Abstracts

Astronomy & Astrophysics

Supernova 2014J: cosmic lighthouse & probe of interstellar dust in the galaxy M82 Poster: A1 Author: Eric Aldieri, Dr. Edward Guinan Advisor: Dr. Edward Guinan

Type Ia Supernovae (SNe Ia) are some of the most helpful objects for astrophysicists in determining stellar distances due to their remarkably similar peak luminosities. A SN Ia is believed to be the product of a white dwarf star overcoming a critical mass (the Chandrasekhar limit), resulting in a runaway thermonuclear explosion. SN 2014J was accidentally discovered by Steve Fossey at University College London on 21 January, 2014. We report on the reddening of SN 2014J, using the stellar explosion as a probe of the interstellar medium in the host galaxy M82. We compare the object to an unreddened SN Ia, SN 2011fe, in order to generate an extinction curve for the light emanating from M82. We then compare this curve to the previously determined extinction curves of the Milky Way Galaxy, Small Magellanic Cloud, and Large Magellanic Cloud.

<u>The secret lives of cepheids: a proof-of-concept study of classical pulsators in the K2</u> <u>engineering field</u>

Poster: A2 Author: Mandi Fry, Cole Johnston, Scott Engle Advisor: Scott Engle

Since their discovery, Cepheids have proved invaluable in the fields of stellar and galactic astronomy. The Period-Luminosity relationship is essential in mapping out the universe and populations of stars due to their apparent long-term stability. However, as we are now finding out, Cepheids may not be as stable as we once thought. A Cepheid pulsates through the kappa mechanism, where opaque layers of ionized Helium II trap radiation inside the star and cause it to expand. Once expanded, the opaque layers thin out and allow radiation to seep through, which then causes gravity to take over and contract the star again. A Cepheid's period and amplitude may change over the course of time due to their evolutionary track. As a B main sequence star burns up all the Hydrogen in its core into Helium, it blows up in size and decreases in temperature, crossing the Instability Strip. Theoretically, as the star crosses the Instability Strip from the hot side to the cold side, its period will increase over long spans of time. However, short-term cycle-to-cycle changes were previously undetectable due to the difficulty in taking continuous and accurate ground-based data. Finally, the space-based K2 mission can allow us to analyze high precision, continuous data on 37 different Cepheid variables. We can search this data to find short-term and long-term changes in the period and amplitude of the stars over time, and determine at which stage of its evolutionary track a Cepheid is on. We developed software specifically to carry out this study, and present the results of K2 engineering data as a proof of concept before the release and study of K2 field zero data. We report new periods for 38 variable stars and an analysis of period modulation in several RR lyrae-type stars, a demonstration of the analysis that will be implemented on the K2 Cepheids.

Biology

<u>The \triangle ydcI, \triangle yaiV, and \triangle STM1266 gene mutations in *Salmonella typhimurium*: can we use these mutations to improve vaccines?</u>

Poster: A3 Author: Kaitlyn Barney Advisor: Dr. James W. Wilson

The design of bacterial vaccines is a delicate process, requiring one to balance the initial virulence of the vaccine strain with attenuation, or the loss of virulence. This balance is critical to the design of an effective bacterial vaccine which will produce a satisfactory immune response with minimal sideeffects. Current Salmonella vaccines suffer from a lack of this balance resulting in vaccines that are either highly immunogenic (capable of producing an immune response) but inadequately attenuated or vaccines that are highly attenuated by insufficiently immunogenic (1,2). Finding the proper balance often involves targeting genes that control or alter the ability of Salmonella to survive in an animal host. Three recently-characterized genes (ydcI, yaiv, and STM1266) have been identified as genes that could play a role in the virulence of vaccine strains. The Δ ydcI mutation has been shown to decrease resistance to acid stress. The Δ yaiV mutation has been shown to increase resistance to oxidative stress. The Δ STM1266 mutation has been shown to decrease biofilm formation which could affect the survival of vaccine strains. My specific aims were (1) to test the effects of current *S. Typhimurium* vaccines in the model organism *C. elegans* and (2) to transfer the Δ yaiV, Δ ydcI, and Δ STM1266 mutations into current *S. Typhimurium* vaccines using P22 transduction. Further work will test the mutated vaccine strains in the model organism *C. elegans*.

Why do sea urchins have rocky diets?

Poster: A4 Author: Tri Nguyen, Alexander Mott, Michael P. Russell Advisor: Dr. Michael Russell

Purple sea urchins (Strongylocentrotus purpuratus) occur on the west coast and occur on rocky substrata. They create cavities or "pits" in sedimentary rock by rasping particles and ingesting them (E. Duwan 2014 senior thesis in Russell lab). This previous study quantified bioerosion rate and explained the mechanism of formation of pits found in the field. Although Duwan's study showed that the sedimentary particles have an organic component, it did not address whether urchins derive any nutritional value from sediment ingestion. We are currently conducting a long-term experiment comparing growth rates of urchins on three different substrates: 1) smooth glass (no particle ingestion = control), 2) sandstone (low organic content), and 3) mudstone (high organic content. Preliminary rock analysis shows that mudstone contains $\sim 5\%$ organic material and sandstone has ~1.5%.We will analyze and compare the organic/inorganic contents of sediments in fecal pellets versus crushed sedimentary rocks. In addition, measure the growth rates of sea urchins living on sediment versus glass. Organic content differences between sediments in fecal pellets and crushed rocks may result in differences in urchin growth rates. This will show whether or not sea urchins are gaining any nutritional value from ingesting sedimentary rocks and help explain the unusual behavior of rock ingestion. It is also possible that rock ingestion is an unintended consequence of urchin behavior and if so, there may be no difference in growth rates between urchins living on sediments versus glass. The urchins used in this experiment have a mean size of 14.12 grams and standard deviation of 2.9 grams.

Identifying gene targets of Brd2a during zebrafish development

Poster: A5 Author: Katrin Heider Advisor: Dr. DiBenedetto

Brd2 is a transcriptional co-regulator and part of the bromodomain-extraterminal domain (BET) family of proteins that act as epigenetic adapter molecules and scaffold proteins for the assembly of regulatory complexes at gene promoters. Brd2 binds to acetylated histones within active chromatin near promoters, and recruits chromatin modifying enzymes to further activate or silence downstream target genes. Brd2 has a known regulatory role in mitosis and apoptosis in adult mammalian tissues, and acts as a maternal factor present in oocytes before fertilization and necessary for proper embryogenesis in flies, mouse, and zebrafish. While Brd2 in Drosophila is a known upstream regulator of homeobox genes that control pattern formation in Metazoans, the downstream effectors of Brd2 in vertebrate development are as yet unknown.

This projects aims to identify novel gene targets of Brd2 during zebrafish embryogenesis using chromatin-immunoprecipitation (ChIP) followed by DNA sequencing, which allows pieces of chromatin that are bound to a target protein to be captured and identified. Known homeobox targets of the Brd2a ortholog in Drosophila will also be tested as candidate genes to see if the Brd2/Hox pathway is conserved. I mated pairs of wildtype strain AB or TU zebrafish, staged and collected embryos at the 48 hour post fertilization (48 hpf), processed them for ChIP by crosslinking of DNA to chromatin using formaldehyde, wash with glycine and stored them in PBS in batches at - 80°C until use. Because it may be difficult to capture chromatin via a protein bound loosely to histones rather than directly to DNA, it was important to first validate the ability of the peptide antibody to pull down Brd2 alone, so that at least that variable could be controlled. To test this, I performed a conventional immunoprecipitation (IP) followed by Western blot using the same antibody and verified the pull-down of Brd2. The next step will be to perform the actual ChIP procedure, using embryos already processed and collected, and the verified anti-Brd2 peptide antibody. I am optimistic to identify new gene targets of Brd2 at the 48 hour stage and therefore further study the function of Brd2 during zebrafish embryogenesis.

Expression and structure analysis of Brd2b in zebrafish oocytes and embryos

Poster: A6

Author: Matthew Haemmerle, Angela DiBenedetto Advisor: Dr. Angela DiBenedetto

Brd2b is a paralogous derivative in zebrafish of Brd2a, an epigenetic transcriptional co-regulator that helps recruit chromatin remodeling complexes to target gene promoters, and is implicated in regulating apoptosis, cellular proliferation, and pattern formation during development. In contrast, little is known about Brd2b's molecular function or role in cellular processes aside from mRNA expression patterns. During zebrafish oocytes development, each paralog's mRNA localizes to different regions in the egg, with brd2b concentrating at the future animal pole and brd2a at cortical periphery; thus, both genes encode maternal factors, but seem to diverge in function. In embryos, transcripts of both paralogs become enriched in the spine and nervous system during segmentation, yet local differences in location and levels are observed. Given these distinct and overlapping mRNA expression patterns, Brd2b may serve shared and distinct functions compared to Brd2a and other proteins in the greater bromodomain family. In order to examine the structure and expression of Brd2b, a more accurate indicator of function than mRNA, Western Blot analysis was utilized.

50kD and 150kD band appear in total ovary and 48 hour embryos while 4 and 24 hour embryos show only one 50kD band. In contrast, the predicted molecular weight of Brd2b is 90.6kD. Given Brd2a binds chromatin via its dual bromodomains, it is possible that Brd2b binds to chromatin in protein preparations, causing it to migrate at a higher molecular weight than predicted; alternatively, covalent modifications or irreversible complex formation may be present. Additionally, multiple potential Brd2b isoforms at the mRNA and protein levels are predicted from the gene sequence by bioinformatics and are being explored for potential differential expression using RT-PCR approaches. Overall, investigating Brd2b will provide insight into its role in oogenesis and vertebrate development, providing an understanding of why chromatin rewiring may be necessary in the egg to embryo transition.

DAF-16-mediated innate immunity and heat stress resistance in C. elegans

Poster: A7 Author: Paul Regan Advisor: Matthew Youngman

Although certain stressors, such as UV light or oxidative stress, damage DNA and other biomolecules, the mechanism that brings about changes in the gene expression of an aging organism is not well understood. DAF-16, a transcription factor in *C. elegans*, mediates the expression of genes involved with stress response, such as protection from infection and heat stress, during aging. When infected with the bacterial pathogen *Pseudomonas aeruginosa*, the wild-type N2 strain outlived both the daf-16::GFP strain, which overexpresses the b isoform of DAF-16, and the daf-16 mu86 mutant strain, which lacks all isoforms of DAF-16. When subjected to heat stress, the daf-16::GFP strain survived longer than both the N2 and daf-16 mu86 strains. These data suggest that DAF-16 is highly regulated with regard to its function in mediating genes that protect the aging worm from bacterial infection and heat stress. The kill assay indicates that DAF-16-mediated innate immunity is activated in an age-dependent manner, and the heat stress assay suggests that the anti-heat stress function of DAF-16 is constitutive during aging. Furthermore, different isoforms may contribute to the specificity of transcriptional regulation by DAF-16 and thus play an important role in determining stress response and lifespan in *C. elegans*.

Plant-soil feedback effects in red mangroves

Poster: A8 Author: Julie Kurtz Advisor: Samantha Chapman

The changes in the chemical, physical, and biological properties of soil that are caused by plants, which in turn can influence the performance of plants, are termed 'plant-soil feedbacks.' Feedbacks can be positive or negative depending upon the effects that the soil biota (e.g. bacteria and fungi) have on plant growth. I examined the impacts of various soil conditions on the growth of red mangrove plants (*Rhizophora mangle*) with the goal of determining if soil biota drives plant seedling growth. I used a greenhouse mesocosm experiment to answer the question: Do the soil biota associated with different species of mangrove plants in soil inoculated with one of four treatments: 1) red mangrove inoculum from the Merritt Island Nature Reserve in Florida, 2) black mangrove inoculum from the Villanova greenhouse for six months, 4) sterilized sand and sterilized inoculum from both black and red mangroves grown at the Merritt Island Nature Reserve. I compared the growth of the

mangroves in these four treatments (n=5) in order to determine if the soil biotas of red mangrove or black mangroves exhibit a positive, negative, or neutral effect on the growth of red mangrove plants. My greenhouse experiment consisted of twenty pots total; five pots for each of the four treatments. At the beginning of the experiment I sterilized silica sand in the autoclave at 160 degrees Celsius for three hours. I measured the original biomass of each plant, and then I recorded a variety of measures of plants growth on three occasions over the course of four weeks (total shoot height, leaf number, and individual node heights). I found that red mangroves grew best in inoculum from black mangrove soil. Further, red mangroves grew the least in soil which had been sterilized. These results show that the soil biota does have an effect on the growth of mangrove plants, and that the soil biotas of red mangrove plants may exhibit negative feedback on its own species. This research could inform managers of mangrove restoration projects about the best soil treatments for the planting efforts of mangroves which are occurring world-wide.

Biochemistry

Antioxidant response element (ARE) assay development reveals surprising trend in catalase-treated cells

Poster: A15 Author: Anna Briker Advisor: Dr. Aimee Eggler

The Nrf2 transcription factor responds to oxidative and electrophilic stress and upregulates the genes that encode for cytoprotective proteins by binding to the antioxidant response element (ARE). In normal cellular conditions, Keap1, the repressor protein of Nrf2, is bound to Nrf2, targeting it for degradation. Nrf2 activators—many of which are found naturally in foods—can act either directly or indirectly on Keap1 to elicit an antioxidant response.

Directly, electrophiles can covalently modify the cysteines of Keap1, preventing it from deactivating Nrf2, and causing Nrf2 levels to accumulate. Indirectly, some compounds can cause the production of reactive oxygen species (ROS) in the cell, either from redox cycling or by stimulating mitochondrial ROS production. However, there are conflicting opinions as to the degree of importance that ROS play in activating antioxidant response elements (ARE).

The long term goal is to assess the role that ROS play in activation of Nrf2 by conducting ARE reporter assays with varying levels of phytochemicals, and including catalase to quench ROS. The extent of ARE activation is measured using a dual-plasmid assay in the cells of interest, human keratinocyte HaCaT. The first plasmid contains an ARE sequence upstream of the firefly luciferase enzyme, and the second control plasmid allows for constitutive express of Renilla luciferase. During the course of developing the ARE assay, it was observed that the Renilla levels on catalase-treated cells were significantly lower than those treated without catalase. Experiments ruled out that lower Renilla values were due to an extra rinse with PBS on the catalase-treated cells, or due to a catalase-related interference in the Renilla-catalyzed light-generating reactions. Thus, Promega's Green CellTox Assay was conducted, and no cytotoxicity of catalase was observed. Regardless, the lower Renilla levels show that the catalase does seem to be affecting the cells; even though they are alive, they may be experiencing a decrease in total protein synthesis. This conclusion led to assay redevelopment. By aspirating the catalase treatment and changing the media after four hours of

incubation, and harvesting the cells after twenty-four hours, catalase was still effective at neutralizing ROS, without affecting the Renilla values.

The generation and purification of recombinant GST-tagged *Trypanosoma brucei* TFIIBassociated factor, 49 kDa.

Poster: A14 Author: William Escobar-Arrillaga, Jennifer B Palenchar Advisor: Dr. Palenchar

African sleeping sickness/Human African Trypanosomiasis is a disease that affects many sub-Saharan African countries. This disease is caused by *Trypanosoma brucei sp.*, single-celled eukaryotic parasites. *Trypanosoma brucei* TFIIB-Associated Factor, 49 kDA (TbTAF49) is a protein that is solely found in the parasites and is essential in all life cycle stages of *T. brucei* studied to date. Thus, TbTAF49 is a potential drug target to treat this neglected tropical disease. Part of the effort to characterize TbTAF49 involves the generation and purification of recombinant protein. Full length GST-tagged TbTAF49 and two truncated version of GST-TbTAF49 were overexpressed. Conditions for the purification of the full-length protein and one truncated version were found and the GST tag was removed. Further, trypanosome whole cell extract was generated and initial protein interaction studies were carried out using the full length GST-TbTAF49 protein. Progress also will be reported on the generation of a GST-TbTAF49 construct to be used to express the tagged protein in the parasites with the goal of identifying interacting proteins.

Understanding specific roles of Rpt subunits in ATP-dependent 26S proteasome

Poster: A13 Author: Hyewon Kim, Dr. Daniel A. Kraut, PhD Advisor: Daniel A. Kraut

ATP dependent proteases are protein complexes that degrade proteins involved in cell regulation and mediation of protein quality control. In eukaryotes, the major ATP-dependent protease is called the 26S proteasome. The 26S proteasome is a highly conserved protein degradation machine that consists of the 20S core particle and 19S regulatory particles on each end. The core particle is the proteolytic active site that is responsible for degradation of the unfolded protein. The base of the 19S regulatory particle consists of six regulatory particle triple-A (Rpt) ATPase subunits. The six Rpt subunits are located at the top of the core particle in a ring formation in the order : Rpt 1, Rpt 2, Rpt 6, Rpt 3, Rpt 4, and Rpt 5. They are responsible for initiating the ATP-dependent unfolding of substrates (Smith et al., 2005, 2006). In order to determine the specific role of individual Rpt subunits, each Rpt will have a single Glutamate to Glutamine mutation in the walker B motif. This mutation within a single subunit will disrupt ATP hydrolysis and may lead to changes in processivity. In 2013, the Martin lab showed that walker B mutations in different Rpt subunits had different effects on degradation, but it is still unclear the effect each Rpt subunit has in terms of processivity. Currently, all the mutations of the Rpt subunits are complete and degradation assays have been performed for proteasomes with mutations in Rpt 1, 3, 5, 6. Eventually, the processivity of the 6 different mutated proteasomes will be compared in order to define the specialization of the individual Rpt subunits.

The effect of Fliz1 deregulation in human and mouse breast cancer cells

Poster: A12 Author: Patrick Frangos, Jiyoung Chun Advisor: Dr. Knepper

Fetal liver zinc protein 1 (Fliz1) has been shown to down regulate GATA-3 in T-lymphocytes. GATA-3 has also been shown to be necessary for the development and maintenance of normal mammary cell differentiation, which is disrupted in cancer. We hypothesized that an increase in Fliz1 expression will repress GATA-3 and cause breast cancer cells to spread more rapidly. However, overexpression of Fliz1 appears to be cytotoxic. An inducible vector was made by cloning human Fliz1 (hFliz1) and mouse Fliz1 (mFliz1) sequences fused to a fluorescent marker into a plasmid that can drive expression in response to doxicylcine. Human and mouse cell lines will be transfected with the inducible vector that was created. In the presence of doxycycline (Dox) the inducible vector will cause the cells to start overexpressing Fliz1. The inducible vector has been made, and transfection of the breast cancer cell lines will begin shortly. We also developed mouse tumor cell lines with reduced levels of Fliz1 expression. Tests, such as wound healing assays, will then be performed on the transfected cells to see how quickly the cells will migrate back together. Western blots will also be performed to measure the levels of Fliz1 in the cells. These experiments will help to define the role of Fliz1 in tumor cell behavior.

Chemistry

<u>The antimicrobial activity of mono-, bis-, tris-, and tetracationic ampiphiles derived from</u> <u>simple polyamine platforms</u>

Poster: A11 Authors: Thomas Paniak, Megan Jennings, Paul Shanahan, Dr. Kevin Minbiole Advisor: Dr. Kevin Minbiole

A series of 35 amphiphilic compounds varying in both number of quaternary ammonium groups and length of alkyl chains has been assembled. These compounds were prepared in a simple and high-yielding fashion in 1-2 steps without the need for chromatography. Antibacterial MIC data was determined, which were single digit against a series of multiple grampositive and gram-negative bacteria in over half of the compounds tested. MIC variation was most dependent on the length of the alkyl chain, with a dodecyl group showing optimal activity and less so, surprisingly, on the number of cations and/or basic nitrogens. Additional structural variation was prepared in a 12,3,X,3,12 series, including a potent amphiphile functionalized with a thiol group which opens the possibility of attachment to surfaces. Tetraamines were also investigated, but showed only modestly improved bioactivity versus amphiphiles with fewer cations.

Synthesis, characterization, and electronic properties of [Ru(bpy)2(33'bpy(OH)2)]2+ (bpy = 2,2'-bipyridine; 33'bpy(OH)2 = 3,3'-dihydroxy-2,2'-bipyridine

Poster: A10 Author: Erin Peterson, Margaret H. Roeder, Jared J. Paul Advisor: Jared Paul We are interested in the study of metal complexes with ligands that can exist in multiple protonation states, which can affect the electronic properties of the complex, potentially leading to pH tunable catalysts. To this end, our lab has studied polypyridyl ligands containing hydroxyl groups that can be readily deprotonated. We report here the synthesis and study of [Ru(bpy)2(33'bpy(OH)2)]2+ (bpy = 2,2'-bipyridine; 33'bpy(OH)2 = 3,3'-dihydroxy-2,2'-bipyridine). This complex is compared to the previously synthesized complexes [Ru(bpy)2(44'bpy(OH)2)]2+ and [Ru(bpy)2(66'bpy(OH)2)]2+ (44'bpy(OH)2 = 4,4'-dihydroxy-2,2'-bipyridine; 66'bpy(OH)2 = 6,6'-dihydroxy-2,2'-bipyridine) where the hydroxyl groups are oriented in different positions on the bipyridine ring. The 3,3' hydroxyl position is unique because the hydroxyl groups are sterically crowded, which makes it difficult to maintain protonation at both hydroxyl positions. This observation is supported by elemental analysis. The deprotonated 3,3'-substituted-complex lacks the resonance structures that exist upon deprotonation in the 4,4'-substitution and 6,6'-substitution, which results in less electron donation to the metal center. [Ru(bpy)2(33'bpy(OH)2)]2+ was synthesized by the complexation of [Ru(bpy)2(Cl)2] with the 33'bpy(OH)2 ligand. The electronic properties of the resulting complex were studied using cyclic voltammetry and UV/visible spectroscopy.

Modeling material properties for lithium rechargeable batteries

Poster: A9 Author: Lauren Raguette Advisor: Ryan Jorn

Lithium batteries, commonly found in cell phones and laptops, are being targeted for use in allelectric cars. Batteries are often seen as the heaviest, costliest, and least green components of any electronic device. To gain a better understanding of battery electrolytes, atomistic molecular dynamics simulations were performed using LAMMPS and a 5nm cube of a lithium ion electrolyte comprised of ethylene carbonate solvent with 1M lithium hexafluorophosphate salt added for conductivity. After the cube was constructed with Packmol, the system was equilibrated and completed production runs, which were then used to create histograms of radial distribution functions (RDF) and the integrated coordination numbers for each atom type. The results from both the simulations and the calculations of RDF and coordination values align with previous results. Changes in solvation structure with salt concentration were then observed with additional simulations of 0.5 M and 2 M solutions. The studies have then been extended to consider the transport of lithium ions from bulk electrolytes into surface films, which required the use of LAMMPS with an additional enhanced sampling method to calculate free energies for ion transport. A surface film consisting of dilithium ethylenedicarbonate (Li2EDC) was generated and equilibrated with the previous simulations of the electrolyte and different lithium ions from the electrolyte were then pulled into the film to obtain free energy curves.

<u>Photochemical degradation of a brominated flame retardant: a study of</u> <u>tetrabromobisphenol A in frozen and liquid aqueous solution</u>

Poster: B16 Author: Garrett Waligroski Advisor: Amanda Grannas

Studies of brominated flame retardants have raised awareness of the potential environmental impact of these toxic compounds. The Polar Regions are recognized for having accumulated significant amounts and traces of brominated flame retardants. Therefore, it is important to analyze the potential environmental dangers of these contaminants. Despite some established knowledge of photochemical reactions in sun exposed snow and ice, published literature regarding the indirect photochemical reactivity of brominated flame retardants is very limited. The purpose of this research is to investigate the direct and indirect photochemical transformation of a popular brominated flame retardant, tetrabromobisphenol A (TBBPA). We have conducted field-based experiments in Barrow, Alaska to investigate the potential photochemical degradation of TBBPA in snow and ice pack samples. Our results show that TBBPA was efficiently and directly photodegraded in frozen aqueous samples under natural Barrow sunlight. In aqueous solution the light absorption properties of TBBPA particles are pH dependent. Therefore, the photodegradation of TBBPA in the environment will be highly pH dependent. Photochemical reactions that are pH dependent may be affected by the nature of the liquid-like layers in snow and ice packs as well as the presence of other solutes that may indirectly affect the pH. In order to establish how the pH of liquid like regions in ice impacts the degradation of TBBPA, various salts (sodium chloride, sodium fluoride, sodium bromide, ammonium chloride, ammonium acetate and ammonium sulfate) were added to aqueous samples of TBBPA. Due to a process known as the freezing potential, the pH of quasi-liquid layers that are produced during the formation of crystalline solid will change with different salts. It is at this microscopic level that TBBPA photodegradation will indirectly be affected by the presence of the salts, if at all, because the solute particles in solution, in theory, are highly concentrated in the liquid like regions of ice. The reactivity of TBBPA particles upon freezing will be assessed and discussed. In addition, natural occurring species such as dissolved organic matter (DOM) have potential, due to their nature, to indirectly affect the photochemical degradation of TBBPA. The presence of a photosensitizer such as DOM could significantly impact TBBPA photodegradation. Laboratory experiments were performed to evaluate the potential for both commercially-derived DOM and DOM isolated from Arctic snow samples to photosensitize TBBPA degradation in liquid and ice.

RT-qPCR assay development to determine the effect of ROS on Nrf2 activation

Poster: B17 Author: Linda Nguyen Advisor: Dr. Aimee Eggler

Phytochemicals found in plants, such as broccoli, kale, ginger, and garlic, incite the activation of the Nrf2 transcription factor. When a cell experiences oxidative stress, Nrf2 escapes repression and binds to and upregulates the antioxidant response element (ARE) found upstream of genes that encode cytoprotective proteins. These upregulated cytoprotective proteins then guard cells against that oxidative stress and the electrophilic species that can contribute to certain chronic diseases, such as cancer and diabetes. A majority of the phytochemicals that target Nrf2 and ARE are oxidizable diphenols that, through redox recycling, can be oxidized into their electrophilic forms, generating reacting oxygen species (ROS). The eventual goal of the overall project is to determine the extent and importance of the contributions of ROS to ARE-activation, and whether or not they promote Nrf2 activation for a series of ARE-regulated cytoprotective proteins.

Over this past summer, we have worked on one particular method to test these queries, developing functioning and robust real-time quantitative PCR (qPCR) assays for eight ARE-regulated genes that encode cytoprotective proteins: AKR1C1 and AKR1C2 (aldo-keto reductases; important for xenobiotic metabolism), GCLC and GCLM (glutamate-cysteine ligase catalytic and glutamate-cysteine ligase modifier; both for GSH biosynthesis), and HO-1 (heme oxygenase 1; for antioxidant functions). SYBR GreenER Dye, which binds to double-stranded DNA, was utilized in the qPCR

performed to quantify the cDNA levels – and therefore gene expression – by measuring fluorescence.

In the data gathered from simply running the qPCR assay to test the relative fold expression of HaCaT cells treated with sulforaphane (a phytochemical) versus DMSO (the control), HO-1 exhibited the largest fold gene expression, followed by the aldo-keto reductases. This can be used for future reference, with the knowledge that the HO-1 data will yield the greatest disparity in the tested results compared to control, affecting how we look at its standard curve. It can be concluded from the process of developing the assay that the RNA extracted and cDNA quantified requires specific and proper treatment, the standard curves must be optimized for each primer set used, and more replicates (biological, unknowns, and standard curve points) must be tested for the assay to successfully yield data.

Anti-fungal defenses of the Panamanian golden frog

Poster: B18 Author: Celina Santiago, Anthony Iannetta Advisor: Dr. Kevin Minbiole

Atelopus zeteki, commonly known as the Panamanian golden frog, has been almost completely eradicated due to an epidemic of chytridiomycosis, a fungal disease lethal to amphibians. This frog is believed to be extinct in the wild, but is housed in survival assurance colonies to preserve the species until reintroduction can be safely accomplished. A key defense against both chytridiomycosis and its causative agent *Batrachochytrium dendrobatidis* (Bd) is the bacteria that inhabit amphibian skin; cutaneous bacteria have been shown to produce antifungal compounds in significant concentrations. This collaborative project aims to inoculate the frogs with anti-Bd bacteria native to Panama, followed by exposure to the fungus, to investigate the effectiveness of bacterial augmentation in this species. Using traditional as well as newly developed sampling techniques, we have performed analysis of amphibian skin in order to identify and quantify antifungal metabolites. We are working to correlate the presence of skin metabolites with both the bacterial species present as well as survival of fungal infection. This work promises to assist in the development of probiotic strategies for amphibian protection. Ultimately we found that addition of the probiotic bacteria was not successful, however, certain pre-existing bacteria on frog skins afforded protection against Bd.

Cloning, expressing, and purification of Drosophila melanogaster Keap1

Poster: B19 Author: Rebecca Lin, Aimee Eggler Advisor: Aimee Eggler

The human Nrf2 transcription factor and its repressor protein Keap1 defend against oxidative stresses in the body, playing an important role in the prevention of diseases including cancers, obesity, and neurodegenerative diseases. The chemopreventive effects of the Keap1/Nrf2 system are activated by various electrophiles that alter the conformation of Keap1 and inhibit repression of Nrf2, allowing upregulation of cytoprotective genes via the antioxidant response element (ARE).

The common fruit fly, *Drosophila melanogaster*, has homologs of the Nrf2 and Keap1 proteins. Studies have shown that Nrf2 plays an important role in various biological functions in the fruit fly, for example, in proteasome dysfunction in the aging process, organismal development and the stress response. *D. melanogaster* is being developed as a model system to test Nrf2 activators that have

promise for disease prevention in humans. Interestingly, while the *D. melanogaster* Keap1 is 38.1% identical in sequence to H. sapiens Keap1, cysteine 151, a major sensor of ARE-activating electrophiles in vertebrates, is not present in the *D. melanogaster*. Research on the mechanisms involved with *Drosophila melanogaster* Keap1 and its chemical inducers can potentially help elucidate human Nrf2 activation mechanisms as well as aid in efforts to avoid crop destruction by insects. In order to begin investigation into the antioxidant response system of fruit flies, the *D. melanogaster* Keap1 must first be cloned, expressed, and purified.

Modeling sodium battery electrolytes and electrode interfaces using classical molecular dynamics

Poster: B20 Author: Jessica Wahlers Advisor: Dr. Ryan Jorn

Sodium battery electrolytes are being studied as an alternative to lithium batteries since there is a larger abundance of sodium which would make batteries more cost effective. Using Classical Molecular dynamics, sodium battery electrolytes comprised of diglyme (C6H14O3) and sodium triflate (CF3SO3Na) were modeled to study the structure of the materials as well as their transport properties. Force fields were developed for the electrolyte based on quantum calculations and were subsequently used to calculate the density, radial distribution functions (RDFs), solvation structure, and diffusion coefficient for sodium electrolyte species. In addition to studying bulk properties, the electrolyte/electrode interface was also considered by implementing an image charge method to incorporate an electric field. The results for distributions of electrolyte species as a function of distance from the electrode were then compared to a lithium electrolyte comprised of ethylene carbonate (C3H4O3) and Lithium hexafluorophosphate (LiPF6).

Investigation of La0.80Sr0.20Ga0.8Mg0.2O3-δ solid oxide fuel cell electrolyte material

Poster: B21 Author: Tim Marshall, Bryan Eigenbrodt Advisor: Bryan C. Eigenbrodt

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

Activation of the Nrf2/ARE pathway through sesquiterpene aminoquinones from the South China sea sponge *Dysidea Fragilis*

Poster: B22

Author: Nicholar Ader, Bing-Nan Han, Zack Kemmerer, Hou-Wen Lin, Aimee Eggler Advisor: Aimee Eggler

Several sesqiterpene aminoquinones from *Dysidea fragilis* (dysidaminoes) were analyzed for Nrf2/antioxidant response element (ARE) activation. Compounds were assayed for ARE activation in HaCaT cells (normal keratinocytes) using a dual-luciferase ARE assay. Two plasmids were transiently cotransfected into the cell, one containing an ARE reporter sequence and a second to act as a control for cell growth levels and cell health analysis. ARE assay results demonstrated one compound in particular, dysidamino 16 (DA16), robustly activated the Nrf2/ARE pathway with relatively low toxicity. Three other structurally similar dysidaminoes, DA14, DA8 and DA9, demonstrated more potent Nrf2/ARE activation, but at the cost of higher cytotoxicity. To assess Nrf2 activation, Western blot analysis was employed. Increased Nrf2 levels in response to DA16 correlated with the ARE response, but the comparatively low accumulation of Nrf2 with respect to (2-tert-butyl-1,4-hydroquinone) tBHQ suggests a mechanism of ARE activation beyond cellular accumulation of Nrf2. The structural differences between DA16 and the other dysidaminoes analyzed appear to be critical to compound activity and provides new insight on structural constraints for Nrf2/ARE activators with low cytotoxicity.

Instrumental analysis of algae growth rates for biofuel generation

Poster: B23 Author: Janelle Gerardi, Tamanna Sultana Advisor: Bryan Eigenbrodt

The purpose of this research is to explore micro-algae as a renewable energy source. Currently most of the world's energy comes from fossil fuels. Two problems are associated with the use of fossil fuels. First, the use of this fuel has increased the concentration of carbon dioxide in the atmosphere, which has been attributed for global warming. In addition, the amount of fossil fuels available to us is unsustainable and depleting. For these reasons, we must find a renewable, environmentally friendly fuel source. Of the various renewable fuel sources that have been considered, like solar power, wind power, or soy bean oil, algae seems to be the most promising. In this research, we grew *Nannochloropis eukaryotum*, a sea water algae. During the first half of the summer a procedure for quantitatively measuring the lipids in the algae was developed and during the second half of the summer this procedure was used to analyze how changing the amount of nitrogen in the nutrient solutions affected lipid production. We examined nutrient solution with 0%, 50%, and 100% nitrogen, as compared to the nutrient solution procedure provided to us by the University of Texas. On the 47th day we found that the two 0% N samples had 16.76 and 29.03 ppm of lipids, the two 50% N samples had 54.74 ppm and 59.29 ppm and the 100% N had 128.91 ppm of lipids.

Solid oxide fuel cells

Poster: B30 Author: Andrew D'Orazio, Bryan C. Eigenbrodt Advisor: Bryan C. Eigenbrodt

Energy sources are currently being depleted, and a need for alternate energy sources is arising. Solid oxide fuel cells (SOFCs) are one sustainable alternate energy source which utilize a variety of fuels

(H2, CO, alcohols, hydrocarbons, natural gas, etc...) and oxygen. Currently solid oxide fuel cells face a number of problems such as: graphite and nickel sulfide formation on the nickel catalyst in these anodes. These problems can ultimately destroy a fuel cell by deactivating the electrode metal catalyst. Research described below will investigate the use to mixed ionic and electronic conducting (MIEC) perovskite materials as potential electrode catalyst that are capable minimizing graphite formation and metal sulfidation. The perovskite material of interest in this research is Sr2Mg1-xNixMoO6 (x=0,0.1). This research will explore the synthesis, and electrochemical activity of this material under SOFC operating conditions. Specifically, the effects of nickel addition into the B-site of this material will be explored at an attempt to increase its electrical and catalytic activity.

Progress towards the synthesis of analogs of Isogemichalcone B and C

Poster: B29 Author: Alicia Angelbello, Sean Longson,

Author: Alicia Angelbello, Sean Longson, Melissa Morales, Eduard Casillas Advisor: Eduard Casillas

Isogemichalcones B & C, metabolites from *Hypericum geminiflorum*, have been shown to have a mild inhibitory effect against aromatase, a late enzyme in the biosynthesis of estrogen, and therefore, a potential therapeutic target against breast cancer. Based on a recently completed synthesis of the Isogemichalcones, analogs in which phenols are replaced with substituents of various stereoelectronic properties are being prepared in order to determine structure activity relationships.

Development of imino and amino pyridine iron (II) catalysts for atom transfer radical polymerization

Poster: B28 Author: Laura Thierer, Lindsey Round, Deanna Zubris Advisor: Dr. Deanna Zubris

Atom Transfer Radical Polymerization (ATRP) is a technique that utilizes a metal catalyst to mediate free radical polymerization to produce polystyrene and acrylic polymers with a narrow polydispersity. Prior studies by Gibson revealed that imino(pyridine) and amino(pyridine) iron (II) complexes have modest ATRP activity, where small electronic changes to the ligands impart large differences in relative polymerization activity. The most electron rich ligands in Gibson's study displayed the highest ATRP activity. In attempt to improve upon these prior studies, we are targeting a series of iron(II) complexes with new imino(pyridine) and amino(pyridine) ligands for ATRP utility. Using our group's previously reported tert-butyl substituted imino(pyridine) ligand, 2-[{(2,6-Me2-C6H3)NC(t-Bu)}C5H4N], as a starting point, synthesis of the amino(pyridine) ligand 2-[{(c-C6H11)NC(t-Bu)}C5H4N] and the imino(pyridine) ligand 2-[{(c-C6H11)NHCH(t-Bu)}C5H4N], metalation of these ligands with iron(II) and subsequent ATRP testing is in progress.

<u>Mid-to-late first-row transition-metal complexes of the Janus head ligand tris(2-pyridyl)phosphine [P(Py)3] and its oxide</u>

Poster: B27

Author: Krystyn Suppa, Carina Fairfield, Danijel Pericic, Nicholar Piro, Scott Kassel Advisor: Dr. Scott Kassel

Pyridylphosphines have gained attention within the last decade due to their versatility, from catalytic properties to the ability to act as precursors in certain pharmaceuticals. Studies of tris(2-pyridyl)

tripodal ligands feature differing central bridging atoms, but tris(2-pyridyl)phosphine has been focused on for its own unique behaviors. The hard nitrogen atoms of the pyridyl rings and the soft phosphorus atom allows for different binding modes, including the N, N', N"- chelating mode of PPy3. The two different donor atoms of this Janus-head ligand can chelate to a metal in four different binding modes.5

Here, tris(2-pyridyl)phosphine (PPy3) reacts with several metal nitrate salts (M= CrIII, CoII, MnII, FeIII), in simple one-pot procedures to yield facially coordinated ligand-metal complexes. Structurally, one or two ligands bind to the metal, forming half-sandwich and sandwich complexes, respectively. The formation of these complexes depend on the ratio of ligand used with respect to the metal salt, and often form equilibrium mixtures in solution.

Novel fluorescent sensors possessing a 1,4-Dihydropyridine core structure

Poster: B26 Author: Danielle Kadish, Sara Zagroba, Sally Zhou, Costas Agrios Advisor: Dr. Costas Agrios

Fluorescence-based detection methods are used extensively and for a variety of purposes such as monitoring Zn2+ in biological samples. We have discovered a new class of fluorescent molecules based on a 1,4-Dihydropyridine core structure. The synthesis of a series of analogs based on this scaffold via a modified Hantzsch reaction will be reported in this poster. UV and emission spectra of selective compounds will also be shown.

Synthesis of tri(pyridylmethyl)phosphine oxide, OP(CH2Py)3, and coordination chemistry with select lanthanide nitrates

Poster: B25 Author: Carina Fairfield Advisor: Dr. Scott Kassell

Tri(pyridylmethyl)phosphine will be prepared using literature methods followed by oxidation with H2O2, as done in the preparation of OPPy3, to form OP(CH2Py)3, tri(pyridylmethyl)phosphine oxide. The coordination chemistry of M(III) nitrates (M = NdIII, SmIII, YbIII) with tri(pyridylmethyl)phosphine oxide and tri(2-pyridyl)phosphine oxide will be investigated. The ability of free pyridyl nitrogens in the M(OP(CH2Py)3)2(NO3)3 to bind MII ions to form heterobimetallic complexes will be investigated as well. The primary characterization of the synthesized compounds will be through x-ray diffraction to determine their 3-dimensional structures. Supplemental characterization of the complexes will be by IR, UV-vis, 1H/31P NMR, and electrochemistry. Investigation of sandwich and half-sandwich equilibrium will be analyzed.

Chemical Engineering

Investigation on the potential of algae as a viable feedstock for the production of fuels and chemicals via fast pyrolysis approach

Poster: B24 Author: Emily Woloshen, Joshua Rickert, Dr. Justinus Satrio Advisor: Dr. Jacob Elmer Fast pyrolysis is a thermochemical conversion process in which organic materials, such as biomass, are decomposed by flash heating at an elevated temperature (300-700°C) in the absence of oxygen to produce a liquid (bio-oil), a solid (bio-char) and a gas mixture (syngas). It is one of the most promising methods to convert biomass for biofuel production due to its ability to process any type of biomass. The potential of selected algae strains as feedstock for the production of bio-oils and chars were investigated in this study. Proximate analysis compositions of the feedstock were determined using thermogravimetric analysis to evaluate the potential oil + gas as well as char yields. Fast pyrolysis experiments were performed using a micro-pyrolyzer/GC-MS system in order to determine the relative composition of the chemical moieties contained in the bio-oil. The results show large variations of the yields and selectivities of the pyrolysis products from different algae strains. It is found that bio-oils produced from algae contained desirable compounds, specifically aromatics that are typically found in pyrolysis of lignocellulosic biomass as products of catalytic pyrolysis. This unique feature makes algae biomass a promising alternative feedstock for the production of bio-oil.

The Effects of ODN sequences on gene expression

Poster: C31 Author: Adam Butchy, Jacob Elmer Advisor: Dr. James Elmer

Cells have an innate immunity that helps protect them from foreign DNA. One way the cell identifies foreign DNA is with the Toll-like Receptor 9 protein, which binds CpG motifs on bacterial DNA and triggers the production of immunostimulatory cytokines. Oligonucleotides (ODNs) with special sequences (e.g. TTAGGG) have been previously shown to bind TLR9 without activating the production of cytokines. The goal of this project was to see if the inhibitory capabilities of these ODN's could help enhance gene therapy by inhibiting recognition of foreign DNA by TLR9. In our experiments, PC3 cells were transfected with plasmid DNA carrying the gene for Luciferase, the cationic polymer PEI, and several ODN sequences. Six different ODN sequences (2088 and TTAGGG) showed significantly higher transgene expression than cells transfected without an ODN present. This shows that ODN's may be promising tools for gene therapy, but more research is required to confirm that ODNs are boosting trans-gene expression through inhibition of cytokines and not by other means.

Synthesis and characterization of hydrothermally stable catalyst supports by carbon deposition

Poster: C32 Author: Sam Chung, Charles Coe, Michael A. Smith Advisor: Charles Coe

Biomass conversion is a promising field in a world moving towards alternative energies. A specific platform of alternative energy science and engineering being developmental within the Department of Chemical Engineering is thermochemical transformations of biomass. Thermal pyrolysis is being used to study the conversion of biomass to bio-oils. These bio-oils derived from biomass unfortunately have properties which make them unsuitable alternatives to currently used petroleum based fuels. Bio-oils contain30% water and water is also a byproduct of the upgrading reactions needed to improve their value and stabilize them for downstream uses. Thus, catalysts used for the upgrading of bio-oils must withstand high temperature steam environments.

The goal of this work was to create a hydrothermally stable support by carbon loading mesoporous silica. The procedure involved loading the silica supports with a carbon precursor (1), pyrolyzing the treated support (2), exposing to steam (3), and analysis of samples before and after steaming (4). Hydrothermal stability was based on retention of surface area, pore volume and mean pore size obtained from standard nitrogen adsorption isotherm measured at 77K. Mesoporous carbon-coated silicas were prepared by pyrolysis from three different carbon precurors: sucrose, furfuryl alcohol (FA) and polyfurfuryl alcohol (PFA). It was determined that PFA was the optimal carbon source for improving hydrothermal stability of the carbon-coated silica supports. The influence of various pyrolysis temperatures and the amount of carbon loaded were also studied. These analyses showed that 900°C was the optimal pyrolysis temperature and a carbon loading of 5wt % was sufficient for the retention of hydrothermal attributes. Lastly, the preferred PFA treated silica was scaled up and is being used in further studies both at Villanova and University of South Carolina.

Isolation of invertebrate hemoglobins for use as a blood substitute

Poster: C33 Author: Jack Dienes, Devon Zimmerman, Dr. Jacob Elmer Advisor: Noelle Comolli

Although donated blood is the preferred material for transfusion, limited availability has motivated the development of hemoglobin based oxygen carriers (HBOC's) that can be used when donated blood is unavailable. To meet a global demand for HBOC's, an easily accessible and equally efficient hemoglobin source is needed. Invertebrates may be the solution to that demand, since they are readily available and efficient oxygen carriers without any significant side effects. In this work, we isolated and purified the hemoglobin from four invertebrate species and compared their characteristics to those of human hemoglobin. We did this via centrifugation and tangential flow filtration, then characterized the hemoglobins by running a variety of assays including oxidation and heme quantification. Our results show that the hemoglobin from earthworms, bloodworms, and ribbon leeches should undergo further study for potential use as HBOC's, whereas the hemoglobin from sandworms is too fragile and difficult to collect. The three hemoglobins which were characterized showed P50 values which would make them viable for oxygen delivery in humans even though they have a slightly lower oxygen affinity (~20-30mmHg, human is ~4mmHg), while also being more stable and resisting oxidation throughout the purification process. These encouraging results show that invertebrate hemoglobins may be promising HBOC's and further motivates the investigation of additional invertebrate hemoglobins in the future.

Development of a fluent-based platform to study the dynamics of microbial fuel cells Poster: C34

Author: Charlotte Eberle Advisor: Dr. Suyi Huang

Microbial Fuel Cells (MFCs) can be used as an alternative energy resource that can produce electricity from organic matter with a low energy input. This work represents an accurate Fluentbased 2D model of a microbial fuel cell which includes an anode chamber, biofilm, anode, membrane, cathode, and cathode chamber. This model integrates mass balances, chemical reactions, and reaction rates with the 2D geometry. A flow of the substrate, acetate, was added in order to increase the current and overall energy production of the MFC. This model was used to analyze the dynamics of microbial fuel cells, and will be used as a platform for a scale-up design of MFCs.

A Simulink-based PID control system for the Operation of Microbial Fuel Cells

Poster: C35

Author: Clement Nevin Ekaputra, Zuyi (Jacky) Huang Advisor: Zuyi (Jacky) Huang

Microbial fuel cells (MFCs) are able to convert the organic compounds in waste water to electricity via the microbial metabolism on the surface of the anode. Since the performance of MFCs depends on the operation conditions (e.g., the substrate concentrations and flow-rates), the design parameters such as external electrical resistance, and the interaction between the microorganism species in the anode compartment, a model-based platform can significantly accelerate the optimization of the design and operation of MFCs. This work presents the first attempt to design a proportional-integral-derivative (PID) control system for regulating a MFC system to the designed current production with a disturbance in the substrate concentration. In particular, a Simulink-based model was developed for a MFC system to describe the growth of both anodophilic and methalnogenic microorganisms, the reduction and oxidation rates of an intracellular mediator protein, and the production of electrical current. A PID-based negative control system was then designed to control the substrate flow-rate for a set-point change in the current production. The performance of MFCs for various values in parameters P, I, and D was investigated and the influence of parameters P, I, and D was evaluated for both set-point change and disturbance rejections. Optimal values for parameters P, I, and D were finally determined for the MFC control system.

Study on non-catalytic and catalytic pyrolysis of lignocellulosic biomass by using a <u>Micropyrolyzer-GC/MS reactor system</u>

Poster: C36

Author: Nicole Hammer, Matthew Pak, Royce Lee, Julie Clarke, Charles Coe, Justinus Satrio Advisor: Justinus Satrio

Throughout our research during the 2014 summer, we investigated both catalytic and non-catalytic pyrolysis of lignocellulosic biomass feedstocks by using a micropyrolyzer-GC/MS reactor system. In the non-catalytic pyrolysis reaction study, we evaluated the performance of three different biomass materials, namely hardwood, switchgrass, and horse manure, as feedstock for producing bio-oil. Analysis of the chemical product distribution in the pyrolytic vapors produced from pyrolysis of these three biomass feedstock showed that the quality and properties of bio-oil are highly dependent on the properties and composition of the biomass feedstock. In the catalytic pyrolysis reaction study, we evaluated the performance of a newly developed ZSM-5 supported Lewis acid catalyst for catalytic pyrolysis of pinewood. The catalyst performance was compared with that of HZSM-5 which is currently considered the best commercial catalyst available for biomass catalytic pyrolysis. Preliminary results showed that relative to HZSM-5, SrZSM-5 may be more stable over time even with a relatively smaller yield of aromatics

Non-catalytic and catalytic pyrolysis of pinewood and *Phragmites australis* by using a batch pyrolysis reactor system

Poster: C37 Author: Charles Ponge, Nicole Hammer, Justinus Satrio Advisor: Justinus Satrio

The purpose of the research is to explore the effects of biomass feedstock properties on the yields and selectivity of bio-oil and bio-char production from fast pyrolysis of biomass by using a batch

pyrolysis reactor system under non-catalytic and catalytic conditions. Two different biomass feedstock, i.e. pinewood (low inorganic mineral contents) and Phragmites australis (common reeds), were used for the study. Pinewood was a woody-type biomass with very low inorganic mineral content and phragmites was a grassy-type biomass having significantly higher inorganic mineral content. A commercially available acid catalyst, namely HZSM-5, was used for the fast pyrolysis performed under catalytic condition. Preliminary results showed significant different product yields and chemical product distribution in the bio-oil produced from fast pyrolysis of these two different biomass feedstocks. Compared to phragmites, pinewood was the better feedstock in producing higher yield of bio-oil, which was due to its very low inorganic mineral content.

Electrical/Computer Engineering

Detecting abnormal behavior of a multithreaded processor

Poster: C38 Author: Matthew Myers Advisor: Danai Chasaki

In traditional multiprocessing, each central processing unit supports a single hardware instruction thread that interfaces with the operating system. This traditional way exhibited performance limitations as more CPUs were added to a configuration. A multithreaded processor allows multiple threads to exist within the context of a single process. The threads share the process' resources, but are able to execute independently. Multithreading allows a program or operating system to manage its use by more than one user at a time and to manage multiple requests by the same user without having to have multiple copies of the programming running in the computer. However, there are many disadvantages to using a multithreaded processor. Multiple threads can interfere with each other when sharing hardware resources, and multithreading creates a lot of overhead for the processor. In addition, sharing the resources among the threads can lead to deadlocks or other unexpected problems. Furthermore, execution times of a single thread are not improved but can be degraded using multithreading. Thus, there are many ways that a multithreaded processor can encounter errors in the system and its programs as well. Additionally, multithreaded processors are susceptible to malicious attacks just like any other processor out there. To remain operational, these multithreaded processors need to detect these failures and recover from them. It is very challenging to identify situations in which a small number of processor threads behave incorrectly, either due to failure or due to malicious attacks. To address these problems, I attempted to collect processing time statistics during the operation of the multithreaded processor, and correlate input and output traffic in order to detect "incorrect" operation of the multithreaded processor. I also attempted to relate these time statistics with the power consumption of the individual threads in the processor.

Mechanical Engineering

Relating energy efficiency to CPU usage in 1U servers

Poster: C45 Author: Kagan Richardson Advisor: Dr. Aaron Wemhoff A data center is a centralized location of computers that generate an enormous amount of heat, requiring complex cooling systems that consume significant amounts of energy. This research is motivated by the need to improve such cooling systems in order to maximize efficiency. In order to do so for air-based cooling systems, the effectiveness of cooling inside a dual-core 1U server is analyzed by measuring air pressure, temperature, and velocity at over 600 points uniformly distributed across the server through a spatial grid. Each measurement is taken one inch above the printed circuit board with one half inch of lateral spacing between each point. Temperature and air speed are measured at each grid point with ATS candlestick sensors, which feature a combined thermistor and hot-wire anemometer. The direction components of air flow velocity are found through the use of air tufts in order to measure air flow direction. The pressure is measured at each node using a Baratron MKS pressure transducer and a MKS Type 670 signal conditioner with a pitot tube. This setup measures static pressure in order to calculate flow work at each node. The experimental data is then used to create a cooling ineffectiveness factor at each grid point across the server, defined as the ratio of flow work to convective heat removal from the surface.

Previous experiments examined the pressure, temperature, and velocity measurements with both CPU's running, while this experiment takes the same measurements with one CPU running. With both CPU's running, the largest pressure loss is seen through the heat sink and a pressure rise is seen near the server outlet due to turbulence created by the partial blocking at the exit. The areas with the greatest ineffectiveness factors are the edges around the heat sink and the gap between heat sinks, and large factors are found near the screw positions on the heat sinks. The goal of taking the same measurements with one CPU running is to compare areas of inefficiency in order to isolate the areas that would need to be improved. It is anticipated that the area above the unused CPU will contain the largest ineffectiveness. The least effectively cooled areas on the server can be modified by reducing the local air flow rate.

AAO template fabrication for the electro-deposition of copper nanowires used for pool boiling

Poster: C44 Author: Matthew Ashcroft Advisor: Dr. Calvin Li

The end goal is to improve the heat transfer characteristics of a copper surface by altering its surface topography. More specifically, the goal is to increase the heat transfer coefficient of the surface, as well as delay the onset of critical heat flux. In the past, the lab has achieved both of these goals by altering the surface with micro-structures (see figure 1). The structures improve heat transfer by increasing the number of nucleation sites and also by creating horizontal and vertical re-wetting channels that keep water flowing to the heated surface. The next step in this research is to move from micro-scale structures to nanoscale. It is hoped that nanoscale structures will provide a further improvement on the heat transfer coefficient and critical heat flux.

The nanoscale structures in question are copper nanowires that are deposited in an anodized aluminum oxide template. The template is an array of vertical nanopores ordered in a hexagonal pattern, resembling a honeycomb. This technique is desirable because it allows for control of the pore diameter and depth, which in turn controls the nanowire diameter and depth.

With increasingly powerful electronic devices, faster processors, higher powered graphics, and larger batteries comes increased heat. To keep these delicate components from overheating, better heat

dissipation is needed. The goal of this research is to improve two phase heat transfer for this purpose. Cell phones and other electronic devices already use two phase heat transfer. Increasing the heat transfer coefficient of the cooling surfaces in such devices would allow for more powerful processors as well as faster chargers that generate more heat. In addition, most of the world's electricity is produced by heat engines. Water is boiled and the steam produced spins a turbine and a generator. Improving the heat transfer coefficient of a boiling surface will produce more steam for the same amount of heat, thus increasing the efficiency of most of the world's power.

Experimental study of various designs for thin film thermal interface materials based on different types of carbon-based nano materials

Poster: C43 Author: Omar Arafa, Dr. Amy Fleischer Advisor: Dr. Amy Fleischer

The thermal management of electronics has become very important as slimmer and more compact electronic devices have been designed. These new advanced designs create higher heat loads within the devices. Failure to remove or manage this heat properly could lead to the failure of these devices.

Thermal Interface Materials are crucial for transferring heat from a die to a heat sink. Thermal Interface Materials are located between the heat source [the processor] and the heat sink in order to fill in the air gaps and irregularities on surfaces resulting in better cooling.

A lot of attention has been given to developing thermal interface materials that are highly conductive and very thin. As a result a lot of research has been put into developing thin films. Adding nanoparticles can improve the performance of these thin films. Nanoparticles provide a greater surface area that is a better conductor when added to thin films.

This research project proposes an experimental study of various designs for thin film thermal interface materials based on different types of carbon based nanomaterials. The thin films will feature various combinations of multi walled carbon nanotubes and a few layer grapheme particles which will be deposited into thin film mats. The mats will be evaluated for their thermal performance in an attempt to determine an optimum combination which maximizes thermal transport. The results of the research will be of significant interest to the thermal research community.

Load capacity and thermal efficiency optimization of a research data center using computational modeling

Poster: C42

Author: Joseph Schaadt, Dr. Kamran Fouladi, Dr. Aaron Wemhoff, Thomas Wu Advisor: Dr. Kamran Fouladi

A data center is a centralized location of networked computer servers that store, process, and distribute data for an organization. In 2007, 1.5% of the electricity consumption in the United States was used for data centers. Of the 1.5%, one-third to one-half of this energy was used for cooling. Data centers are most commonly cooled by air delivered to electronic equipment from centralized cooling systems. This research is motivated by the need for strategies to improve and optimize the load capacity and thermal efficiency of data centers by using computational fluid dynamics (CFD) simulation software. In the last decade, CFD has been used extensively to study

the cooling issues and thermal management in data centers. The program 6SigmaRoom by Future Facilities was chosen as the computational fluid dynamics simulation software for modeling and optimizing the Villanova Steel Orca Research Center (VSORC). Presently in the design stages, VSORC will be a research data center to provide an environment with the capability to test industry's best practices as well as state of the art strategies in order to measure and validate the characteristics of the proposed strategies in a data center facility. These strategies, which include hybrid cooling, IT load distribution, density zones, hot aisle and cold aisle containments, and hot aisle and cold aisle layouts are employed in the design of data centers to reduce the power needed to cool IT equipment and prevent damage to the IT equipment. The results of this study will be used in the overall design and construction of the research data center. The objective of this study will be to find the optimal operating points and design layout of a data center while still meeting the design constraints. A focus will be on finding both the ideal total supply flow rate and supply-side control temperature of the air conditioning units in VSORC under different data center design configurations and load capacities. A hybrid cooling strategy made up of computer room air condition (CRAC) units and in-row cooling units will be employed in VSORC while investigating effectiveness of various hot aisle and cold aisle containment arrangements. The flow rate and supply-side control temperature of the air conditioning units will be varied as design parameters in separate simulation cases in order to systematically determine the optimal operating points. The study will also examine the influence of hot aisle and cold aisle containment in full containment, half containment, and no containment configurations on the determined optimal operating conditions for the modeled research data center.

Impact of intra- and extracellular ice on zebrafish oocytes during cryopreservation Poster: C41

Author: Anthony DeCamillo, Fatemeh Jalali, Angela DiBenedetto, Jens O.M. Karlsson Advisor: Jens O.M. Karlsson

The ability to cryopreserve the eggs of aquatic species would benefit a wide range of fields, including biomedicine, aquaculture, and conservation. For example, in genomic research, zebrafish are becoming an increasingly popular and viable animal model. This is primarily because they are one of the few vertebrate species that develop outside of the uterus, which allows their development to be more easily studied. Zebrafish also have a short gestation period and produce many offspring, again contributing to their increasing popularity in the scientific community. However, there has yet to be a report of the successful cryopreservation of fish oocytes, necessitating poorly controlled and costly maintenance of live zebrafish stock in aquaculture. In contrast, cryopreservation of oocytes would allow for their long-term storage and subsequent thawing to produce live fish when needed. Thus, the goal of my proposed research is to lay the groundwork for successful cryopreservation of zebrafish oocytes. Using high-speed video cryomicroscopy, it was observed that contact with extracellular ice preceded damage to the oocytes. Because of the importance of ice crystal growth in this phenomenon, we conducted separate experiments to study the nucleation and growth of ice crystals in microscale water droplets. Using a microfluidic device, an emulsion of water in oil was generated and made into a sample suitable for cryomicroscopy. The average temperature at which ice crystals began to form was -41.20 °C \pm 3.82 °C. The speed of the ice growth was measured by tracking a point that moved linearly from initial crystal formation until it reached the farthest point along the edge of the droplet. The average duration of this event was 400 µs which shows the need for the high-speed imaging. In a graph of Speed vs. Temperature it was difficult to see a negative linear trend as expected. This may be explained by the fact that ice growth in directions outside of the plane of view would distort speed measurements. Also, the shape of the crystals may impact the

speed with which they grow. Plans for future analysis include correlating crystal growth velocity and oocyte damage.

Light-weight stereo vision system for a micro-quadrotor helicopter

Poster: C40 Author: John Bellizzi Advisor: Garrett Clayton The purpose of this research is to find the image processing capabilities of a light weight cameramicrocontroller system that can potentially be used for stereo-vision applications on small aerial craft such as micro-quadrotor helicopters. The main focus of this project concentrated on the maximum data transfer and processing speeds of a Toshiba TCM8230MD camera controlled by the Atmel AT91SAM ARM microcontroller on an Arduino Due board. The limits of data transfer were tested to find an appropriate rate to send out image frames while still leaving enough time for the images to be manipulated by image processing algorithms.

Geography and the Environment

<u>Growing a greener lawn: encouraging change through scientific monitoring and community</u> <u>involvement</u>

Poster: C39 Author: Kaitlyn McGrath, Dr. Steven T. Goldsmith Advisor: Dr. Steven T. Goldsmith

Although several studies have documented how nutrients in lawn fertilizers can make their way into water systems, relatively little information exists linking historical lawn maintenance practices and impairments to surrounding bodies of water. Furthermore, an even smaller amount of studies document how one's perception of their lawn drives this over application process. The East Branch of Indian Run in Lower Merion Township, PA largely traverses neighborhoods dominated by singlefamily homes with lawns dating back to the early 1900s. The stream has been deemed "impacted" by the PADEP due to excess nutrient input form stormwater runoff, thus providing an ideal location to examine the link between historical fertilizer application rates and streamwater quality. This study bridges existing knowledge gaps through the administration of a series of household surveys and collection of lawn core and streamwater samples for nutrient analysis in two residential areas which boarder the East Branch of the Indian Creek, Narbrook Park and Shortridge Park. Cumulative average scores on a scale of 1 to 10 revealed that while the residents largely feel a visually appealing lawn can positively affect home value (5.8) they tended to be dissatisfied with both the appearance (4.6) and perception of health (4.9) of their lawn. Furthermore, many residents were in tune with their surroundings and had a somewhat negative perception of the health of Indian run (4.6). Surprisingly, a low level of the residents in these communities (31.6%) actively apply fertilizer to their lawns; however this does not preclude the idea that fertilizer from previous owners could be contributing to the streams nutrient content via storage in shallow groundwater. Therefore, soil core and water samples collected over the summer will continue to be analyzed to determine whether historical application of fertilizer is the main cause of nutrient impairment in the East Branch of Indian Run.

<u>Pre- and post-storm morphological analysis of sand dune effectiveness and regeneration in</u> <u>Mid-Atlantic barrier island systems</u>

Poster: D46 Author: Samantha Blemker, Francis Galgano Advisor: Dr. Francis Galgano

Dunes are an essential morphological component of barrier islands. Dunes are an important buffer to storm energy and are a natural part of the barrier beach ecosystem. The vital importance of sand dunes was underscored during Hurricane Sandy in October 2012. Sandy damaged much of the Mid– Atlantic coastline with a 12 to 14 foot storm surge. There was a clear and dramatic difference communities that maintained vital and healthy dune systems did not suffer as much damage as those that did not. Our understanding of the importance of dune systems as a storm buffer is not new. Nevertheless, the maintenance of dune systems is a matter of some contention and the real question is why, in the face of long–standing evidence, would coastal communities fail to maintain their dune systems? This project evaluated pre– and post–storm performance of dune systems in three New Jersey barrier island systems: (1) Sandy Hook; (2) Long Beach Island; and (3) Brigantine. I evaluated the status of the dunes at each location before and after Sandy and correlated the level of storm– related damage to the health of the dune system today adjacent to each of three land use types: urban/residential, semi natural/recreational, and natural ecosystem.

Accumulation of heavy metals in freshwater clams from the East Branch of the Brandywine Creek: cause for concern

Poster: D47 Author: Danielle Radomile, Steven Goldsmith, Stephen Levas Advisor: Stephen Levas

Anthropogenic land use and management practices such as agriculture, urbanization, and deforestation negatively impact essential natural resources. These practices often introduce various pollutants into nearby waterways, which have the potential to alter both water quality and chemistry. Heavy metals are of particular concern due to their ability to bioaccumulate in the tissues of organisms when consumed and because of their toxicity to humans. Freshwater clams have a significant ability to bioaccumulate metals with no evident danger to themselves, making them excellent indicators of stream health. The Brandywine Creek of Southeastern Pennsylvania has become inhabited by the invasive Corbicula fluminea, also known as the Asian Clam. In order to determine potential impacts of land use change on the East Branch of the Brandywine Creek freshwater ecosystem, we sampled 6 sites differing in their land use patterns along the creek, and 2 sites from a tributary, collecting 10 Asian Clams from each site. Using an ICP-MS, whole clam tissues were digested in nitric acid and analyzed for concentrations of Ni, Cu, As, Cd, and Pb. Ni and Cu were the two most present metals at each site while Cd was present in the lowest concentrations. Sites 2 and 6 revealed noticeably higher concentrations of heavy metals than the other six sites. Interestingly Site 2, located just above the wastewater treatment plant, showed higher concentrations of heavy metals than Site 5, located just below the treatment plant. Presumably, this difference can be attributed to the effectiveness of the treatment plant in removing metal pollutants. Clams from the tributary, Beaver Creek, exhibited the least bioaccumulation of metals. Overall, the highest concentrations of heavy metals were found at sites located in close proximity to highly developed and urbanized lands.

Effects of hydraulic fracturing on surface water

Poster: D48 Author: Stephanie Dantos Advisor: Nathaniel Weston

The Marcellus Shale is one of the largest natural gas deposits in the U.S., and extraction of natural gas is becoming increasingly prevalent in rural regions of Northeastern Pennsylvania. The process of drilling and hydraulic fracturing or "fracking," remains a highly controversial environmental issue. Most of the controversy focuses on the potential negative impacts on groundwater, such as unusually high levels of methane and chemicals used in the fracking process that renders the water undrinkable. However, the impacts of fracking on surface water quality remains largely unknown, and our research focused on the relationship between natural gas drilling and surface water quality. To address this, we sampled water from 36 stream sites draining small watersheds representing a gradient of natural gas extraction well densities in three counties in NE Pennsylvania. We measured water quality data including stream-water conductivity at each site. We hypothesize that stream conductivity is significantly correlated with well pad densities across the sites due to land-use change and possible contamination from fracking flow-back water.

Humanities

Defining grace: a theo-literary analysis

Poster: D49 Author: Jessica Swoboda Advisor: Dr. Helena Tomko

Drawing on the Thomistic account of nature, grace, and art in Jacques Maritain's Art and Scholasticism, I will provide an analysis of Flannery O'Connor's *A Prayer Journal* that focuses on her gradual understanding of the workings of grace in her young artistic life. Throughout *A Prayer Journal*, O'Connor asks for grace to help to strengthen her intellect and to develop greater knowledge of her soul. I argue that in her earlier journal entries, her invocations for grace reveal a struggle to comprehend the meaning of grace in her life in relation to its role in her artistic life. Since we do not have definitive proof of when O'Connor first read Maritain's *Art and Scholasticism*, I conjecture that her journal seems to either reflect her reading of the text or show her intuiting the arguments Maritain will affirm when she does read it. I will also contend that in the course of writing the journal she seems to be slowly and, at first, imperfectly, and perhaps unknowingly, assimilating the Thomistic account of grace, art, and virtue that Maritain interprets and describes in *Art and Scholasticism*. I will then claim that O'Connor's admission that she is "to be an artist" represents the moment in her journal where this assimilation seems to occur. This entry signifies a transformative moment in her life in which her human life and artistic life converge, and in which she properly orders her art so that it transcends our humanity.

Unto this beginning: the Ruskinian effect on social and economic thinking

Poster: D50 Author: Christopher Gelardi Advisor: Dr. Eugene McCarraher John Ruskin was, among many other things, a mid-nineteenth century art and architecture critic famous for his keen eye and his peculiar philosophy of the union of morality and aesthetics. When he turned to social critique in the late 1850s, he adhered to his hard-held belief that morality, both on a societal and an individual scale, should be the most penetrating and central element of every aspect of life, including the noble art of socioeconomics. Ruskin abhorred the "scientists" of political economy of his time for stripping anything human out of economic thought, and in 1860 he published Unto This Last, a series of essays in response to the modern trends in political economy he saw as destroying civil society. "There is no Wealth but Life," he wrote, for societal happiness rather than material productiveness should be the guiding principle behind socioeconomic theory and practice.

Although Ruskin was unable to reverse the popular modern trend in socioeconomic thinking, he was able to inspire a tradition of dissenters. The Ruskinian spirit of moralism, humanism, and anticapitalism has lived on in twentieth-century writers and social movements more so than Ruskin's specific prescriptions and dogma. This research thus attempts to trace the influence of Ruskinian moralism through a close reading of the most important texts of certain countercultural social movements that either directly recognize Ruskin as an influence or that have been deduced to be part of the Ruskinian tradition. The purpose of this research is to firstly establish John Ruskin as one of the most influential catalysts of anti-capitalist moralism, and secondly to develop a narrative not often told of capitalist critique in order to open more widely the discussion of its discontents.

The study begins with William Morris, perhaps the most influentially Ruskinian thinker, and his political radicalization of Ruskin's socioeconomic teachings, from where the study then moves to the Arts and Crafts Movement and the call for the humanization of production. Next, a Ruskin-inspired socialism is explored and contrasted with Marxist socialism, taking into account writers such as G.D.H. Cole and R.H. Tawny. Then, environmentalism and economics of scale are explored through writers such as E.F. Schumacher and Mohandas Gandhi. And finally, the watered-down contemporary version of the Ruskinian spirit is explored through writers such as Tibor Scitovsky.

Mathematics and Statistics

Lyme Borreliosis prevalence in the dogs and humans of Bucks County, Pennsylvania and the environmental factors affecting risk of infection

Poster: D51 Author: Darby McDermott Advisor: Dr. Michael Posner

Since its emergence in 1975, Lyme borreliosis has become one of the leading zoonotic diseases to watch in the United States. Though its geographical distribution continues to increase, 95% of all cases remain in 13 states, Pennsylvania having one of the highest rates of prevalence. In order to yield a more accurate representation of the prevalence of Lyme borreliosis in certain locations, dogs and horses have been used as sentinels for the disease, this method of surveillance being favored to passive surveillance of human cases (B. Wagner, Lindenmayer). My research had the objective of studying the rates of prevalence during the year 2013 in the population of dogs and humans living in the area of Bucks County, Pennsylvania. Using statistics obtained from six small animal veterinary hospitals, along with the human cases of Lyme disease reported to the Bureau of Epidemiology in

Pennsylvania's Department of Health, I tested for a correlation between the prevalence of Lyme in humans and dogs living in the different zip codes of Bucks County. Environmental factors collected from the 2010 U.S. census data, along with the 2006 Land Use Land Cover data on ArcGis, were used to determine whether these factor affect prevalence rates. Additionally, a pilot survey was launched at Quakertown Veterinary Clinic to begin research on whether owners of pets with Lyme disease are more likely to have Lyme disease as well. This project had the intention of promoting a One Health approach to the surveillance and diagnosis of Lyme Borreliosis, and furthering the information on factors affecting prevalence of a leading zoonotic disease.

Physics

Structural properties of distorted perovskites (Sr,Ca)(Fe,Co)O2.5+&

Poster: D52

Author: Joseph Pollichemi, Michael Evans, Ian Leahy, Jeremy Carlo Advisor: Jeremy Carlo

Many materials, both natural and manmade, crystallize in the perovskite structure, named after the naturally occurring mineral CaTiO3. Perovskite structures exhibit a wide range of interesting properties such as superconductivity, colossal magnetoresistance, and multiferroicity. This study was concerned with the structural and magnetic properties of the oxygen deficient perovskites of the form $(Sr,Ca)(Fe,Co)O2.5+\delta$.

SrFeO2.5+ δ crystallizes into an ideal cubic (Pm3m) perovskite structure while CaFeO2.5+ δ crystallizes into a distorted orthorhombic (Pnma) perovskite structure, also known as the brownmillerite structure. Synthesis under standard pressure without powerful oxidizers yields oxygen deficient perovskites of the form (Sr,Ca)FeO2.5+ δ . Oxygen deficient perovskites show potential applications for energy storage in fuel cells due to their oxygen mobility properties.

The synthesized oxygen deficient perovskites exhibit a variety of structures depending on the ordering of oxygen vacancies. SrFeO2.5+ δ indexes to an ideal cubic structure while the crystal structures of the doped intermediaries between SrFeO2.5+ δ and CaFeO2.5+ δ change progressively as the 'A' site progresses from all Sr to all Ca.

The Sr(Fe,Co)O2.5+ δ series exhibits an ideal cubic perovskite structure down to 10% Fe composition, whereas SrCoO2.5+ δ exhibits a distorted perovskite structure. SrCoO2.5+ δ and up to 7.5% Fe composition indexed to a orthorhombic unit cell, but the space group, basis, and relation to the parent structure have not been determined.

There seems to be some instability with regards to the magnetism of the CaFeO2.5+ δ sample. Mossbauer on one sample indicates ~100% ordered volume fraction at 300K, while another indicates coexistence of ordered and paramagnetic phase fractions.

Special Appreciation to the Following Sponsors:

Office of Research and Graduate Programs

Center for Undergraduate Research and Fellowships

College of Engineering

College of Liberal Arts and Sciences