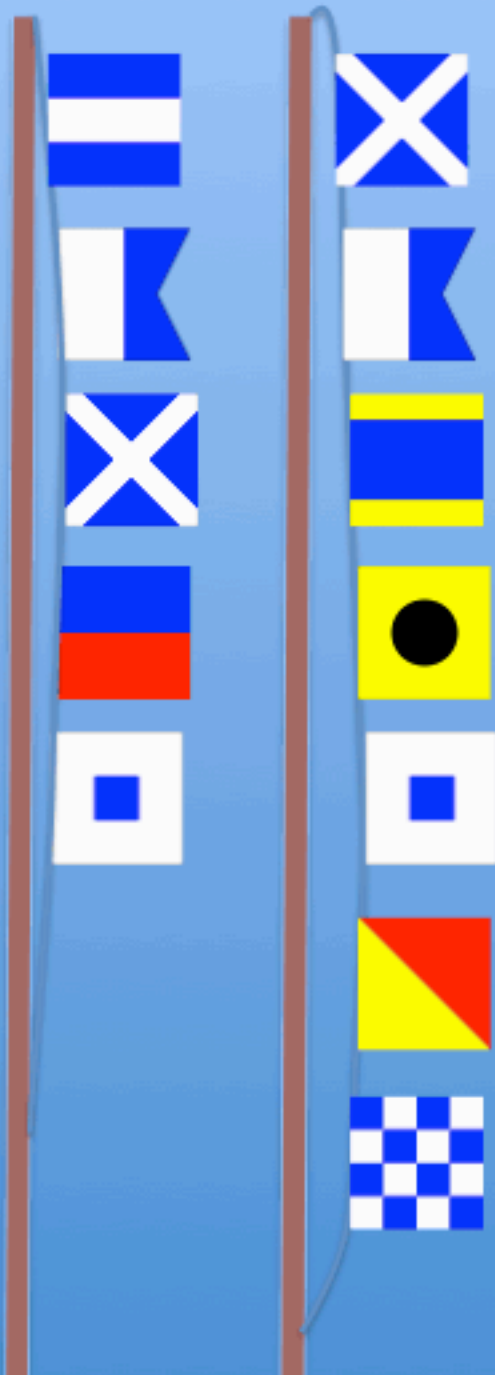


2011 SUMMER REU RESEARCH SYMPOSIUM



*Friday, July 29, 2011
Thursday, August 4, 2011
Friday, August 5, 2011*

*Roop Hall &
Festival Conference
Center*

*James Madison University
Harrisonburg, VA*

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

Allegheny College	Longwood College	SUNY-New Paltz
American University	Lynchburg College	Technical University of Denmark
Benedictine College	Mary Baldwin College	Towson University
Bethany College	Merrimack College	University College, Galway (Ireland)
Bethel College	Miami University	University of Alabama
Blue Ridge Community College	Millersville University	University of Belgrade (Serbia)
Bridgewater College	Mississippi State University	University of Dayton
Boston College	Montana Tech	University of Evansville
California State - Channel Islands	Mount Holyoke College	University of KwaZulu-Natal (South Africa)
California State—Long Beach	Mount Union College	Univ. of London—Royal Holloway (UK)
Catawba College	New River Community College	University of Mary Washington
Central State University	Niagara University	University of Maryland, Baltimore Co.
Central Michigan University	Norfolk State University	University of Maryland, College Park
Chapman University	Northern Virginia Community College	University of Missouri—Rolla
The College of New Jersey	Paul Quinn College	University of North Carolina— Asheville
College of William and Mary	Piedmont Virginia Community College	University of North Carolina— Wilmington
Clarkson University	Pomona College	University of Plymouth (UK)
Clemson University	Pontifical Catholic University of Puerto Rico	University of Rochester
Davidson College	Princeton University	University of San Diego
Drake University	Providence College	University of Virginia
Eastern Mennonite University	PUC-Campinas (Brazil)	Villanova University
East Tennessee State University	Queen's University, Belfast (UK)	Virginia Union University
Edgewood College	Radford University	Washington & Lee University
Elizabeth City State University	Ramapo College of New Jersey	Western Carolina University
Elon University	Randolph College	West Virginia University
Fairfield University	Randolph-Macon College	Wheaton College
Florida Atlantic University	Rochester Institute of Technology	Willamette University
Framingham State University	Rutgers University	Winona State University
Gallaudet University	St. John Fisher College	Winston-Salem State University
Grove City College	Saint Joseph's College	Worcester Polytechnic Institute
Hampden-Sydney College	St. Vincent College	Xavier University
Hanover College	Salem College	
Harvey Mudd College	St. Olaf College	
High Point University	Southern Illinois University	
Hood College	Stevenson University	
Illinois Wesleyan University	Sweet Briar College	
Ithaca College		
James Madison University		
KAIST (Korea)		

Mathematics - Oral Presentations

Friday, July 29

11:00 AM - 1:20 PM

103 Roop Hall

11:00 - 11:20

Periodicity and asymptotics of Tchoukaillon sequences.

David Creech*, Central Michigan University

Jeff Anway*, Longwood University

Tchoukaillon is a single-player sowing game in which there is a unique board for each natural number, indexed by board size. We will examine the global periodicity properties of Tchoukaillon and the long-term asymptotic behavior that describes the surprisingly complicated relationship between board size and board length.

11:25 - 11:45

Algebraic Tchoukaillon representations.

Benjamin Warren*, Ramapo College of New Jersey

Fanya Wyrick-Flax*, Bard College

We present three algebraic representations of the sowing game Tchoukaillon and construct maps translating between each representation. These maps yield information about the relationships between the pit size and move sequences and in addition enable us to construct a binary addition operation on Tchoukaillon boards.

11:50 - 12:10

Permutations avoidance and the Catalan triangle.

Wesley K. Hough*, Hanover College

Jacob W. Ziefle*, The College of New Jersey

Some of the first questions regarding permutation pattern avoidance arose from sorting methods in computer science. In one-line notation, a permutation of n letters avoids a pattern of k letters if every subsequence in the permutation has at least two elements out of order relative to the pattern. It has been previously shown that the size of the set of permutations of n letters that avoid a 3-letter pattern is equal to the n -th Catalan number. In this paper, we refine this result for all patterns of size 3 by intuitively partitioning the set of permutations of n letters that avoid a given pattern and relating these partitions to some well-known refinements of the Catalan numbers.

12:15 - 12:35

Homology of pattern avoidance.

Derek DeSantis*, California State University Channel Islands

Rebecca Meissen*, Worcester Polytechnic Institute

In this presentation, we explore the relationship between topology and partially ordered sets. We consider the symmetric group S_n under the Bruhat partial order. Björner and Wachs showed that any interval in S_n is homotopic to a single sphere. We examine the topology of $S_n([p])$, the symmetric group on n letters which avoids a specific permutation pattern p . Babson and Hersh introduced a method for analyzing the homology of a poset via Discrete Morse Theory. We use this to study $S_n([321])$.

12:40 - 1:00

A different view of Bruhat ordering.

Bill Rau*, James Madison University

Bruhat ordering is an intuitive way to partially order permutations, creating interesting combinatorial objects. However, combinatorialists are not the only ones who find this form of ordering interesting and useful. This presentation will focus on some other ways Bruhat ordering is used in modern mathematical research, delving into group theory and algebraic geometry to reveal new ways to look at an already-familiar concept.

NOTES

Chem/Mats - Oral Presentations Session I

Thursday, August 4

8:30 AM - 10:00 AM

Festival Ballroom A

Dr. Kevin Caran, Presiding

8:30 - 8:45

Characterization of deposited Alumina (Al_2O_3) on Gallium Nitride (GaN) Substrate using Electron Beam Vapor Deposition

Bojan Ljubovic*, Dept. Of Physics, James Madison University

Costel Constantin, Dept. Of Physics, James Madison University

Metal oxide semiconductor field effect transistors (MOSFET) made with Silicon as a semiconductor and SiO_2 as a gate dielectric approaches the physical minimization limit of ~ 25 nm gate width. This limit is mainly due to the current leakage through the SiO_2 gate dielectric which in turn increases the power consumption, and consequently decreases the total efficiency of the MOSFET. Recently scientists look into creating gallium nitride (GaN) based MOSFETs that use the same SiO_2 as a gate dielectric. One solution that can alleviate the current leakage in MOSFETs is to replace the SiO_2 layer with a high-k dielectric constant material. Alumina has a dielectric constant of ~ 16 which is much larger as compared to the one of SiO_2 (~ 3.9). In this study, we present preliminary results of Al_2O_3 deposited on SiO_2 and GaN substrates by the use of electron beam vapor deposition chamber.

8:45 - 9:00

Effect of Protic and Aprotic Solvents on Negative Ion ESI Response for a Physiochemically Diverse Group of Acidic Compounds.

Brian Huffman*, Dept. of Chemistry and Biochemistry, James Madison University

Christine Hughey, Dept. of Chemistry and Biochemistry, James Madison University

Negative ion electrospray ionization (ESI) is commonly used to convert acidic molecules from the liquid phase to the ionized gas phase for mass spectrometric detection. Despite ESI's wide use, little is understood about the mechanism through which various physiochemical properties influence response. Many properties have been studied individually, but this study seeks to observe the collective impact of chemical attributes such as pKa, log P (log of the octanol-water coefficient), gas phase proton affinity, total polar surface area, capillary voltage and solvent composition. An Agilent triple quadrupole mass spectrometer with a Jet Stream ESI source was used to measure the response of 37 physiochemically diverse acidic compounds in methanol, water, acetonitrile and acetone. For most compounds, the highest response was in methanol. A positive correlation was identified between log P and response when looking at compounds with similar pKa's. However, little correlation was observed when comparing compounds with different pKa's and log P values. The lack of trend suggests the need for a multivariate approach. The end goal is to produce a practical multivariate computational model, which takes into account these various physiochemical properties to predict negative ESI response. This model will aid in optimization of LC-MS method development, allowing reproducible instrument operation and increased sensitivity.

9:00 - 9:15

Characterizing the movement of grains in a 2D rotating drum with imposed vibrations.

Nora Swisher*, Dept. of Physics, James Madison University

Brian Utter, Dept. of Physics, James Madison University

We study particle trajectories and surface behavior of photoelastic grains in a 2D circular rotating drum subjected to imposed vertical vibrations. Jamming appears in many granular systems (grain silos & chutes, landslides, mixing industrial materials, etc.) and vibration (granular temperature) is a primary factor in the jamming/unjamming transition. For granular materials, flow is characterized by sudden avalanches, large shear gradients, and history dependence and these characteristics make it difficult to form general equations of flow. To quantitatively measure the flow, jamming, and mixing properties of the grains, images are taken and each particle's position and velocity are found for each frame. External vibration leads to increased compaction of the grains, larger rearrangements, and a narrower shear band. Particle tracking will allow us to closely analyze the velocity profiles, trajectories of individual grains, and separation and diffusion of originally neighboring grains.

9:30 - 9:45

Distribution of Almond Flavonoids in Blanch Water and Skins as a Function of Blanching Time and Temperature.

Rima Januszewicz*, Dept. of Chemistry and Biochemistry, James Madison University

Jenny Phung*, Dept. of Chemistry and Biochemistry, James Madison University

Brian Huffman*, Dept. of Chemistry and Biochemistry, James Madison University

Christine Hughey, Dept. of Chemistry and Biochemistry, James Madison University

The distribution of polyphenols in blanched almond skins and blanch water as a function of time and temperature was quantified using negative ion electrospray time-of-flight mass spectrometry (ESI TOF-MS). Almonds were blanched in room temperature and 100°C water for up to 10 min. Measurement of the total phenolic content of the skins and water showed that the high temperature of the blanch water leached 90% of the phenolics from the skins during the first 240 s of blanching. LC-TOF measurements showed that most of the polyphenols quantified leached from the skins and then precipitated from the 100° blanch water due to limited water solubility as evidenced by a logarithmic fit to kinetic data (concentration vs. time). This fit is indicative of first order kinetics. We also found that hydration and temperature affected the extraction efficiency of the polyphenols from the skins. For the phenolic acids and flavanols, the sum of the concentration in the skins and blanch water at 25°C and 100°C was significantly greater than the untreated control, indicating that both hydration and temperature increase extraction efficiency. For the flavonol rutinosides, hydration was a greater factor in increasing extraction efficiency as the sum of the water and skins concentrations were similar at 25°C and 100°C. For the flavonol glucosides, the sum of the water and skins concentrations was similar to the control, indicating that hydration and temperature did not significantly effect extraction. This work shows that the blanch water, in particular the 100°C blanch water, is rich in polyphenols and may potentially be used for nutraceutical purposes since polyphenols have been shown to lower risk for inflammatory diseases.

9:45 - 10:00

Investigating Protease Digestion of RecA Using SDS gel electrophoresis.

Mika Bennett-Fraychineaud*, Model Secondary School for the Deaf

Amber Marchut, Model Secondary School for the Deaf

Gina MacDonald, Dept. of Chemistry and Biochemistry, James Madison University

RecA is a DNA repair protein from *E. coli*. SDS gel electrophoresis was used to study Trypsin digestion of RecA. Trypsin cleaves RecA into smaller peptides. Experiments were done to find out how much digestion would occur when Trypsin is added to RecA. SDS gel electrophoresis separates proteins by size. The SDS gel electrophoresis separates Trypsin and RecA bands. RecA runs in the middle of vertical lanes as its' molecular weight is 38 kDa. Trypsin is close to the bottom of the gel because its' molecular weight is 23.8 kDa. Additional information was found about Trypsin and RecA by changing incubation time and concentrations. For example, increasing the concentration of Trypsin, results in increased RecA digestion time. Decreasing the concentration of Trypsin slows digestion of RecA so the incubation time can be varied. In several experiments, Trypsin was added to RecA and incubated for varying times. The results showed how changes in the experimental conditions change RecA digestion over time.

Chem/Mats - Poster Session A

Thursday, August 4

10:00 AM - 11:00 AM

Festival Ballroom B/C

Tracking Antifungal Metabolites on Amphibian Skin through Use of Q-TOF High Performance Liquid Chromatography/Mass Spectroscopy (LC/MS).

Alison L. Blackman*, Dept. of Chemistry and Biochemistry, James Madison University

Thais L. Teotonio*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin P.C. Minbiole Dept. of Chemistry and Biochemistry, James Madison University

Batrachochytrium dendrobatidis (Bd) is a fungal pathogen that has played a major role in the steep decline of amphibians worldwide. It has been found that the presence of certain species that reside on the skin of amphibians serve as a natural defense mechanism against this pathogen. Such bacterial species protect against Bd by producing antifungal compounds. With almost 40% of amphibians facing extinction, the identification of these metabolites and the bacteria that produce them is crucial for finding

ways to protect amphibians that do not maintain such residential bacteria. Due to its high sensitivity, the use of a Q-TOF high performance liquid chromatography/mass spectroscopy (LC/MS) allows for easy detection of such compounds. Using Agilent MassProfiler software, samples obtained from newts and bullfrogs were analyzed and found to have an array of unidentified metabolites. In addition, violacein, an antifungal compound known to be produced by certain bacterial species, was detected in three of the provided samples. The use of the LC/MS, with support of a high performance liquid chromatography (HPLC) with UV-Vis, revealed that the BOH3 strain of *Pseudomonas fluorescens* produces DAPG, another known antifungal metabolite produced by bacteria. Though satisfactory results were obtained, sample preparation needed to be modified in order to obtain optimal results while using the LC/MS. The incorporation of the 13mm PTFE 0.2 μm filter in sample preparation was found to serve as an effective filtration device that withstood methanol, the solvent used in the extraction of metabolites from the sample, and did not prohibit the passage of our known antifungal compounds. In addition, a polyurethane foam swab was found to be the preferred swab regarding absorption and release of three antifungal compounds known to be produced by bacteria.

Synthesis of Ruthenium Dinitrosyl Compounds with Phosphine/Phosphine Oxide Ligands; Potential NO Releasing Drugs.

Duane Bock*, Dept. of Chemistry and Biochemistry, James Madison University

Donna Amenta, Dept. of Chemistry and Biochemistry, James Madison University

John Gilje, Dept. of Chemistry and Biochemistry, James Madison University

NO is an important cellular messenger molecule involved in many physiological and pathological processes. Low levels of NO production are important in protecting an organ such as the liver from ischemic damage.¹ Chronic expression of NO is associated with various carcinomas and inflammatory conditions including juvenile diabetes, multiple sclerosis, arthritis and ulcerative colitis.¹ A number of ruthenium nitric oxide complexes are of interest as drugs as they are known to release NO under certain conditions. In our lab, we have evidence that NO is released from $\text{Ru}(\text{NO})\text{Cl}_3[\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2]_2$ during a reaction with AgBF_4 . We postulate that this reaction is aided by the ability of the $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ ligand to convert from mono to bidentate coordination. In this project we have looked into the preparation of ruthenium dinitrosyl complexes with $\text{P}(\text{Ph})_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$, $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$, and $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ ligands. Reactions similar to those used to prepare $\text{Ru}(\text{NO})_2(\text{PPh}_3)_2$ failed.² From there, the reactions of $\text{Ru}(\text{NO})_2(\text{PPh}_3)_2$ with $\text{P}(\text{Ph})_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$, $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$, and $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ were investigated. In NMR tube experiments using $\text{P}(\text{Ph})_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$, mixtures of $\text{Ru}(\text{NO})_2(\text{PPh}_3)_2$, $\text{Ru}(\text{NO})_2(\text{PPh}_3)(\text{P}(\text{Ph})_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2)$ and $\text{Ru}(\text{NO})_2(\text{P}(\text{Ph})_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2)_2$ were observed. However, pure samples could not be obtained from bulk scale reactions. With $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ similar NMR tube results were obtained, but through careful manipulation of solvents and other conditions relatively pure $\text{Ru}(\text{NO})_2(\text{PPh}_3)(\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2)$ or $\text{Ru}(\text{NO})_2(\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2)_2$ can be isolated. Experiments using $\text{P}(\text{Ph})_2\text{CH}_2\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ are in very initial stages. Details of these experiments will be discussed.

¹ http://en.wikipedia.org/wiki/Nitric_oxide, Retrieved July 28, 2011.

Synthesis and characterization of hybrid organic-inorganic frameworks using the hydrotris(triazolyl)borate ligand.

Caroline Campbell*, Dept. of Chemistry and Biochemistry, James Madison University

Dr. Barbara Reisner, Dept. of Chemistry and Biochemistry, James Madison University

Zeolitic imidazolate frameworks have captured a great deal of attention because of their potential for gas storage, separations, and catalysis. A new material, $\text{K}[\text{BH}(\text{trz})_3]$, ($\text{trz}=1,2,4\text{-triazolate}$) was synthesized from the reaction between potassium borohydride (KBH_4) and excess triazole (Htrz). $\text{K}[\text{BH}(\text{trz})_3]$ (KL) was crystallized from acetonitrile, producing clear, transparent hexagonal rods about 0.2 mm in length. The FTIR and NMR spectra confirmed that the compound was present without excess triazole or solvent. TGA data indicated that the compound is stable to 250 °C. Single crystals have been grown for elemental analysis and single crystal structure determination. Three new frameworks containing transition metals ($\text{M} = \text{Co}, \text{Ni}, \text{Cu}$) were synthesized by layering. $\text{Co}[\text{BH}(\text{trz})_3]_2$ was synthesized by the slow diffusion of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and KL in DMF and hexanes, producing 0.5 mm yellow rods. $\text{Ni}[\text{BH}(\text{trz})_3]_2$ was synthesized by the slow diffusion of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ and KL in DMF and hexanes, producing 2 mm purple rods. $\text{Cu}[\text{BH}(\text{trz})_3]_2$ was synthesized by the slow diffusion of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ and KL in DMF and hexanes, producing 1 mm blue rods. Analysis of these materials in progress.

Submerged granular flow of hydrophobic and hydrophilic sand

Benjamin Foltz*, Dept. Of Physics, James Madison University

Dr. Brian Utter, Dept. Of Physics, James Madison University

We experimentally investigate submerged granular flows of hydrophobic and hydrophilic grains in a rotating drum. While slurry and suspension flows are common in nature and industry, effects of surface chemistry on flow behavior have received little attention. The experiment consists of a cylindrical drum containing various concentrations of hydrophobic and hydrophilic grains of sand submerged in water and rotated at a constant angular velocity. Images of the resulting avalanches are taken and analyzed. While it is known that at slow speeds, submerged avalanches appear qualitatively similar to dry flows, our results suggest that the surface properties of the grains affect underwater flow significantly. High concentrations of hydrophobic grains result in the formation of aggregates. At concentrations larger than 75% hydrophobic sand, the avalanches do not behave in a manner which is typical for sand, but as the concentration decreases, the aggregates are smaller, the angle of repose decreases, and the grains start showing properties similar to those in regular sand. We believe that the behavior of the grains and aggregates is controlled primarily by an inability for the water to penetrate as well as the presence of an air/water interface in the drum. We present data on the size of the aggregates, slope, and contact angle measurements with changes in concentration of hydrophobic sand.

Characterization of Thin-Film Bismuth Vanadium Oxide (BiVO_x) Semiconductors for Photoelectrolysis Applications.

Brandon H. Journell*, School of Engineering, James Madison University

Milan Y. Patel*, General Studies, New River Community College

Dr. David Lawrence, ISAT, James Madison University

Dr. Keith Holland, School of Engineering, James Madison University

Hydrogen is one of the most promising renewable and sustainable clean energy carriers. For hydrogen energy to be truly “green” it needs to be produced by methods that do not pollute the environment. Work this summer was focused on the methods necessary to develop a characterization system for semiconductor photo-electrodes. Characterization methods include measuring the photocurrent density as a function of the bias voltage, X-Ray diffraction, SEM imaging, and UV/VIS spectroscopy. Along with developing methods for characterizing the semiconductor materials, the testing procedures were refined to ensure repeatability. Bismuth Vanadium Oxide (BiVO_x) was characterized using these techniques. Results from testing will be presented. BiVO_x was investigated for comparison with theoretical performed by a group at NREL (National Renewable Energy Laboratory) on dopants and their effect on electrical properties.

Infrared studies of the effects of salts on amino acid side chains.

Alesha May*, Department of Chemistry, Rochester Institute of Technology

Gina MacDonald, Dept. of Chemistry and Biochemistry, James Madison University

There are twenty common amino acids. Each amino acid consists of a carboxyl group and a side chain or “R” group. At pH level of 7, the carboxyl group exists as –COO⁻ and the side chain as –NH₃⁺. Previous studies in the MacDonald lab have focused on salt interactions with proteins. The amino acids with salt solutions will be used as a model to help with future studies of proteins. Fourier transform infrared (FTIR) spectroscopy allows the study of different vibrations of amino acids and salts. Here we studied twelve different amino acids in six different salt solutions. We compared our results to previous studies of amino acids obtained in the absence of salts. Data shows slight changes in frequency are observed in the presence of salt. These shifts range from 1-10 wavenumbers difference from the amino acids vibrations in the absence of salts. Therefore, we can determine that the salts are interacting with the amino acid structures. The Hofmeister Series is an arrangement of salts, anions, or cations in descending order of their effect upon protein precipitation. Anions tend to have a larger effect than cations on protein structures. Hofmeister ions are known to change water structures and have specific interactions with proteins. Some ions increase the solubility of nonpolar molecules. In most cases addition of salts resulted in the amino acid vibrations shifting to lower wavenumbers ranges, showing a large shift to the right compared to amino acids in the absence of salt. However, in some solutions of amino acids, the salts caused small shift to the higher frequencies. In all cases we can see that the salt solutions have some interactions with the amino acids, which result in observable changes in infrared spectra.

Elemental Analysis of *Didymosphenia geminata* (Didymo)

Phillip Chambers*, Dept. of Chemistry and Biochemistry, James Madison University

Waleed Ahmad*, Dept. of Chemistry and Biochemistry, James Madison University

Joline McNece*, Dept. of Chemistry, RIT/NTID

Daniel Downey, Dept. of Chemistry and Biochemistry, James Madison University

The single celled freshwater algal diatom, *Didymosphenia geminata* (didymo) is an invasive algal species that produces large and repugnant stalk mats or 'blooms' in streams. Didymo was first observed in the Faroe islands (Scotland) in the early 19th century, has been spread worldwide and identified in four rivers of Virginia. Basic biological and chemical data are being collected to provide a better understanding of this pest with the hope that future mitigative measures may be developed. The goal of our project was to determine an "elemental fingerprint" for didymo collected from the Jackson River in Bath County, Virginia. A two step process of base and acid digestion to dissolve silica (SiO₂) and organic matter, respectively, with microwave assisted digestion was successful in preparing aqueous solutions that were subsequently analyzed by Inductively Coupled Plasma – Mass Spectrometry (ICP-MS). Water chemistry was also determined for the reach of the river where Didymo was found. The concentrations and ratios of 29 elements in the didymo and water samples were evaluated for this project.

Depth and temperature of the mantle beneath Mole Hill, an Eocene basalt near Harrisonburg, VA.

Brittany Sacco*, Dept. Of Geology and Environmental Science, James Madison University

Elizabeth A. Johnson, Dept. Of Geology and Environmental Science, James Madison University

Harvey E. Belkin, US Geological Survey, Reston, VA

Mole Hill is a 48 Ma basaltic neck near Harrisonburg, VA, located in the Shenandoah Valley. Mantle xenocrysts of clinopyroxene (Al-augite), olivine, spinel, and rare plagioclase are trapped within the basalt. Clinopyroxene-melt and olivine-melt geothermobarometry were used to determine the pressure and temperature at which these xenocrysts formed and, implicitly, the depth and temperature in the mantle from where they originate. Clinopyroxene and olivine compositions were determined using the JEOL 8900R Electron Microprobe at 20 kV, 20 nA and a 2 μm spot size at the USGS in Reston, VA. Whole-rock compositions were used to represent the melt composition. Olivine xenocryst rims in equilibrium with the host magma have compositions from Fo₆₄₋₈₈. Clinopyroxene rims have an average composition of Wo₄₆En₄₂Fs₁₂ while clinopyroxene cores have an average composition of Wo₄₁En₄₉Fs₁₀. The clinopyroxene, olivine, and melt compositions were input into a set of geothermobarometers summarized in Putirka (2008). The average temperature calculated using clinopyroxene-melt thermometry is 1227±41 °C and using olivine-melt thermometry is 1222±62 °C. The average pressure using clinopyroxene rim compositions is 10±2 kbar. The average pressure determined for the cores of clinopyroxene xenocrysts is slightly higher, 13±1 kbar. These pressures are within the stability field of spinel peridotite (clinopyroxene cores) and at the boundary between the plagioclase and spinel peridotite stability fields (clinopyroxene rims), consistent with the observed xenocrystic mineral assemblage. The corresponding depth of ~36 km for the clinopyroxene xenocryst cores is consistent with seismic data indicating the Moho is ~40 km below the Blue Ridge region (TEENA experiment). The calculated temperature places the mantle xenocrysts close to the solidus for Al-augite for these depths. Our data places important constraints on the depth and characteristics of the mantle beneath the Shenandoah Valley.

Synthesis of RNA Analogues.

Brooke Stevens*, Dept. of Chemistry and Biochemistry, James Madison University

Debra Mohler, Dept. of Chemistry and Biochemistry, James Madison University

The synthesis of stable RNA analogues that can bind via Watson-Crick base pairing is a goal of therapeutic siRNA treatments. Our proposed synthesis of the siRNA analogues entails using a single step polymerization. Progress in the synthetic approach of using ring opening metathesis on synthetic monomers will be presented.

Phase Behaviors of PEO-PPO-PEO Triblock Copolymer in the Presence of Osmolytes.

Emigdio E. Turner*, Dept. of Chemistry, James Madison University

Yanjie Zhang, Dept. of Chemistry, James Madison University

Osmolytes have significant effects on protein folding and stability. For example, urea is widely used as a denaturant, while trimethylamine N-oxide (TMAO) is a powerful stabilizer. Work studying the effects of osmolytes on protein stabilization/denaturation goes back more than half a century. Despite this, the

mechanisms by which osmolytes affect protein structure still remain elusive. Herein, we employ a model system, the phase behavior of poly-(ethylene oxide)-b-poly(propylene oxide)-b-poly(ethylene oxide) (PEO-PPO-PEO) triblock copolymers in the presence of osmolytes, to investigate the mechanism of osmolytes-protein interactions. The phase transition temperatures of PEO-PPO-PEO in the presence of 12 osmolytes were measured by using an automated melting point system. It was found that the polymer undergoes a two-step phase transition in solutions containing all the protein stabilizers used in this study. On the other hand, protein denaturants showed an interesting trend in affecting the phase transition of the polymer. The polymer shows a two-step phase transition in solutions containing urea up to 6 M. When the hydrophobicity of the denaturant increases, switching from urea to 1,3-diethylurea, the polymer shows only one step in phase transition. Further research will be done to determine the molecular level interactions of triblock copolymers with osmolytes.

Chem/Mats - Oral Presentations Session II

Thursday, August 4

11:00 AM - 12:00 PM

Festival Ballroom A

Dr. Brycelyn Boardman, Presiding

11:00 - 11:15

Chemical Demonstrations – Developing an Infrastructure for Outreach.

Casey Rogers*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin L. Caran, Dept. of Chemistry and Biochemistry, James Madison University

This project, which has been ongoing for close to two years, aims to aid and provide resources to people interested in using chemistry demonstrations in a variety of venues. Specifically, we are targeting college professors, college students and K-12 teachers, largely within the state of Virginia. We have made significant progress over the last year. A new website was developed (Summer 2011), with improved functionality and appearance compared to the original site (Summer 2010). This website includes over 50 demonstrations with instructions on how to perform them, including downloadable and editable Word formats. In addition the website contains lesson plans and problem sets corresponding to selected demos for ease of use in the classroom. The Second Annual Chemistry Demonstration Workshop for High School Teachers was held for 20 participants on July, 15th, 2011. The workshop (9am-3pm) included hands-on demonstration instruction, a presentation on the importance of demos, and opportunities to discuss demos with other high school teachers. Videos for demos using liquid nitrogen and dry ice were recorded and produced in collaboration with JMU's Center for Instructional Technology (CIT). These videos were incorporated into the website, and DVD copies were given to participants of the workshop.

11:15 - 11:30

Development of a Point Source Photoacoustic Greenhouse Gas Sensor for CO₂

Chae yeun Jeon*, Dept. of Chemistry and Biochemistry, James Madison University

Colin Wallace*, Dept. of Chemistry and Biochemistry, James Madison University

Daniel Havey, Dept. of Chemistry and Biochemistry, James Madison University

Greenhouse gases, most notably carbon dioxide, are important species in atmospheric chemistry and climate change. There is growing concern that their continuously increasing concentrations will lead to global surface temperatures producing major climate changes. A key issue for the next few decades will be to accurately measure the amount of atmospheric CO₂ produced at the local, national, and international scale. Motivation has been amplified since the passage of the American Clean Energy and Security Act of 2009 by the United States House of Representatives. The bill, now under consideration by the United States Senate, could create a type of cap and trade program utilizing carbon emission credits. If an emissions trading system is implemented then American taxpayers and private industry will likely both demand accurate and precise measurements of local CO₂ concentrations. However, this is a difficult technical problem because useful measurements involve quantifying small changes on top of a relatively large atmospheric background of approximately 385 parts per million. Current portable measurement systems used to quantify CO₂ concentrations may suffer from low sensitivity and/or high costs and typically require calibrations against reference gas standards. A major obstacle for utilizing state-of-the-art greenhouse gas detectors is resource investment. Current state-of-the-art instruments are relatively

expensive and this prohibits their deployment on a large scale. Thus, there is an urgent need for new robust, yet simple and affordable, high-performance analytical instruments to measure greenhouse gases in both laboratory and field environments. In this work, progress in the development of a new portable greenhouse gas measurement instrument based on photoacoustic spectroscopy is discussed. Specifically, the effects H₂O on measured CO₂ signals near 1.57 mm were quantified. H₂O broadening as well as direct spectral interferences were observed and have been characterized.

11:30 - 11:45

Fingerprinting Limestone in an Archeological Study.

Rebecca Shifflett*, East Rockingham High School

Tammy L. Stone, East Rockingham High School

Julie Ritchie, Turner Ashby High School

Daniel M. Downey, Dept. of Chemistry and Biochemistry, James Madison University

The Shenandoah Valley is underlain by limestone rocks which have been used as a construction material for buildings and roads. Limestone varies in the amount of calcium, magnesium and other elements from one location from other. The focus of this study was to see if variations in the ratios of calcium to magnesium and concentrations of some trace elements could be used to match rock used in historic building construction with the quarry location. We developed a Flame Atomic Absorption (AA) method to determine the magnesium and calcium ratios using the calibration curves from the AA to calculate parts per million (ppm) for calcium and magnesium. In addition, we used Inductively Coupled Plasma- Mass Spectrometry (ICP-MS) to determine trace elements at parts per billion (ppb) levels found in the rock. We tested limestone rock samples taken from several structures on the Stickley House property including a chimney, the foundations of the Stickley Mill and the Old Bowman Mill, and the abutment for an old bridge where the Valley Pike had once crossed Cedar creek. These structures were significant features during the War Between the States. We also tested rock samples taken from three possible quarry sites with exposed bedrock that showed signs of block removal. The results of this study will be shared with the US National Park Service as part of historical interpretation of the site.

11:45 - 12:00

Real-Time Micro-Phase Separation Kinetic Analysis of POSS-MA Thin Films Using Atomic Force Microscopy.

Skylar White*, Dept. Of Chemistry and Biochemistry, James Madison University

Brian Augustine, Dept. Of Chemistry and Biochemistry, James Madison University

Chris Hughes, Dept. Of Physics and Astronomy, James Madison University

Poly(propylmethacrylisobutyl POSS co-methylmethacrylate) (POSS-MA) is a co-polymer that contains polyhedral oligomeric silsesquioxane (POSS) cages co-polymerized to a poly(methyl methacrylate) (PMMA) backbone. 2 mg/mL solutions of 20 – 70 wt% POSS-MA are dissolved in chloroform and deposited onto samples of oxidized Si wafers using spin casting. Immediately after spin casting, these samples are analyzed using atomic force microscopy (AFM) while being heated in a range of 25-90° C. Typical 30 – 70 wt% POSS-MA thin films exhibit varying rates of micro-phase separation. Once this micro-phase separation is complete, the pixel areas of the dendritic structures are measured using the AFM software on the complete time-series of AFM scans. These varying area determinations are normalized and then fit to the Avrami plot by graphing $\ln(-\ln(1-f))$ vs. $\ln(\text{time})$ with “f” being the normalized area and the time being time after deposition. From this graph, the resulting slope is the dimensionality of growth constant and the y-intercept is the natural logarithm of the rate constant ($\ln k$). Data shows the dimensionality of growth constant to vary from 1.72 to 2.15 and the $\ln(k)$ to vary from -9.02 to -14.14 when the scan is conducted at 35° C for 30 wt% POSS-MA thin films. This data is consistent with the literature values of two dimension micro-phase separation in polymer thin films. Current work involves characterization of the silicon composition of the dendritic structures present on the POSS-MA thin films using energy dispersive spectroscopy (EDS).

Chem/Mats - Oral Presentations Session III

Thursday, August 4

1:00 PM - 2:00 PM

Festival Ballroom A

Dr. Brian Utter, Presiding

1:00 - 1:15

Constructing Devices to Measure the Torsional Properties of Carbon Nanotubes.

Anthony N. Speziale*, Department Of Physics, James Madison University

John Bridstrup*, Department Of Physics, James Madison University

Phillip Meyerhofer*, Department Of Physics, Saint Vincent College

Dr. Scott Paulson, Department Of Physics, James Madison University

Multiwalled carbon nanotubes act much differently than their single walled counterparts when submitted to successive torsional forces. The torsional properties of single walled carbon nanotubes are naturally perspicuous. When a torsional force is applied to a single walled nanotube, much like any string or rope, the nanotube relaxes to its previous state when that force is removed. Successive twists of the nanotube show no difference in behavior. On the other hand, with each successive application of a torsional force, multiwalled nanotubes exhibit some form of torsional friction. It becomes more difficult to twist the nanotube the same amount. This phenomenon is theorized to occur from the chirality of the nanotubes and the interaction between the carbon atoms. Our experiment develops a structure that will suspend a nanotube between two electrically conductive leads and attempts to use a magnetic field to twist the nanotube and concurrently use a transmission electron microscope to observe how the changing carbon lattice affects the magnitude of the torsional friction.

1:15 - 1:30

The Synthesis of Novel Polycephalic and Gemini Amphiphilic Derivatives of Mesitylene.

Jhosdyn Barragan*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin L. Caran, Dept. of Chemistry and Biochemistry, James Madison University

Derivatives of mesitylene were synthesized in order to prepare a series of amphiphiles with n benzylic quaternary ammonium headgroups and $3-n$ pyridinium headgroups, where $n = 0-3$. The series includes compounds with tail lengths from 8 – 16 carbons. Nine compounds in this series have been prepared, including derivatives where $n = 0, 2$ and 3 . The preparation of compounds in the remaining subset ($n = 1$) are still in progress. Reaction temperature, water content, and solvent polarity were found to be key factors in controlling the synthesis of various derivatives. Preliminary studies, in collaboration with JMU Biology, suggest that antibacterial activity was inversely proportional to tail length for compounds where $n = 2$.

1:30 - 1:45

Measuring 3-D Grain Sizes for Crystal Size Distributions Analysis Using Singular Value Decomposition for Recovering Crystallization Rates

Theresa Dalmut*, Department of Mathematics and Statistics, James Madison University

Brittany Wilhelm*, Department of Mathematics and Statistics, James Madison University

Roddy Amenta, Department of Geology & Environmental Science, James Madison University

Crystal size distribution (CSD) analysis is used to recover quantitative crystallization information from the microstructures of igneous rocks. Current methods of analysis are based on 2-D grain size measurements in slices through the microstructure. We explored a new application of singular value decomposition (SVD) for measuring 3-D grain sizes directly. To validate the SVD method, we used data sets of irregular grain shapes taken from computer generated microstructures. The irregularities in the modeled grain shapes appeared similar to grains found in real microstructures. Seven microstructures were generated, each from one of seven classes of crystal shapes, prisms (1:1:3, 1:1:5), plates (1:1:3, 1:5:5), and cuboids (1:2:5, 1:3:5, 1:4:5). The governing equations for crystal nucleation rate ($N_t=e^{at}$) and growth rate ($G=\Delta L/\Delta t$) predicted ideal linear CSDs with slopes equal to $-a/G$ if the crystals were to form freely, i.e. not in microstructures. The predicted ideal CSDs were used as standards for comparing our measured CSDs from the grains in the microstructures. The database for each grain was a 3-D matrix containing the (x,y,z) coordinates of its unit cells. The importance of the SVD method is that it works with any general

matrix (not necessarily square) to extract its singular values which relate to the diameters of an ellipsoid (Moshtag, 2006) which approximates the grain shape. We found that one of the diameters (intermediate versus long) of the ellipsoids inscribed within the grains consistently yielded CSDs close to the predicted CSDs. The best diameter can be predicted from the average of the axial ratios of the ellipsoids for each bin size. We anticipate that application of this method to measuring CSDs of silicate minerals in real igneous rocks will follow advances in new high energy X-ray tomography.

1:45 - 2:00

Dynamics of Polydisperse Foam-Like Emulsion.

Harry Hicock*, Dept. of Physics, James Madison University

Dr. Klebert Feitosa, Dept. of Physics, James Madison University

Foam displays complex fluid behavior. Under different circumstances it may display plasticity or fluidity. The complexity emerges from the interactions between individual bubbles which are disordered and whose interaction energy is greater than the thermal energy. As the foam ages, coarsening induced rearrangements lead the foam to a relaxation process akin to glassy materials. Here we study the dynamics of an index matched, buoyantly neutral emulsion that coarsens like foam. We use confocal microscopy to image the droplets, measure their positions and radii, and track their evolution in time. We find that the droplet size distribution fits a Weibull distribution also seen in foam systems. Additionally, in spite of the large number of droplets, we find relatively small number of large rearrangements suggesting a slow continuous relaxation process.

Chem/Mats - Oral Presentations Session IV

Thursday, August 4

2:30 PM - 4:00 PM

Festival Ballroom A

Dr. Christine Hughey, Presiding

2:30 - 2:45

Electrical Characterization of Zinc Nanowires Grown on PEDOT:PSS/SiO₂ Conductive Polymer Thin Films by Vapor Phase Deposition.

Matthew P. Chamberlin*, Dept. of Physics and Astronomy, James Madison University

Costel Constantin, Dept. of Physics and Astronomy, James Madison University

Easily available spin coating and vapor phase deposition techniques offer tremendous possibilities in fabricating inorganic/organic heterojunctions. In this study we examine films of inorganic conductive zinc and semiconductive zinc-oxide nanowire arrays grown on organic conductive PEDOT:PSS polymer films using the above methods. Understanding the electrical properties of these hybrid films are of particular interest for applications in organic electronics. However, traditional systems for measuring conductivity and resistivity of thin films by the Van Der Pauw method prove problematic when dealing with soft polymeric surfaces. We present here novel techniques for measuring electrical properties of thin films with a focus on ZnO- and Zn-nanowire/PEDOT:PSS heterojunctions using a modified 4-point probe method.

2:45 - 3:00

Investigation of N-Sulfide Bond Formation in Soluble Precursors for Metal Chalcogenide Thin Films.

Brian Reeves*, Dept. of Chemistry and Biochemistry, James Madison University

Brycelyn M. Boardman, Dept. of Chemistry and Biochemistry, James Madison University

Developing soluble inorganic precursors for metal chalcogenide thin films requires fundamental knowledge and control of the precursor's ligand chemistry. This study involves the investigation of the formation of pyridine N-sulfide (S-Py) bonds from elemental sulfur and pyridine in a range of solvents with increasing polarity. Variable temperature nuclear magnetic resonance (VT-NMR) spectroscopy was used to monitor the formation of S-Py in d-toluene, d-tetrahydrofuran (THF) and d-dichloromethane (DCM). The largest chemical shift was observed in toluene, while minimal shifts were observed in both THF and DCM. UV-Visible spectroscopy was also used to probe the formation of S-Py by titration of sulfur solutions with pyridine in toluene, THF, and DCM. In all solvents an increase in absorbance and molar

absorbitivity was observed when compared to sulfur or pyridine alone. Modeling of the UV data with the SIVVU software determined Gibbs free energy values of -16.94 kJ/mol, -19.40 kJ/mol, -27.02 kJ/mol, as well as K values of 1046, 2873, 65510 for the formation of S-Py in toluene, THF, and DCM respectively. Free energy and equilibrium constants increase with solvent polarity, which suggests the N-sulfide bond exists as a charged species. Finally the formation of S-Py was confirmed by GC-MS with a M+ of 111 m/z, corresponding to a single sulfur bonded to a single pyridine.

3:00 - 3:15

Is Extragalactic Maser Activity Dependent on Galaxy Morphology?

James Corcoran*, Dept. of Physics and Astronomy, James Madison University

Thomas Redpath*, Dept. of Physics and Astronomy, James Madison University

Nathan DiDomenico*, Dept. of Physics and Astronomy, James Madison University

Anca Constantin, Dept. of Physics and Astronomy, James Madison University

Currently the most accurate way to measure the distance to another galaxy, and thus precisely determine the Hubble constant, H_0 , is through water mega-masers detected near the center of galaxies in a disk-like distribution. An accurate determination of H_0 would allow for a better understanding of dark energy, which accounts for ~74% of the composition of the universe. Finding galaxies that host these mega-maser disks has proven difficult and hence we need to improve our searches by understanding the relation between mega-maser phenomenon and their galaxies' properties. We use the Sloan Digital Sky Survey (SDSS) Data Release 7 to statistically compare the optical characteristics of both galaxies which host mega-masers and those that have been surveyed for mega-maser activity, but have shown none. We aim to reveal the most statistically significant connections between mega-maser emission and their host optical properties by exploring the role of environment as an indicator of mega-maser activity and comparing optical spectral classifications, central black hole masses, luminosities of specific emission features, and masses and ages of associated stellar populations. The focus of this presentation is on the morphology and photometric colors of galaxies with and without mega-masers. The trends we find with these comparisons will offer improved ways of finding new mega-masers, and therefore, a better hope of understanding dark energy, and thus determining the ultimate fate of our universe.

3:15 - 3:30

Properties of a Propargylic Alcohol Gelator and its Derivatives in a Water/Ethanol System.

Ivan A. Liapin*, Dept. of Chemistry and Biochemistry, James Madison University

Misha Salim*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin L. Caran, Dept. of Chemistry and Biochemistry, James Madison University

The design and control of self-assembly of low molecular weight gelators offers a powerful tool for the development of functional supramolecular nanostructures. In this study novel gels were prepared using a ternary mixture of a gelator, a good solvent (EtOH), and a poor solvent (H_2O). This allowed the gelator to spread throughout the solvent prior to gelation. A closer investigation of this system showed that the optimum percentage of ethanol is between 20% and 40%. Minimum concentrations of gelator were determined for a range of EtOH/ H_2O ratios. Robust gels were prepared at gelator concentrations as low as 2 mg gelator per mL of liquid. A Scanning electron microscopy (SEM) study confirmed that the gel is composed of long fibers. A number of derivatives were prepared, starting from the parent propargylic alcohol gelator, with yields ranging from insignificant to almost quantitative; none of these new compounds yielded a better gelator than the parent compound. Additionally, we have prepared a novel polymer by the reaction of a bis(propargylic alcohol) and a diisocyanate.

3:30 - 3:45

Chiral Interactions at the Air/Water Interface.

Justin Hagerman*, Dept. of Chemistry and Biochemistry, James Madison University

Melissa Palmer*, Dept. of Chemistry and Biochemistry, James Madison University

Leigh Matano*, Dept. of Chemistry, The College of New Jersey

Yanjie Zhang, Dept. of Chemistry and Biochemistry, James Madison University

Chiral interaction is a fundamental phenomenon that is observed in all biological systems, ranging from single cell organisms to the most complex of animals. Herein, amino acid surfactants were synthesized and employed as a model system to understand the chiral recognition phenomena at the air-water interface. *N*-stearoyl-glutamic acids with different chirality (L-, D-, and DL-) were spread at the air-water interface on subphases containing varying concentrations of L-arginine at pH 5. The pressure-area (*II-A*)

isotherms of these chiral monolayers were used to study the interactions between amino acids. *N*-stearoyl-glutamic acids with different chirality displayed varied affinity to L-arginine. A fluorescence microscope was used to observe the domain formation of these chiral molecules at the air-water interface. We are trying to investigate the correlation between the amino acid-amino acid binding affinities and the surface morphology of the monolayer.

Chem/Mats - Poster Session B
Thursday, August 4
4:00 PM - 5:00 PM
Festival Ballroom B/C

Interaction Between Pairs of Bubbles floating on a Bubble Raft.

Joice Bigon*, Dept. Of Chemistry, Pontificia Universidade Católica de Campinas
Klebert Feitosa, Dept. Of Physics, James Madison University

A random packing of bubbles display complex behavior, such as “jamming”, due to the bubble’s mutual interactions. In this present work, we study the interaction between a single pair of bubbles floating at a liquid-air interface using video photography. Left by themselves, the bubbles slowly move towards each other and merge due to capillary attraction. We investigate the capillary attraction as a function of size of the bubbles and find that the attraction increases with bubble size. Additionally, the measured capillary forces follow the same trend of Nicolson’s approximation for two floating bubbles.

Microfluidic Device for High School Laboratories.

Kevin G. Carini*, Dept. Of Science, Luray High School
Chris W. Hughes Professor, Dept. Of Physics, James Madison University
Brian H. Augustine Professor, Dept. Of Chemistry, James Madison University

The purpose of this project was to fabricate a practical microfluidic “lab on a chip” for use in high school laboratories. The microfluidic device is comprised of four layers: one layer of glass and three layers of PDMS (polydimethylsiloxane). These devices are to work in tandem with an optical microscope. The microfluidic devices will provide high school laboratories with the ability to demonstrate fluid phenomena on the micro scale, the ability to use cost prohibitive precious metals, the ability to reduce the amount of chemical waste, the ability to provide laboratory experiences that are consistent with science standards of learning, and the ability to drastically reduce the time required for labs.

Synthetic Modification of PCPDTBT for Improved Film Morphology in Organic Photovoltaics

Mae Alexandra Carpenter*, Dept. of Chemistry, University of Mary Washington
Brycelyn M. Boardman Dept. of Chemistry and Biochemistry, James Madison University

Poly(3-hexylthiophene) (P3HT) and poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl]] (PCPDTBT) are commonly used donor materials in bulk heterojunction solar cells. P3HT forms ordered domains producing efficient cells but are plagued by a small range of absorption; PCPDTBT however suffers for the reverse. Functionalization of the alkyl chains of PCPDTBT with phenyl groups was investigated, to probe whether pi-pi stacking of the phenyl groups would increase the ordering of the polymer domains. The synthesis of the model monomer 3-(6-phenylhexyl)thiophene (**1**) was used to determine the most efficient reaction pathway. The synthesis of **1** was performed in a one-pot reaction by sequential addition of 3-bromothiophene and bromobenzene to an in-situ generated alkyl bisgrignard. GC-MS was used to monitor the progress and to identify the side products of the reaction. Separation of **1** from 1,6-dithienylhexane, the main side product, has proven to be a significant challenge due to similar polarity. Optimizing reaction conditions are currently being investigated.

Infrared Studies on the Effects of Salts on Nucleotide Binding to RecA.

Brittany Danzig*, Dept. of Chemistry and Biochemistry, James Madison University

Gina MacDonald, Dept. of Chemistry and Biochemistry, James Madison University

The *Escherichia coli* RecA protein is a multifunctional enzyme that is involved in homologous recombination, DNA repair, and initiating the SOS response. RecA is typically a DNA-dependent ATPase. However, high salt concentrations are known to activate RecA mediated ATP hydrolysis in the absence of DNA. Previous experiments in our lab followed the thermally induced unfolding of RecA in various salt solutions and found that RecA stability is dependent on the concentration and nature of the salt ions present in solution. In order to better understand the nature of the salt ion-RecA interactions this study continues to monitor RecA using Fourier transform infrared spectroscopy (FTIR). FTIR was used with a caged ADP nucleotide to observe the effects of pH and buffer salts on the conformational changes of RecA. Salts appear to influence the structure of nucleotide binding; however, more studies are necessary to evaluate the dependent nature of ion-RecA interactions that alter structure, aggregation, nucleotide binding, and ATP hydrolysis.

Vibrated Granular Systems.

Rachel Derby*, Department of Physics, University of Maryland Baltimore County

Brian Utter, Department of Physics and Astronomy, James Madison University

Despite the strong fluctuations in a rapidly moving granular material, dissipation and correlations in collisions can lead to long range forces in granular materials. In this experiment, we study the long-range attraction between two objects when immersed in a vibrated granular system. Depending on the degree of vibration, a granular system can take the form of a gas, or be fluidized. We place two large intruders in each of these systems to track the effective interactions between the intruders, varying frequency, amplitude, size of grains, and the shape of the intruder. Using image processing, we track the separation of the intruders over time. We find that parallel plates come together if they are separated by less than approximately 16 particle diameters between them and reach a final position in which one ordered layer of grains is between them. Future work will focus on varying the amplitude and frequency and driving the system with random noise rather than periodic vibration.

The Synthesis of Tripodal Sensitizer for the Study of Long-Range Electron Transfer across Molecule-Nanocrystalline Semiconductor Interfaces As model solar cells.

Jindong Kang*, Dept. of Chemistry and Biochemistry, James Madison University

Debra Mohler, Dept. of Chemistry and Biochemistry, James Madison University

A series of a compound of 1-(ethynylphenyl)-3,5,7-tris(4-carbomethoxyphenyl)adamantane have been synthesized to study the relationship between molecular structure and electron transfer (ET) rate in ultrafast interfacial processes occurring between semiconductor nanoparticles and molecular adsorbates. Interfacial ET from molecular adsorbates and semiconductor nanoparticles is an important step in the function of solar cells, photocatalysis, and many other molecular devices. Since the rate of ET plays a significant role in determining the efficiency in these systems, significant efforts have focused on this phenomenon. It has been found that rigid linkers between semiconductor and sensitizer modulate efficiency; the compounds that we have made contain rigid tripods, having a tetrahedral core made of 1,3,5,7-tetraphenyladamantane, three COOR surface binding groups, and a rigid rod arm carrying the sensitizer. These rigid tripods are also able to position the linker perpendicular to the surface. Characterization of the compound was accomplished by ¹H and ¹³C NMR, IR, and UV-vis spectroscopy.

The origin of sandstone xenoliths at Mole Hill, an Eocene volcanic neck near Harrisonburg, VA.

Zachary A. Kiracofe*, Dept. Of Geology and Environmental Science, James Madison University

Elizabeth A. Johnson, Dept. Of Geology and Environmental Science, James Madison University

John T. Haynes, Dept. Of Geology and Environmental Science, James Madison University

Mole Hill, located four miles west of Harrisonburg, VA, in the Shenandoah Valley, is a volcanic neck of Eocene age (48 Ma). The Mole Hill basalt exhibits moderate to poor columnar jointing in outcrop, and includes sandstone xenoliths and mantle-derived xenocrysts. Mole Hill is surrounded by limestone and dolostone of the Ordovician Beekmantown Formation and a thin contact zone of hydrothermal quartz. To constrain the origin of the sandstone xenoliths, petrographic and whole-rock geochemical analyses were performed on 23 samples from 14 regional sandstone units, 7 sandstone xenoliths from Mole Hill, and 8 samples of the Mole Hill basalt. Grain size distributions and sphericity were also determined for the framework grains of the sandstone xenoliths and 5 of the most similar sandstone units. The xenoliths are

comprised mainly of monocrystalline quartz, commonly with undulose extinction. The matrix and grain boundaries of most xenoliths were partly to completely infiltrated with magma, but quartz overgrowths are observed on some quartz grains. The average xenolith grain size is 0.32 ± 0.12 mm (n=4) to 0.49 ± 0.27 mm (n=1) (longest axis), with an average long/short axis ratio of 1.98.

Compositionally, the xenoliths form mixing trends on chemical discrimination diagrams between the basalt end member and an unknown sandstone end member. Al_2O_3 , La, Zn, and Ce concentrations are the best geochemical discriminators between possible sandstone units. Combining results from the three types of analysis shows that the Devonian Oriskany Sandstone and Silurian Tuscarora Formation are most similar to sandstone xenoliths. The Tuscarora Formation is exposed in the North Mountain thrust zone, both as a coherent unit and in breccias; the Tuscarora is a more indurated unit than the Oriskany and its sandstones are more likely to form xenoliths that preserve original textures when placed into an igneous environment. The structural evidence supports the hypothesis that the Eocene magma exploited the deep-seated thrust system to make its way to the surface, and strengthens the argument that the Mole Hill xenoliths are fragments of Tuscarora sandstone.

Educational Interpreting in Chemistry: Iconicity and Sign Recall for Explained and Non-explained Signs.

Sean McKinley*, James Madison University

Laura O'Connor*, James Madison University

Steven Kulsar, James Madison University

As student interpreters in the chemistry program, our goal was to track our improvement in voice-to-sign, sign-to-voice, and platform interpreting throughout the 10-week program via videotaped analyses and consumer assessments. By the end of the program, we aimed to achieve 80% accuracy in each domain of educational interpreting. Researchers and users of American Sign Language (ASL) have debated whether or not various levels of iconicity affect accurate sign recall. For this experiment, a test was designed to investigate two components of sign recall; if first, iconicity of a sign and second, explaining a sign origin or development, affect the ability of individuals with no prior sign language exposure to recall the meaning of an ASL sign. Forty-eight signs were selected based on varying levels of iconicity. These signs were videotaped and administered across four weeks of teaching and testing (12 words each week). Two sets of vocabulary words were provided only with the English word equivalent in print while the other two sets were provided along with a verbal explanation/manual demonstration. Participants were 15 college-level students, between the ages of 20 and 25 participating in a chemistry research program. Results suggest that given no explanation, the more iconic signs were more accurately recalled. When provided an explanation of how a sign was developed, participants were better able to accurately recall the less iconic signs.

Polycationic Polycephalic (and other) Amphiphiles.

Daniel Moon*, Dept. of Chemistry and Biochemistry, James Madison University

Jhosdyn Barragan*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin Caran, Dept. of Chemistry and Biochemistry, James Madison University

Polycationic polycephalic amphiphiles have two or more cationic head groups and one non-polar tail group. Previous studies have shown that cationic amphiphiles exhibit antimicrobial properties on both gram-positive and gram-negative bacteria. The goal of the experiments was to study the antimicrobial activities of amphiphiles and to relate this activity to molecular structure. Variations in amphiphile structure include the number and relative position of cationic head groups and as well as the number of carbons in the tail. For comparison, gemini amphiphiles (with multiple heads and multiple tails) having analogous core structures were also prepared. Dr. Seifert's group (JMU Biology) tested the aqueous amphiphile samples for antimicrobial activity. From these data, we have begun to develop an understanding of the trends of antimicrobial activities based on the structure of the amphiphile for two Gram-positive and two Gram-negative bacteria.

Deposition of BiVO₄ Thin Films for Photoelectrochemical Water Splitting.

Milan Y. Patel*, New River Community College

Brandon H. Journell*, School of Engineering, James Madison University

Dr. David Lawrence, ISAT, James Madison University

Dr. Keith Holland, School of Engineering, James Madison University

Bismuth vanadate (BiVO₄) has been proposed as a photoanode for photoelectrochemical water splitting to convert solar energy into hydrogen for future renewable energy applications. BiVO₄ absorbs more visible spectrum than many early material (e.g TiO₂, WO₃). We prepared thin films of BiVO₄ using the spray pyrolysis technique. Films were made using different precursors in efforts to vary film morphology and doping. The resulting films were characterized by measuring their thickness and UV/Visible light transmission spectra. Films were examined with the scanning electron microscope. We will describe the spray pyrolysis technique and show how the choice of precursors affects the morphology and optical transmission of the thin films.

Synoptic Sampling of Little Stony Creek, Mountain Run and Smith Creek.

Michael Morris*, Dept. of Chemistry and Biochemistry, James Madison University

Caitlyn Siemans*, Dept. of Chemistry, NTID/RIT

Daniel M. Downey, Dept. of Chemistry and Biochemistry, James Madison University

Monthly water quality samples have been collected for a number of streams in the Shenandoah Valley of Virginia for water quality and environmental assessment. Unfortunately, due to time, effort and budget limitations only a small number of sites are repeatedly sampled. To gain a more detailed assessment of environmental influences for water quality, synoptic samples were collected for three streams during the summer of 2011. A synoptic sampling involves taking water samples and physical measurements at two or three hundred meter intervals in a fixed reach of stream in as short a time as possible to provide a “snapshot” of detailed water quality data. Little Stony Creek in Shenandoah County is an acid sensitive stream that has been treated with limestone. We sampled 4,800 meters from the downstream US Forest Service boundary to upstream of the limestone treatment site in June 2011. Mountain Run is another acid sensitive stream that has been treated with limestone. It discharges into Smith Creek in the valley floor of Rockingham County, Virginia, where it turns into a meandering stream that flows through agricultural land. We collected synoptic samples along 8,420 meters on these two streams in July 2011. Water chemistry parameters included pH, temperature, acid neutralization capacity (ANC), conductivity, and the concentrations of sodium, potassium, magnesium, calcium, chloride, sulfate, nitrate and aluminum. These parameters and on-site physical observations were used to evaluate geology, soils, land use and pollution on the water quality of the above streams.

Comparative in-vitro Study on the Hemodynamics of a Mechanical and Biological Prosthetic Heart During Healthy and Diseased Cardiac Flow Conditions Using Particle Image Velocimetry

Kritika Vayur*, School of Engineering, James Madison University

Dr. Olga Pierrakos, School of Engineering, James Madison University

Dr. Michelle Xiao, School of Engineering, James Madison University

It is estimated that 23.6 million people will die by the year 2030 from some form of cardiovascular disease (CVD), which includes deep vein thrombosis, embolism, and rheumatic heart disease [1]. These types of diseases are a result of adverse flow dynamics that can be devastating to the heart's functionality, particularly the left side of the heart which is the workhorse of the heart. In a diseased heart, change in the hemodynamics creates turbulence which can cause cavitation, high shear stresses, and unfavorable vortices [3]. By understanding these disturbances in the heart, we gain insight into the hemodynamics of the heart at a macro-level. This study can also lead to the creation of innovative tools to resolve some of the tribulations presented in the heart. The knowledge gained from this study can further lead to solutions that can be used in in-vivo studies as well.

To examine the flow field in greater detail we use the Time-Resolved Digital Particle Image Velocimetry (TRDPIV) as a tool to quantify the downstream flow of the valves in the mitral position. TRDPIV allows us to estimate shear stresses, turbulence levels, vortical characteristics, etc. at different stages of heart conditions. This measurement technique enables us to estimate planar velocity distributions for the flow downstream of two heart valves; the Bjork Shiley mechanical tilted disc and a St. Jude Medical porcine trileaflet valve. By changing the heart rate and stroke volume, we will induce a normal heart as well as a diseased heart. Many studies have been done on prosthetic hearts valves using Digital Particle Image

Velocimetry (DPIV), but most of these studies have focused on the hemodynamics during normal and resting heart conditions. There are limited DPIV studies focused on comparing both normal resting cardiac flows with diseased ones, and this is a main objective of this study. Previous studies have shown that orientation as well as the valve design highly influence turbulence levels and vortical characteristics downstream of a valve [2]. To study further characteristics of the hemodynamics, this study will focus on both healthy as well as diseased heart conditions by varying the stroke volume and heart rate.

1. World Health Organization. "Cardiovascular diseases (CVDs)." *World Health Organization*. January 2011. July 22 2011. <<http://www.who.int/mediacentre/factsheets/fs317/en/index.html>>
2. Pierrakos O., P. Vlachos, Aug. 2006, "The Effect of Vortex Formation on Left Ventricular Filling Energetics," *ASME Journal of Biomechanical Engineering*, Vol. 128, pp. 1-15.

Chem/Mats - Oral Presentations Session V

Friday, August 5

8:30 AM - 10:00 AM

Festival Highlands Room

Dr. Brian Augustine, Presiding

8:30 - 8:45

Monitoring the Effect of Salts on the Aggregation and Unfolding of the *Escherichia coli* DNA repair protein, RecA.

Karen Corbett*, Dept. of Chemistry and Biochemistry, James Madison University
Nate Talley, Dept. of Chemistry and Biochemistry, James Madison University
William Cannon, Dept. of Chemistry and Biochemistry, James Madison University
Vince LiCata, Dept. of Chemistry, Louisiana State University
Gina MacDonald, Dept. of Chemistry and Biochemistry, James Madison University

RecA, a DNA repair protein from *Escherichia coli*, is known to hydrolyze adenosine-5'-triphosphate (ATP) during the DNA strand exchange process. Although the presence of DNA is usually required for RecA to hydrolyze ATP, high concentrations of salt have been shown to induce the active, ATP-hydrolyzing form of RecA. Previous Circular Dichroism (CD) studies in our lab have shown that salts affect the structure and stability of the RecA protein. Attenuated total reflectance (ATR) Fourier transform infrared (FT-IR) spectroscopy was used to track changes in the RecA protein unfolding and aggregation in presence and absence of different salts. Various peaks from the IR spectra were fit to a modified van't Hoff equation to determine the melting temperature (T_m) of RecA in different concentrations of salt. The T_m data for the IR coincided with the CD data. RecA in the absence of salt was shown to undergo two transitions upon heating. RecA in the presence of sulfate salts only had one transition, and in the presence of chloride salts, the protein never completed unfolded.

8:45 - 9:00

Optical Electronegativity Trends of Semiconducting and Insulating Binary Oxides.

Kristen Dagenais*, Dept of Chemical Engineering, University of Maryland Baltimore County
Dr. Costel Constantin, Dept of Physics and Astronomy, James Madison University

Binary oxides have always had useful electronic properties, specifically their status as semiconductors. Their wide energy band gap allows them to be used as insulators, while still retaining important conductor behavior. Predicting the value of an oxide's energy band gap can be difficult as the ionization of oxygen gives oxides unique electronegative behavior. Taking this into account, this study took a critical look at oxide semiconductors and found several trends to describe it. This included an attempt to account for the differences in band gap caused by defects in a substance, growth method and crystalline structure. Alkali earth metal and poor metal oxides are modeled with linear equations, while transition and rare earth metal oxides were found to be lie within certain ranges of values.

9:00 - 9:15

Title: Structure of Polydisperse Dry Foam

Anthony Chieco*, Dept. of Physics, James Madison University

Dr. Klebert Feitosa, Dept. of Physics, James Madison University

Aqueous foams are a disordered packing of bubbles. When they are dry, i.e. the liquid fraction is less than 1%, the bubbles distort into polyhedral shapes. We use optical tomography to reconstruct horizontal cross sections of a dry foam system by adding a series of successive projections of the foam. Image analysis of the cross sections is then used to identify the plateau borders and vertices of the foam. Reconstructing the foam in three dimensions is accomplished by using Plateau rules to connect vertices in 3D. We obtain statistics on the number of sides, nearest neighbors and volume of the bubbles. Our preliminary analysis found that the average number of sides is 5.66, the average number of nearest neighbors is 5.82 and the average volume of is 1.18 cm cubed.

9:15 - 9:30

The Perception of Warped Nanotubes

Phillip M. Meyerhofer*, Department of Physics, Saint Vincent College

John Bridstrup*, Department of Physics, James Madison University

Anthony Speziale*, Department of Physics, James Madison University

Scott A. Paulson, Department of Physics, James Madison University

Carbon nanotubes, being approximately one nanometer in diameter, present certain challenges in order to view as well as ascertain the location of the nanotubes. Because of a nanotube's properties it is desirable to integrate them into electromechanical devices but the extreme precision needed to do this at the one nanometer length scale requires exact knowledge of the location of the nanotubes. The scanning electron microscope can be used to mark the surface with reference markers as well as the other required structures however the SEM is unable to see the nanotubes. Nanotubes are many times smaller than the wave length of light meaning the best optical microscopes are also useless. Images were needed which could show the nanotubes in relation to the markers whose position was known. The AFM needed to take images large enough to include all the markers as well as images of a small enough area so the nanotubes were visible. These images needed to be combined to make a useful picture of the location of the nanotubes but due to drift, hysteresis and differences in calibration, images from the AFM would not agree with SEM images or even other AFM images. A program will be presented which solved this problem.

9:30 - 9:45

Organogel Formation by Amino Acid Surfactants.

Anthony DiDomenico*, Dept. of Chemistry, Western Connecticut State University

Yanjie Zhang, Dept. of Chemistry, James Madison University

In recent years, much emphasis has been placed on the formation of gels and specifically gels in organic solvents. The unique structures and self-assembly of gels give rise to a wide variety of potential applications and models for understanding cell growth and sol-gel structures. Potential applications could include sensor fabrication, liquid crystallines, electrophoretic and electrically conductive matrices, cosmetics, oils, and foods. In this study, organogels were prepared by combining amino acid surfactants with different amines in a variety of non-polar organic solvents. X-ray diffraction (XRD), scanning electron microscopy (SEM), FT-IR, and an automated melting apparatus (OptiMelt) were employed to characterize the structure of the gels. The mechanisms of gels formation by amino acid surfactants will be explored.

9:45 - 10:00

Identifying Radiative Polaritons in Thin Oxide Films through Experimental and Simulated Dispersion Relations.

Anita Vincent-Johnson*, Dept. of Physics, James Madison University

James S. Hammonds Jr., Dept. of Mechanical Engineering, Howard University

Giovanna Scarel, Dept. of Physics, James Madison University

Solar radiation serves as an alternate energy source; presently, photovoltaic cells are used to convert absorbed visible photons into usable energy through, e.g., the formation of excitons. Interest in capturing infrared (IR) radiation for energy conversion, IR sensing, thermal photovoltaic's and enhanced thermal transport at interfaces has led to the study of polaritons. Polaritons form when IR photons couple with phonons present in thin oxide films where ionic bonds are present. Multiple types of wave-propagating polaritons exist, including surface phonon polaritons (SPP) and radiative polaritons. Radiative polaritons have the unique property that their phase velocity is faster than the speed of light. Theory states that absorbed IR photons are readmitted as radiation at lower frequencies. We hypothesize that, in addition to radiation, some of the absorbed IR photons are converted into heat. Before testing this hypothesis, it is necessary to prove that the polaritons present in thin oxide films are radiative polaritons with the characteristics predicted by theory. To accomplish this, simulated and experimental IR spectra of Al_2O_3 grown by atomic layer deposition (ALD) on Al were studied. Radiative polaritons are characterized by a complex frequency, which can be derived from IR spectra; the real part is the location of the peak, and the imaginary part is the width of the peak. Dispersion relations were obtained by plotting the real and imaginary parts of the frequency versus the angle of incidence of the IR radiation. Three different polaritons: the oTH, 2TL and 3CL modes were studied with Transverse Magnetic (TM) and Transverse Electric (TE) polarized IR light. The close agreement between simulated and experimental data as well as between our data and theory allow us to conclude that the polaritons present in thin oxide films are radiative polaritons.

Chem/Mats - Poster Session C

Friday, August 5

10:00 AM - 11:00 AM

Festival Highlands Room

Photoacoustic Measurements of Collisional Widths and Shifts of Water Vapor near 7180 cm^{-1}

Victoria Awadalla*, Dept. of Chemistry and Biochemistry, James Madison University

Daniel Havey, Dept. of Chemistry and Biochemistry, James Madison University

Remote sensing of Earth's atmosphere typically utilizes optical spectroscopy. In this context, the climate science community needs to know how certain spectroscopic transitions change shape (width, position, area, etc.) as a result of atmospheric conditions before accurate retrievals can be made. Certain parameters, such as collisional shifting, are extremely difficult to measure due to the small absolute shift values (typically just ≈ 300 MHz per atmosphere). Photoacoustic spectroscopy is a powerful analytical tool for making measurements on spectral line parameters. In this work, a set of experiments was designed that exploits the benefits of photoacoustic spectroscopy in order to quantitatively determine the collisional widths and shifts for a collection of water vapor transitions between 7178 cm^{-1} and 7185 cm^{-1} . Low-uncertainty line parameters are extracted, compared to existing standard reference data, and discussed in terms of impact on remote sensing campaigns that aim to measure atmospheric water vapor.

Fabrication of Micro-Electromagnetic Devices for the Actuation of Carbon Nanotubes.

John Bridstrup*, Dept. of Physics and Astronomy, James Madison University

Phillip Meyerhofer*, Dept. of Physics, St. Vincent College

Anthony Speziale*, Dept. of Physics and Astronomy, James Madison University

Scott Paulson, Dept. of Physics and Astronomy, James Madison University

With advances in microscopy techniques, such as transmission electron and scanning transmission electron microscopy, it has become increasingly more interesting to study and manipulate the structures of solid state materials at the atomic scale. One of the issues with the study of these properties is that these advanced microscopes require that the sample be confined to a space not very conducive to

traditional methods of actuation, such as atomic force microscopy and electrostatic methods. In our research, we are primarily focused on building tiny “electro-magneto-mechanical” devices on carbon nanotubes in order to manipulate them without breaking vacuum or removing them from the microscope. Our current project is primarily focused on putting small, magnetizable paddles on to the carbon nanotubes, using an SEM for electron beam lithography and a metal evaporation deposition system, then running current to induce a magnetic field with which the paddles, which can have any magnetic dipole we want, will align. In order to create these devices we must first choose a type of material and a method for creating the magnetic paddles, in our work we use iron. The main problem with iron is the rate at which it oxidizes at the nanoscale, it is practically instantaneous. Because of this we have developed a method, using what basically amounts to simple geometry, for encasing our iron paddles with gold and thus preventing the oxidation. It is our hope that this research opens the doors for many new opportunities in nanoscale materials science, and at the least greatly reduce the time required for many current experiments.

Polycephalic Amphiphiles as Novel Antimicrobial Agents

Melissa C. Grenier*, Dept. of Chemistry, Villanova University

Robert W. Davis*, Dept. of Chemistry and Biochemistry, James Madison University

Kevin P.C. Minbiole Dept. of Chemistry and Biochemistry, James Madison University

With increasing bacterial resistance to antibiotics throughout the world, the development of novel antibiotics has become an important area of research. Our group is investigating the synthesis and antimicrobial properties of a series of viologens, more specifically symmetric and asymmetric paraquats. For our research, the starting material 4,4'-bipyridine was alkylated using electrophiles of various chain lengths and counterions to generate over thirty different cationic amphiphiles. These compounds were then sent to our collaborators in the JMU Biology Department for evaluation against four bacterial species. Results show that our compounds vary in their effectiveness against gram-positive and gram-negative bacteria, as well as their MIC and time kill properties. Initial biological results have led to the following initial hypotheses: longer hydrophobic chain length offers greater activity until solubility begins to decrease; counterion identity has minimal effect on activity; and gemini structures, in comparison with bicephalic amphiphiles, have shown greater activity for this series. Further examination of the biological activity of these compounds will be conducted. The continued development of new antimicrobial structures is crucial for slowing the spread of bacterial disease and resistance.

Surface Modification and Au Thin Film Deposition in Microfluidics

Stefan D. Jobe*, School Of Engineering, James Madison University

Brian H. Augustine, Dept. Of Chemistry and Biochemistry, James Madison University

W. Christopher Hughes, Dept. Of Physics and Astronomy, James Madison University

Rapidly prototyped poly(methyl methacrylate) (PMMA) microchips are modified for microfluidic projects involving the deposition of Au thin films. These PMMA chips are cut using a laser cutter and annealed in an oven for 30 minutes for stress relief. The deposition of Au is used for thin film infrared reflective mirrors to help improve the heating rate for polymerase chain reaction (PCR) on a microfluidic platform. Au thin film adhesion is tested for strength using a commercial grade tensile tester. Two 1in x 1in Au deposited PMMA substrates are pressed together with a layer of adhesion between them. A sample mount was designed and fabricated to measure the Au film adhesion strength using a tensile tester. The tensile tester then pulls these pieces apart to test the adhesion force between the PMMA and the thin film of Au. The remaining Au is measured to determine the maximum stress and strain on each substrate. Au infrared mirrors were integrated into a microfluidic PCR platform and results of DNA amplification will be shown. 600um thick PMMA with a 4.5mm diameter hole are used for creating wax membranes. Thin membranes are then created using benzoin methyl ether (BME) as the photo initiator over the wax filled hole. The photo initiator is cured under 75% intensity UV light for 900 seconds. The wax is micro pipetted out by heating a hot plate to 90°C. These techniques and potential applications for microfluidics will be further discussed in the poster.

Quantitating Neurotransmitters and their Metabolites in Urine.

Jarvis Mitchum*, Dept. of Chemistry and Biochemistry, James Madison University

Gina MacDonald, Dept. of Chemistry and Biochemistry, James Madison University

Serotonin (5HT) is a heterocyclic amine that is synthesized from the amino acid tryptophan and is metabolized by monoamine oxidase (MAO). One product of serotonin breakdown is 5-Hydroxyindoleacetic acid (5-HIAA) that is excreted in urine. Quantitation of serotonin levels have been

studied in relation to many physiological and behavioral functions including: carcinoid tumors, aggression, depression, and appetite. Many studies have shown the links between increased aggression and differing levels of neurotransmitters/metabolites in body fluids. Our studies use ELISA (Enzyme-Linked Immunosorbent Assay) to quantify serotonin levels in urine. In addition, the LC-MS (Liquid Chromatography–Mass Spectrometry) was used for serotonin and metabolite quantitation. LC-MS has the potential to measure the concentrations of many different neurotransmitters and their metabolites of interest. These measurements were used to determine if we were able to observe differences in serotonin and metabolite levels between animals.

Design, Development, and Investigation of a Multi-Directional Spray Cooling Device.

Christen Rhodes*, School of Engineering, James Madison University

Dr. Heather Watson, School of Engineering, James Madison University

Spray cooling research has increased in popularity as a possible solution for cooling advanced electronics. As electronics become smaller and smaller, the amount of heat generated per area, or heat flux generated, will become greater and thus a new cooling method that can handle these large heat fluxes is necessary. Spray cooling is the process of forcing liquid through a nozzle to create fine droplets which then impact a heated surface. The energy required to evaporate the drops from liquid to vapor form is extremely high and thus the surface is cooled as the liquid evaporates. Convection within the liquid film that forms on the surface from the droplets is also known to contribute to the cooling. Currently, most research is conducted on small surfaces approximately 1- to 2-cm² in size. The present investigation focuses on studying spray cooling over larger surfaces, up to 10-cm², incorporating various spray impact angles and requires the development of a unique testing apparatus. Existing literature on spray cooling was reviewed to establish other possible requirements pertinent to the design of our device. It was determined that the nozzle would need the flexibility to change positions in the x, y, and z directions. The spraying assembly also needed to be modularized so that it could hold various sizes of nozzles or a multi-nozzle array, should this become another area of research. Finally, the spraying assembly should be able to switch easily between a downwards, upwards, and sideways spraying configuration. Design ideas were drawn and modeled in the 3D software design program SolidWorks, and an optimized design was chosen. Major component parts of the design were machined and assembled using equipment in the ISAT Machine Shop. The final product is a cube-like frame with a nozzle angling device that will help the James Madison University School of Engineering conduct further research into an infrequently studied area of spray cooling.

The Synthesis of Tripod Molecules for Ultrafast Photolysis Studies.

Michelle Rudman*, Dept. of Chemistry and Biochemistry, James Madison University

Debra Mohler, Dept. of Chemistry and Biochemistry, James Madison University

A 1,3,5,7-tetraphenyladamantane tripod with carboxymethyl anchoring groups and a photoactive perylene complex was synthesized according to literature. The purpose of this system is to keep the light-sensitive perylene complex perpendicular to the semiconductor surface in order to study the effects of distance on solar cell efficiency. By varying the distance between the perylene “dye” and the molecular anchoring groups, improvements may be made in solar cell technology. Further studies of this molecule via femtosecond IR spectroscopy will be conducted at Emory University.

Synthesis of a New, Square Planar Nickel(II) Acetylacetonate Complex.

Scott A. Steehler*, Dept. of Chemistry and Biochemistry, James Madison University

Barbara A. Reisner, Dept. of Chemistry and Biochemistry, James Madison University

In an attempt to produce hybrid inorganic-organic frameworks, a new polymorph of the square-planar nickel(II) acetylacetonate solvate complex, Ni(acac)₂·xsolvate, was synthesized. This complex was crystallized from a solution containing derived from sodium dihydrobis(imidazolyl)borate, Na[H₂B(im)₂], which was used in an attempt to make new framework materials. Sodium dihydrobis(imidazolyl)borate, Na[H₂B(im)₂], was synthesized by reacting NaBH₄ in an imidazole flux under N₂. The ligand was characterized by NMR and FTIR spectroscopy. Ni(acac)₂·xsolvate was synthesized through a solvothermal reaction between Na[BH₂(im)₂] and Ni(acac)₂ yielding yellow octahedral crystals. On heating, Ni(acac)₂·xsolvate is volatile and can act as a chemical vapor deposition (CVD) precursor to deposit nickel-containing films. Preliminary structural characterization of this material indicates that the material crystallizes in a tetragonal unit cell, I₄/a with *a* = 14.3154(6) Å and *c* = 17.2950(7) Å. The molecular Ni(acac)₂ units pack in a herringbone-like lattice and disordered solvent molecules are present. The thermal

properties of this material have been studied by thermogravimetric analysis and evolved gas analysis-FTIR.

Hydration profiles in clinopyroxene mantle xenocrysts from the Eocene Mole Hill basalt, Rockingham County, VA.

Victoria A. Stempniewicz*, Dept. Of Geology and Environmental Science, James Madison University

Elizabeth A. Johnson, Dept. Of Geology and Environmental Science, James Madison University

Mole Hill, located west of Harrisonburg, VA, is a 48 Ma basaltic neck formed by intraplate volcanism. Little is known about the cause of the eruption or the source of the magma. In this study we determine the water content of the mantle beneath Mole Hill and the ascent rate of the magma by measuring the concentration of structurally bound OH (hydroxyl) in clinopyroxene (Al-augite) mantle xenocrysts entrained in the basalt. Infrared spectra of OH bands were obtained at 4 cm^{-1} resolution averaging over 256 scans using a Nic-Plan microscope attachment on a Thermo-Nicolet Magna 750 FTIR spectrometer at JMU. Concentration gradients of OH were measured in transects across 6 clinopyroxene xenocrysts with shortest diameter between 0.61 and 1.42 cm. Quantitative polarized measurements were obtained from the center of each crystal using a custom-mounted wire grid on CaF_2 polarizer. The clinopyroxene xenocrysts exhibit hydration profiles, with the highest OH concentrations (up to 425 ppm H_2O) found at the rims and near large fractures in the crystals. The OH concentrations in the cores of the xenocrysts are low (18-37 ppm H_2O) and represent the water content of the clinopyroxenite mantle beneath Mole Hill. The hydration profiles of two xenocrysts were modeled using a 1D infinite slab model from Crank (1975) using 4 different sets of diffusion data for diopside (Ingrin & Blanchard 2006) and a magmatic temperature of 1220°C (Sacco 2011). The initial OH concentration is taken to be the concentration preserved in the center of the crystal; the OH at the very edge of the crystal is assumed to be in equilibrium with the water concentration of the host magma. The calculated magma ascent time is highly dependent upon diffusivity and ranges from 0.03 to 4.21 hours. Since the Mole Hill basalt originated from a depth of $\sim 30\text{ km}$ (Sacco 2011), the ascent rate of the Mole Hill basalt is estimated to be 2-278 m/s, with a median value of 17-34 m/s. The ascent rate for the Mole Hill basalt is equal to or faster than rates previously reported for alkali basalts (1-6 m/s) and kimberlite magmas (4 m/s).

Chem/Mats - Keynote

Friday, August 5

11:00 AM - 12:00 PM

Festival Highlands Room

Zeric Hulvey (JMU-REU '01 & '02, JMU '04)

Gas adsorption and separation in porous metal-organic frameworks

Metal-organic frameworks (MOFs) are a relatively new class of crystalline materials composed of metal cations or clusters connected through coordinating organic ligands. As virtually any organic molecule which contains a coordinating functional group can be used in conjunction with most metals to make a MOF, they display a considerable amount of structural and chemical diversity. The applications MOFs have attracted are just as diverse, as materials have been developed with interesting catalytic, electronic, spectroscopic, magnetic, and adsorptive properties. Many of these properties depend on the synthesis of structures with nanoporosity, which is achieved through the post-synthetic removal of solvent or template molecules without destruction of the framework crystallinity. The majority of this talk will focus on the synthesis of porous MOFs designed to address two specific issues in the field of gas adsorption and separation. First, I will address the large effort behind developing MOFs for use as hydrogen storage materials in fuel cell applications. Problems in this area arise from the relatively weak binding interaction of H₂ with the surfaces of MOFs. I will highlight my past work which focused on the development of MOFs with fluorinated pore surfaces in an effort to increase the strength of this interaction. Second, I will describe the potential for porous MOFs to be used to separate mixtures of gases, specifically my current work which is aimed at screening various MOF materials for the separation of Krypton and Xenon, a component of spent nuclear fuel.

Chem/Mats - Pizza Luncheon

Friday, July 30

1:00 PM - 3:00 PM

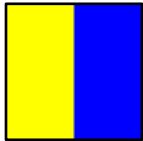
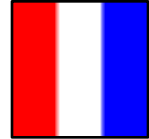
Dave's Taverna , Downtown Harrisonburg

Dr. Dan Downey, Presiding

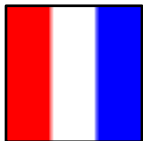
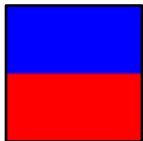
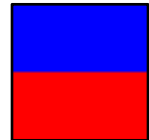
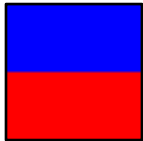
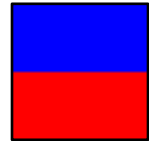
NOTES



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 2011 marks the 21st 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 and the chemistry program is in its 6th funded REU grant. 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. While the biology program is between funding as of the summer of 2011, the other three continue on supporting students from not only JMU but numerous other colleges throughout the country. 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. The REU is just one of many programs at NSF from which JMU faculty currently draw funding.



This symposium will feature the work of students who participated in the REU programs during the summer of 2011. 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, Engineering, Geology, ISAT, and Physics Departments. All of these students worked together this summer and deserve to be commended for their accomplishments.



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Research Corporation

USDA Forest Service

Virginia Department of Environmental Quality

Virginia Department of Game and Inland Fisheries

