H NMR). NMR experiments

demonstrate that dynamic processes within the colloidal aggregates range between slow and fast, relative to the NMR timescale. Results show that the relative positions of the head groups affect the  $T_k$ , CMC, and exchange rate of the monomers into micelle.

### 31 Proton Chemical Shifts for Alcohols in the Vapor Phase and Dilute Solutions.

Curtis White and \*Thomas C. DeVore

James Madison University

Alcohol molecules form hydrogen bonded clusters in solution and the chemical shift observed for the OH proton is known to depend on the concentration of the alcohol and provides an indication of the amount of cluster formation. Quantitative information can be obtained if the chemical shifts for the pure species can be established, for instance by using high level Hartree-Fock or density functional theory calculations. Calculations at various levels of theory are compared to the measured chemical shifts in the proton NMR spectrum of methanol, ethanol, 2-propanol, and 2-methyl 2-propanol in the vapor phase and 2-methyl 2-propanol in dilute toluene, chloroform, and acetone solutions. While the relative chemical shifts agree well with the measurements made for the vapor molecules, the absolute chemical shifts differ by ~2 ppm, suggesting that the air introduces an absolute shift to the spectrum. The high level calculations for methanol are fast enough for use in a laboratory.

### 32 Identifying antifungal metabolites from *Pedobacterium cryoconitis*.

Patrick Wiggins, Christian Schwantes, and \*Kevin Minbiole

James Madison University

Metabolites from *Pedobacterium cryoconitis* were examined in an attempt to discover a probiotic antifungal treatment against the fungus *Batrachochytrium dendrobatidis*, or Bd. Bd is associated with the disease chytridiomycosis, one of the leading factors for amphibian decline all over the world. However, according to past research, several surviving amphibians house cutaneous bacteria on their skin that inhibits the growth of the invading Bd. *Janthinobacterium lividum* and *Pedobacterium cryoconitis* were among the protective bacteria living on the amphibians' skin. In a previous study, it was discovered that *Janthinobacterium lividum* produced violacein, an anti-chytrid metabolite. This metabolite was tested on the frog *Rana muscosa* before Bd exposure; the presence of violacein was a major factor in the survival of all those infected. Using the success of our previous experiment, tests utilizing a 96 well-plate were run to isolate different anti-chytrid metabolites produced by *Pedobacterium cryoconitis*. Bd zoospores in 1% tryptone solution were exposed to metabolites dissolved in DMSO/sterile deionized water, and absorbance difference indicated growth or lack thereof. This systematic approach was taken in order to isolate, identify, and to eventually test anti-chytrid metabolites on amphibians.

### 33 Fabrication of buried magnetic structures in PMMA microfluidic devices.

Jon Willcox and \*Chris Hughes

James Madison University

The control of fluids in microfabricated structures by electric and magnetic fields is important for a variety of applications for microfluidic devices. In this project we fabricate a device with magnetized iron (III) oxide nanoparticles embedded just beneath the surface of an approximately 120  $\mu\text{m}$  wide x 50  $\mu\text{m}$  deep channel. The magnetic field from these nanoparticles can then be used to filter magnetic particles out of a fluid which is flowed through the channel without reacting with the fluid. The fabrication of these devices begins by cutting wells about 300  $\mu\text{m}$  deep into a strip of poly(methyl methacrylate) (PMMA) to be used as a cover plate over top of the channel. Both the wells and channels are made by CO<sub>2</sub> laser engraving. The wells are then filled with a mixture of iron (III) oxide nanoparticles and a 20% PMMA/methyl methacrylate precursor solution with benzoic methyl ether (BME) as a photoinitiator for polymerization. The solution is then placed under an ultra violet light so that it photopolymerizes. A thin layer of the precursor solution is spread over top of the iron (III) oxide and similarly photopolymerized to make a barrier between the well and the channel. The Fe<sub>2</sub>O<sub>3</sub> nanoparticles are then magnetized and the cover plate is bonded to the channel plate. Further work will be done to test the filtering capacities of these devices.

## Chem/Mats - Session IV - Oral Presentations

Friday, July 31

9:30 AM - 12:00 PM

ISAT/CS 159

Dr. John Gilje, Presiding

### 9:30 A Quantitative Study of Gold Adhesion to PMMA and POSS-MA Surfaces.

Laura Lee<sup>1</sup>, Jon Willcox<sup>2</sup>, and \*Chris Hughes<sup>2</sup>

<sup>1</sup>High Point University, <sup>2</sup>James Madison University

The deposition of gold layers onto polymer surfaces has many applications such as the fabrication of reflective layers and electrical contacts. However, metals do not adhere well to the non-polar surfaces of most polymers. In this project, we investigated the adhesion of gold to a poly (methyl methacrylate) or PMMA, and methods to improve this adhesion. Different treatments to PMMA were explored including exposing PMMA samples to a 5%O<sub>2</sub>/95%N<sub>2</sub>, 25W remote plasma and/or spin coating 45wt% poly[(propylmethacryl-heptaisobutyl-polyhedral oligomeric silsesquioxane)-co-(methylmethacrylate)] (POSS-MA) on the samples. Previous experiments have shown that plasma treatment of POSS-MA coated PMMA creates a Si-O terminated surface while untreated PMMA is terminated by hydrocarbons. Thus the plasma treated surface should provide better adhesion for Cr/Au layers deposited on it. Four different treatments groups were used: untreated PMMA, PMMA exposed to plasma, PMMA spin coated with POSS-MA, and PMMA treated with POSS-MA and plasma. After gold deposition in a magnetron sputtering system, these samples were put through a 'tape test' where the gold was forcibly removed by peeling scotch tape off the PMMA sample. To quantify the data, the program Image J was used to calculate the area of the deposited gold on the sample before and after the tape test. It was shown that PMMA samples that were coated with POSS-MA and exposed to plasma had more gold remaining after the tape test than samples from the other groups.

### 9:45 Ruthenium Complexes Containing PPh<sub>2</sub>(CH<sub>2</sub>)<sub>n</sub>P(O)Ph<sub>2</sub> Ligands.

Nicole Ando<sup>1</sup>, \*Donna S. Amenta<sup>1</sup>, \*John W. Gilje<sup>1</sup>, and Glenn P. A. Yap<sup>2</sup>

<sup>1</sup>James Madison University, <sup>2</sup>University of Delaware.

The reactions of Cl<sub>2</sub>Ru(PPh<sub>3</sub>)<sub>3</sub> with 1 or 2 equivalents of PPh<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>P(O)Ph<sub>2</sub> or PPh<sub>2</sub>CH<sub>2</sub>P(O)Ph<sub>2</sub> were run in toluene at room temperature. From the reaction of Cl<sub>2</sub>Ru(PPh<sub>3</sub>)<sub>2</sub> with 1 equivalent of PPh<sub>2</sub>CH<sub>2</sub>P(O)Ph<sub>2</sub>, Cl<sub>2</sub>Ru(PPh<sub>3</sub>)<sub>2</sub>(PPh<sub>2</sub>CH<sub>2</sub>P(O)Ph<sub>2</sub>) was characterized by <sup>31</sup>P NMR spectroscopy and by a crystal structure. When the reaction is run in acetonitrile or with benzonitrile as a reagent, Cl<sub>2</sub>Ru(PPh<sub>3</sub>)(PPh<sub>2</sub>CH<sub>2</sub>P(O)Ph<sub>2</sub>)

(NCR) is observed. The chemical shifts of the  $\text{PPh}_2$  and  $\text{P(O)}$  moieties indicate that both the phosphino phosphorus and phosphoryl oxygen are bonded to the ruthenium. We postulate that the basicity of acetonitrile or benzonitrile facilitates the dissociation of the second  $\text{PPh}_3$ . The reaction of  $\text{Cl}_2\text{Ru}(\text{PPh}_3)_3$  with 2 equivalents of  $\text{PPh}_2\text{CH}_2\text{P(O)Ph}_2$  and excess acetonitrile or benzonitrile produces  $\text{Cl}_2\text{Ru}(\text{PPh}_2\text{CH}_2\text{P(O)Ph}_2)_2(\text{NCR})_x$ . The  $^{31}\text{P}$  NMR spectrum contains two peaks, one due to the phosphine and the other to the phosphoryl phosphorus of the ligands. Chemical shifts indicate both coordinate to the ruthenium. The structure of the product from the reaction of  $\text{Cl}_2\text{Ru}(\text{PPh}_3)_3$  with 2 equivalents of  $\text{PPh}_2\text{CH}_2\text{CH}_2\text{P(O)Ph}_2$  has not been completely characterized. However, the low temperature  $^{31}\text{P}$  NMR spectra shows an AB pattern characteristic of a *trans* P-Ru-P unit. The  $^{31}\text{P}$  NMR spectra of the product from the reaction between  $\text{Cl}_2\text{Ru}(\text{PPh}_3)_2$  with 1 equivalent of  $\text{PPh}_2\text{CH}_2\text{CH}_2\text{P(O)Ph}_2$  is not well defined even at low temperatures.

**10:00 Amphibian chemical defense: repelling *Batrachochytrium dendrobatidis* with the metabolites of cutaneous bacteria.**

Christian R. Schwantes, \*Kevin P. C. Minbiole, and \*Reid N. Harris

James Madison University

Amphibians worldwide are facing extinction at an alarming rate. The decline has been attributed to deforestation, pollution, global climate change, and recently, emerging disease. Chytridiomycosis, an amphibian disease caused by the fungal pathogen *Batrachochytrium dendrobatidis* has been linked to a number of extinctions. Some cutaneous bacteria, found naturally on amphibians, can inhibit the fungus via antifungal metabolites. *Lysobacter gummosus* produces 2,4-diacetylphloroglucinol, an antifungal compound with a minimum inhibitory concentration (MIC) of 136  $\mu\text{M}$ . *Janthinobacterium lividum* produces indole-3-carboxaldehyde (MIC = 69  $\mu\text{M}$ ) and violacein (MIC = 2  $\mu\text{M}$ ). In addition, red back salamanders from the wild have been observed to have detectable amounts of violacein in their mucus. These concentrations have been above the MIC of violacein. Since the antifungal metabolites from *J. lividum* are so potent, the bacterium was used in a bioaugmentation experiment with frogs (*Rana muscosa*) and salamanders (*Plethodon cinereus*). The bacterium was able to protect all frogs and most salamanders exposed to the fungus. These results indicate that bioaugmentation with antifungal bacteria is an effective way of protecting individuals from mortality associated with chytridiomycosis. Currently, investigations into the metabolites of *Chryseobacterium sp.* are underway. The bacterium is known to be antifungal, but no antifungal metabolites have been identified. Further research into these and other antifungal bacterial species is necessary to develop this bioaugmentation method for application to wild species.

**10:15 Material characterization of emplaced landmine components.**

Kevin Cabaniss and \*Kevin Davies

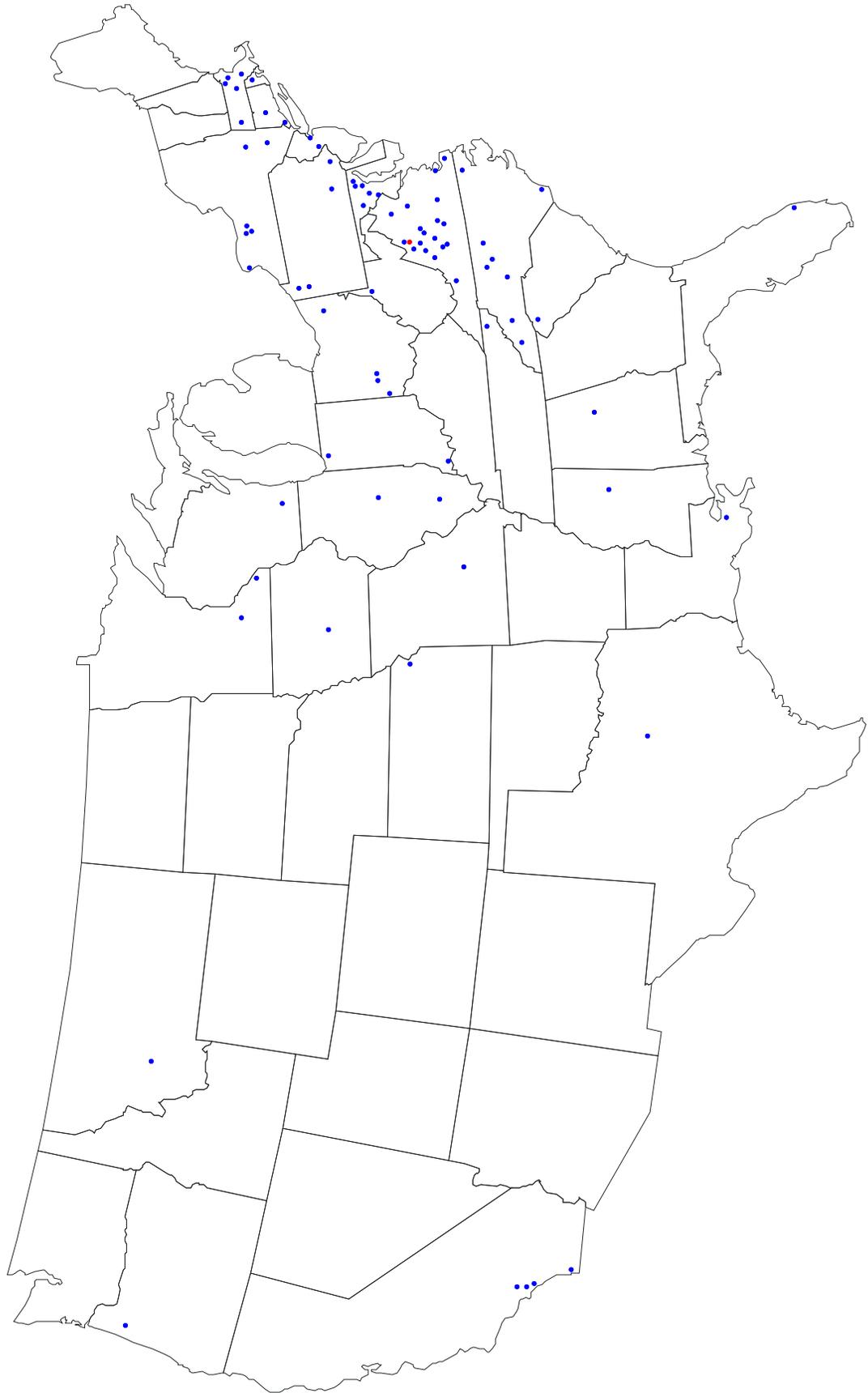
James Madison University

In many countries military conflicts have lead to the large-scale deployment of landmines. These sites often remain active for many years, causing harm to innocent life long after the hostilities have officially ended. Many countries and private groups have attempted to remove these weapons, but the process is slow and costly. During this process, it has become apparent that time and environmental conditions have some effect on the condition of the mines. Through the use of electron microscopy, infrared spectroscopy and colorimetric identification reactions, degraded landmine components have been analyzed and identified. With this data, the cause of the observed degradation can be determined, where the cause is environmental degradation, interactions between different associated components, or simply time itself. This data could lead to a better process of landmine removal, potentially making the process both less expensive and more efficient.

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|   | <p><b>Chem/Mats - Keynote Address</b><br/> <b>Friday, July 31</b><br/> <b>11:00 AM – 12:00 PM</b><br/> <b>ISAT/CS 159</b></p> |  |
| <p><b>Nickel Initiators for Olefin Polymerization and The Synthesis and Electronic Properties of Metal Chalcogenide Clusters</b><br/> <b>Dr. Brycelyn Boardman ('03)</b><br/> <b>Dept. of Chemistry</b><br/> <b>Columbia University</b><br/> <b>(Host: Dr. Donna Amenta)</b></p>   |   |   |
| <p>My seminar will focus on two different areas of research. The first will concentrate on the development of catalysts for olefin polymerization. This research is aimed at coordination complexes that utilize bi, tri, and tetradentate ligands that are easy to synthesize, are inexpensive to produce, and allow for controlled symmetry at the metal center. Different methods of catalyst activation as well as polymer products and their properties will be discussed. The second topic is focused on the on going struggle of the photovoltaic industry. Obtaining materials that can compete with crystalline silicon is an area of active research that spans a wide range of disciplines. Many promising metal chalcogenide semi-conducting materials have been developed, but have been plagued by processing issues and device lifetimes. Many of these problems arise from a lack of understanding of the fundamental properties of these materials. Having a better understanding of the growth of these materials as well as the influences of structural relationship on electronic properties could greatly impact the field of solid-state semiconductors and photovoltaic devices. To probe some of these problems metal chalcogenide clusters have been synthesized. The synthesis of these clusters is described as well as some investigation into their electronic properties.</p> |   |   |

**Chem/Mats - Pizza Luncheon**  
**Friday, July 31**  
**1:00 PM – 3:00 PM**  
**Dave's Taverna, Downtown Harrisonburg**  
**Dr. Dan Downey, Presiding**





Just as a dancer or musician can't learn their art simply by watching, students in the sciences must actively participate in a scientific pursuit to truly understand their craft. Undergraduate research has long been a critical part of the education of undergraduate scientists at James Madison University. The faculty, who care deeply about both being active scholars and excellent teachers, combine with students who desire to go beyond the typical classroom experience to create a unique atmosphere in which student and professor can both feel a sense of pride and ownership in high level scientific research. The primarily undergraduate focus of JMU means that undergraduates have the opportunity to learn how to be scientists in a nurturing but challenging atmosphere.

The summer of 2009 marks the 17th in which the Chemistry Department at JMU has hosted a Research Experiences for Undergraduates (REU) program funded by the National Science Foundation (NSF). The REU program is designed to give students from both JMU and other institutions the opportunity to do summer research. Since 2000, the Chemistry program has been joined by one in materials research which has included faculty and students from not only Chemistry but also Physics, Geology, ISAT, and Mathematics. This program was initially funded by the NSF program through the Division of Materials Research, but now receives funds from the Department of Defense (DoD) ASSURE (Awards to Stimulate & Support Undergraduate Research Education) program. In 2002, REU programs were started in Biology and Mathematics. The Biology program includes not only James Madison but also the biology departments at Eastern Mennonite University and Bridgewater College. These students are added to the many who work on other grants received by the faculty of James Madison University so that there are well over 100 undergraduate students each summer participating in scientific research which leads to publications, presentations, patent applications, collaborations with other institutions, and service to our community. JMU is one of only 2 primarily undergraduate institutions in the United States to have four funded REU programs at one time.

This symposium will feature the work of students who participated in the REU programs during the summer of 2009. This not only includes students who were supported directly by the grants from the NSF and the DoD which fund the REU and ASSURE programs, but also the many others funded through other research grants and internal JMU funds. This includes other students from the Biology, ISAT, and Physics Departments. All of these students worked together this summer and deserve to be commended for their accomplishments.

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