University of Minnesota

2006
Institute of Technology
Summer Undergraduate Research Expo

Thursday, August 10, 2006
4:00-6:00 p.m.
Memorial Hall, McNamara Alumni Center
**Poster Presentations**
Listed by presenting author and sponsoring program.

1. **Allen, Joshua, Linli Meng, L. E. Scriven, Juan de Santos**  
   *A Model of Network Flows in Convective Assembly*  
   Home Institution: University of Minnesota  
   Sponsor: Chemical Engineering and Materials Science  
   Abstract: A photonic crystal is a material made up of particles around one micron in size. Some of these crystals exhibit a photonic band gap - a range of wavelengths that cannot propagate through the crystal - and have the potential for a variety of uses. Convective assembly is a possible method for producing crystals with a photonic band gap because the resulting crystal tends to form a face-centered cubic structure. My project was to mathematically model the flow of solvent through the porespace of a photonic crystal during convective assembly and explore how the flows are affected by crystal growth.

2. **Vagias, Apostolos, Zhen Whu, Lorraine Francis**  
   *Scale Growth Formation in Polypropylene Tubes for Water Heating*  
   Home Institution: National Technical University of Athens  
   Sponsor: Chemical Engineering and Materials Science/support from IREE (Initiative for Renewable Energy and the Environment) and NREL (National Renewable Energy Laboratory of the Department of Energy)  
   Abstract: The research object involves the study of scale formation into polypropylene tubes for water heating. In hard water flowing through water heating tubes, decipitation of calcium carbonate is possible to occur, when supersaturation ratios are above 1. This has to do with the supersaturation ratio of the ions dissolved in the water, the pH of the water solution, as well as the roughness of the inner surface of the tube. Literature studying has taken place, regarding roughness obtaining, evaluation, measurement and controlling, as well as supersaturation of the water solution. Our research is focused on the control of surface roughness, as well as the reproducibility of pH, so as conclusions about the efficiency of polymer tubes instead of copper tubes could be drawn.

3. **Jundt, Adam, Amy Coddington, Nick Voshell, Yousef Saad**  
   *Calculating and Visualizing the Properties of Atomic Systems*  
   Home Institution: University of Minnesota  
   Sponsor: Computer Science  
   Abstract: PARSEC represents more than a decade of work at the University of Minnesota and the University of Texas on electronic structure calculations. However, due to PARSEC's complexity, it can be time consuming to test new approaches on solving atomic systems. For this reason, we developed MATLAB scripts based off of PARSEC that can be used by researchers for rapid prototyping. These will help reduce the typical time it takes to test a conceptual idea, before developing a full-fledged code in a programming language such as C or FORTRAN. We also revisited and modified a program, PVOX, that interns built last year that allows for the visualization of the generated output of PARSEC and the newly developed MATLAB version of PARSEC.
4. apRoberts-Warren, Nicholas, Vincent Noireaux  
*Biomimetics and Evolution*  
Home Institution: Wheaton College  
Sponsor: Physics  
Abstract: We investigated the idea of using robotics as a conveyor of information—an imitation of DNA in cells. We started to build two different devices of approximately one centimeter scale and both using solar cells as a source of energy. Our first idea was to make a robot that can exhibit phototaxis; it can guide and propel itself along a gradient of light, and be power-independent. The second system was to see how a group of small, vibrating robots (approximating Brownian motion) will behave under a selection pressure. This involves in seeing if their bonding would be a positive or negative adaptation via the pressure.

5. Becket, Elizabeth A., Shaul Hanany  
*Ebex: Studying the Universe Through Cosmic Microwave Background Radiation*  
Home Institution: Colorado College  
Sponsor: Physics  
Abstract: Approximately 10-35 seconds after the Big Bang, the universe is believed to have inflated—a new state of existence—increasing in size exponentially within a fraction of a second. This inflation should have created ripples in space, leaving a signature any near-by photons, more specifically in their polarization. These photons surround us today in the form of the Cosmic Microwave Background radiation. Ebex, the E and B experiment, has been created to study the polarization modes of the CMB radiation. We hope to improve our knowledge of the inflationary period and potentially confirm our current cosmological paradigm. This summer I have worked to model and test pieces of the experimental set-up. This poster will explain parts of that set-up and the theoretical background of the Ebex experiment.

6. Broaded, Laura, Roberta Humphreys  
*Mapping the Asymmetry of the Milky Way with IRAF*  
Home Institution: Butler University  
Sponsor: Physics  
Abstract: A significant excess of stars has been found in the first quadrant of the Milky Way above and below the galactic disk. This asymmetry is not only spatial, but kinematic as well, having a significantly slower rotation than the galactic disk. The goal of our research is to determine the extent and shape of this asymmetry. We will do this by performing star count ratios between the first and fourth quadrants of the sky. My research consisted of analyzing and calibrating CCD images from the fourth quadrant of the galaxy in preparation for conducting star counts. A detailed map of this asymmetry will help determine the cause of this feature and has implications for galactic formation, the history of the Milky Way, cosmology and dark matter. Possible causes for the asymmetry are a merger galaxy, interaction with the stellar bar and a triaxial thick disk.

7. Collier, Jennifer, John Wygant  
*An Analysis of a CME Shock in the Magnetosphere*  
Home Institution: Carthage College  
Sponsor: Physics  
Abstract: A survey of four CME shocks in the magnetosphere was conducted using ACE, WIND, and CLUSTER satellite data. The CME shocks caused magnetic storms in the magnetosphere which all had the following properties: sharp peak in the ZGSE direction of the magnetic field, similar (but oppositely directed) peak in the Edusk direction of the electric field, and sharp peaks in the ion density and solar wind speeds, making them good candidates to be analyzed with higher resolution data. The higher
resolution data from the CLUSTER satellite was used to look for interesting phenomena occurring in the solar wind.

8. **Krzyzewski, Sean, Joachim Mueller**  
**Supercontinuum Generation**  
Home Institution: Marquette University  
Sponsor: Physics  
Abstract: Recent advances in photonic crystal fibers allow the generation of supercontinuum at moderate powers with ultrashort laser pulses. We are exploring supercontinuum generation by coupling light from a Ti:Saph laser into a commercially available photonic crystal fiber (Femtowhite 800) and present initial experiments that test its suitability for running multiple wavelength fluorescence spectroscopy experiments. Super continuum was generated; however, a significant amount of light with the input wavelength passed through the fiber and dominates the spectrum, making it difficult to observe other wavelengths without the aid of extremely sensitive detectors. The power output was also too low and could not be compensated for by increasing the power without damaging the fiber. Further tests are being done to improve the power output, stability and spectrum.

9. **Larkoski, Andrew, Tony Gherghetta**  
**A Schroedinger Approach to Holography**  
Home Institution: University of Washington  
Sponsor: Physics  
Abstract: The Randall-Sundrum solution to the hierarchy problem has incited much further research into consequences of the model, both motivated by the hierarchy problem and holography. Here, we review scalar and fermion fields in the bulk, studying the Kaluza-Klein modes of both fields. We introduce a Schroedinger approach to studying the fields and the corresponding potential for each. We review the AdS/CFT holography for both fields and find that remarkable information about the dual theory can be obtained by considering the Schroedinger potential.

10. **Legursky, Katrina, Priscilla Cushman**  
**Cryogenic Dark Matter Search**  
Home Institution: Benedictine College  
Sponsor: Physics  
Abstract: The CDMS project is a collaboration experiment that is actively searching for dark matter candidates called WIMPs, or Weakly Interacting Massive Particles. My part in this project has been twofold. My primary task was to define a data cut using calibration data that defines the range in which WIMPs are expected to interact. This range distinguishes electron recoil background from neutron and WIMP interactions. I also worked on a simulation that is trying to reproduce results from the CDMS runs at the Stanford Underground Facility(SUF) to check the simulation run for the deeper Soudan site. My primary task with the simulation was to extract information from multiple data sets as they were produced while we tried to get the simulation to work properly.

11. **Rustan, Gustav E., Allen Goldman**  
**Looking for Signatures of Superconductivity in Laser-Processed Strontium Ruthenate**  
Home Institution: University of Minnesota - Morris  
Sponsor: Physics  
Abstract: Physicists working at Naval Research Laboratory claim to have found signatures of superconductivity at high temperatures in specially processed samples of strontium ruthenate, which is a known superconductor with $T_c \approx 1.5$ K. Three techniques were used to measure the critical temperature, resulting in a range for $T_c$ of 200:250 K. Another signature of type-II superconductivity, a butterfly
curve, was also found, however it was not found directly through M(H) measurements as would be typical. To verify the existence of superconductivity, samples were sent to the University of Minnesota for magnetization measurements. After a series of measurements, it was found that the butterfly cannot be taken as a signature of superconductivity; M(T) and STM data also fail to show signs of superconductivity.

12. Simones, Jacob, Russell Palma, Robert Pepin  
*Measuring Noble Gases In Coma Samples From Comet Wild 2*  
Home Institution: Minnesota State University, Mankato  
Sponsor: Physics  
Abstract: Since comets are relics of the early solar system, the formation of the solar system can be better understood through compositional analysis of cometary material. In 2004, NASA's Stardust spacecraft used aerogel (a low density, silicon-based material) to collect coma samples from comet Wild 2 that were then returned to earth for analysis in 2006. Aerogel not from the spacecraft has no embedded cometary material and was investigated initially to determine the possibility of measuring noble gases in Stardust samples. Non-flight aerogel samples were heated and the evolved gases measured using a mass spectrometer. The helium and neon levels observed were low enough that measuring helium and neon in Stardust samples using the same method is viable. The first Stardust samples are currently being examined.

13. Sperling, Jonathan, E. Dan Dahlberg  
*Research and Development of Magnetic Tunnel Junctions*  
Home Institution: University of Wisconsin - Madison  
Sponsor: Physics  
Abstract: Magnetic tunnel junctions (MTJs) belong to a class of spintronics (spin transport electronics) devices that may soon have important technological applications; for example, as components of nonvolatile magneto-resistive random access memory (MRAM) and magnetic sensors. By taking advantage spin-dependent tunneling, MTJs exhibit a phenomenon known as tunneling magnetoresistance, in which the probability of charge transport between two insulated ferromagnets is dependent on their relative magnetizations. To be discussed are the physics of MTJs, the progress that has been made in MTJ fabrication, and the role of MTJs in MRAM applications.

14. Tenenbaum, Alex, Daniel Cronin-Hennessy  
*NOvA*  
Home Institution: Connecticut College  
Sponsor: Physics  
E-mail: alexander.tenenbaum@gmail.com  
Abstract: The NOvA (Neutrino Oscillation ne Appearance Experiment) project is a second generation neutrino oscillation experiment utilizing the NmMI neutrino beam at Fermilab. The detection of neutrino oscillations has necessitated the attainment of certain physical observables and the fulfillment of NOvA is critical to gaining a clearer understanding of these radical particles. The detector is designed to primarily track ne events based on the oscillation of nm ÔÇ£ne at peak probabilities. Fundamental and longterm objectives include but are not limited to the following: the measurement of the final mixing angle ÔÇ£13, ÔÇ£Nm2, and the CP-violation phase factor. The detector is presently in the design phase and a multitude of projects are currently active, which includes the development and prototype construction of a wavelength shifting fiber spooling machine. The machine will thread thousands of kilometers of fragile wavelength shifting fiber through each of the 32 cells for each of the 23,000 extrusions that make up the bulk of the detector.
15. **Vo, Pamela, Cindy Cattell**  
*Magnetospheric Impacts on Earth's Aurora*  
Home Institution: Baylor University  
Sponsor: Physics  
Abstract: Magnetic reconnection occurs in order to form a more stable magnetic configuration between the interplanetary magnetic field and that of Earth. Dayside reconnection allows solar wind plasma into the magnetosphere, and upon a second reconnection in the magnetotail, newly closed field lines heading toward the earth compress the plasma. Energetic particles are sent toward Earth and strike the atmosphere, causing the aurora. Picture data at a period of strong aurora are collected by the IMAGE spacecraft and are compared with satellite data from the magnetosphere.

16. **Weiss, Claire, Paul Crowell**  
*Spin Ejection in Ferromagnet-Semiconductor Heterostructures*  
Home Institution: Lawrence University  
Sponsor: Physics  
Abstract: Spin transport is an important area of research in physics because its applications could be useful in creating new types of electronic devices in which both charge and spin could be manipulated. Spin transport of charge carriers across a potential barrier is studied here in several different samples. The samples are all ferromagnet-semiconductor heterostructures. An external cavity tunable diode laser was used to send polarized light into the heterostructures. The current through the quantum well barrier was then measured to study the effectiveness of spin transport of the charge carriers. Although we did not observe spin ejection by these methods, we did observe electro-absorption, Zeeman splitting, and Landau diamagnetism, which make us hopeful as to the success of future measurements.

17. **Anderson, Eric, R. Lee Penn**  
*The Effect of Ionic Solutions on Titanium Dioxide Nanoparticles*  
Home Institution: Winona State University  
Sponsor: MRSEC  
Abstract: Titanium dioxide, or Titania, has three different polymorphs: Anatase, brookite, and rutile. A sol-gel synthesis resulted in the formation of anatase and brookite at different ratios. It is unclear when ionic strength of the suspension is most critical, the synthesis or aging process. TiO2 nanoparticles were aged in NaNO3 and NaCl ionic solutions with concentrations ranging from 0.01-1.0M. X-Ray Diffraction systematically calculated the ratios of polymorphs, as well as the particle size by a Rietveld Refinement method. TEM verified the polymorph ratios as well as confirmed particle size, growth mechanism, atomic structure, and crystallography. Results show that increasing the concentration of ionic solutions during the hydrothermal aging step had no effect on the ratios of anatase to brookite. The presence of ionic solutions during synthesis is more critical than during the hydrothermal aging process.

18. **Aubain, Max, Adam Meuler, Frank Bates**  
*Investigations of the Morphological Behavior of Poly(lactide)-b-poly(styrene)-b-poly(isoprene)-b-poly(styrene)-b-poly(lactide) Pentablock Copolymer*  
Home Institution: Cornell University  
Sponsor: MRSEC  
Abstract: Block copolymers are useful materials because of their variable mechanical, chemical and structural properties. Capable of forming self-assembling network morphologies, such as core-centered gyroid and recently the discovered O-70 phase, it is feasible that when one of the domains is removed the copolymer will become nanoporous. One material that may exhibit these properties is the poly(lactide)-b-poly(styrene)-poly(isoprene)-b-poly(styrene)-b-poly(lactide) [LSISL] pentablock
copolymer. This material is thought to be mechanically robust from a combination of the glass-like styrene block and the rubber-like isoprene block in conjunction with the pentablock structure that immobilizes the polymer chain ends. If the [LSISL] copolymer forms network, removal of the lactide blocks on both ends could provide a pathway that allows for transport of small molecules, making it a candidate for membrane applications.

19. Beaulieu, Michael, Christopher Macosko  
*Effects of Polyethylene Naphthalate-Clay Nanocomposites on Young's Modulus and Coefficient of Thermal Expansion*  
Home Institution: University of Massachusetts - Amherst  
Sponsor: MRSEC  
Abstract: Mixing a clay nanocomposite or filler with a polymer can increase the mechanical properties, such as: Youngís modulus and coefficient of thermal expansion (CTE). The polymer of that we will be trying to increase the mechanical properties of is polyethylene naphthalate (PEN); PENís industrial application is in the data storage industry, in the form of magnetic tape. The samples of PEN-clay nanocomposites will be made through melt intercalation by a small scale extruder. After the samples have been made we will begin measuring the Youngís modulus, CTE, and degree of crystallinity. The goal is to find which type of clay yields the highest Youngís modulus and lowest thermal expansion coefficient.

20. Bryant, Benjamin, Chris Leighton  
*Ferro/AntiFerro Coupling and Exchange Bias of Co/FeMn and Fe/Cr*  
Home Institution: University of Pittsburgh  
Sponsor: MRSEC/ITAMIT  
Abstract: The coupling of Ferromagnetic and Antiferromagnetic materials in thin films has lead to novel spin interactions and exchange bias that can be exploited for memory storage and other applications. In this project, the FM/AFM materials Fe/Cr and Co/FeMn are studied for their underlying mechanisms and physics. The main goal at this stage was producing clean surfaces on the materials to allow for better viewing of these base mechanisms and to eliminate extraneous surface interactions.

21. DeVries, Lucas, Xiaoyang Zhu  
*Charge Carrying Species of PTCDI-C8 when used as a Semiconductor Material in a FET*  
Home Institution: University of Northern Iowa  
Sponsor: MRSEC  
Abstract: The goal of this project is to create an apparatus that can fabricate a polymer FET on a silicon waveguide and analyze its operation in situ. An infrared radiation beam is projected into the waveguide and evanescent waves penetrate into the substrate of the polymer FET. These waves can be detected and analyzed by an FT-IR in the same way as normal IR waves. This method allows the potential charge carrying species of the polymer, PTCDI-C8, to be examined while the polymer FET is operation. The low permeability of the evanescent waves (~1 micron) necessitates a balance between dielectric thickness and IR signal strength. A side project will investigate the use of a nanolayer technique to create a very thin dielectric layer.

22. Di Marco, Aniello Scotto, Chun Wang  
*Investigation on Thermal and Electrochemical Properties of Some Organic Semiconductors*  
Home Institution: Pennsylvania State University  
Sponsor: MRSEC  
Abstract: Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were used along with cyclic voltammetry (CV) to investigate the thermal and electrochemical properties of several
oligothiophenes, and oligoacenes and some of their derivatives. Thermal stability as well as sublimation temperatures, and crystals and thin films are important factors in this area of research. Cyclic voltammetry provides oxidation/reduction potentials of the compounds which can be used as a predictor of how well they will behave as semiconductors.

23. **Drexler, Jason, Michael Tsapatsis**  
*Optimizing the Swelling Procedure for a Layered Silicate*  
Home Institution: Washington State University  
Sponsor: MRSEC  
Abstract: Zeolites are micro porous crystalline framework materials with many applications including catalysts, absorbents, and ion exchangers. Recently a material composed of many flat stacked zeolite layers has been synthesized. For several applications, it would be beneficial for the layers to be separated thus increasing the surface area and decreasing the time for molecules to pass through the pores. In order to separate the layers the crystal will undergo a process known as swelling. The swelling will occur when the layer spacing is increased by organic molecules. A procedure was created to perform the swelling of similar layered crystals. To improve upon this, systematic variations of the procedure will be performed to further improve the swelling technique. X-ray diffraction and Scanning Electron Microscopy analysis will be used to characterize the material.

24. **Emery, Jonathan, Lorraine Francis**  
*Correlations Between Hardness and MFFT and CPVC of Latex/Ceramic Composite Coatings*  
Home Institution: Carleton College  
Sponsor: MRSEC  
Abstract: The goal of this research is to further investigate the correlation between hardness of polyvinyl acetate (PVAc)/alumina composite coatings with the Minimum Film Formation Temperature (MFFT) and Critical Pigment Volume Concentration (CPVC). Based on research conducted by Ming Lei et al. (2003), the hardness of the composite coatings should experience significant increase at the MFFT and CPVC. By using methods and techniques from Leiís masterís thesis, it should be possible to use nanoindentation, as opposed to Vickersí hardness testing, to investigate the characteristics of the coatings. The poor correlation between the data from the Vickers and nanoindentation tests are likely not results of the misunderstanding of film formation and microstructure, but rather are caused by the differences between the characterization instruments themselves.

25. **Halsey, Christopher, Kent R. Mann**  
*Synthesis and Characterization of Pyrene-Capped Oligothiophenes for Use as Organic Semiconductors*  
Home Institution: Truman State University  
Sponsor: MRSEC  
Abstract: Organic semiconductors offer cheaper manufacturing alternatives to silicon-based materials due to their mechanical flexibility and processibility. Oligothiophenes show promising characteristics needed to produce efficient semiconductors. X-ray crystallography demonstrates several close intermolecular contacts make oligothiophenes with aromatic capping groups good candidates for organic semiconductors. This research will explore the effects of capping oligothiophenes with pyrene groups. Previous work has shown that mobility improves with increasing either the number of thiophene rings in the oligomer or the number of aromatic rings on the capping groups. This goal of this research in synthesizing pyrene-capped oligothiophenes is a step in both directions. Successful syntheses were confirmed by 1H NMR, cyclic voltammetry, and UV-Vis spectroscopy.
26. **Hovlid, Marisa, Mark Distefano**  
*Design, Synthesis, and Biological Applications of DATFP Containing FPP Analogues With Enhanced Stability*  
Home Institution: University of Minnesota – Twin Cities  
Sponsor: MRSEC/Department of Chemistry - HEISIG  
Abstract: Protein prenylation is a post-translational modification involving the addition of either a 15 or 20 group to the cysteine residue of a protein. Prenylated proteins are of great interest because they are involved in numerous biological activities including the development of cancer. Photoaffinity labeling is a useful method for determining specific binding sites. This is done by irradiating the photoaffinity labeled compound which forms cross links with nearby residues. The specific amino acids active in binding events may then be determined. The purpose of my research is to synthesize a dihydro geranyl pyrophosphate (GPP) with a diazotrifluoropropionyloxide (DATFP) photolabel. Previous experiments using DATFP-geranyl-pyrophosphate which contains a double bond at the C-6 carbon. DATFP-dihydro-GPP, which lacks the C-6 double bond, is expected to be more stable.

27. **Hsu, Tienyi Theresa, Nathaniel Lynd, Timothy Lodge**  
*Dependence of Critical Micelle Temperature on Polydispersity in Dilution Solutions of Diblock Copolymers*  
Home Institution: Cornell University  
Sponsor: MRSEC  
Abstract: Diblock copolymers are hybrid materials consisting of two distinct polymer species covalently bounded at one end. When a block polymer is dispersed into a selective solvent, meaning that the solvent has a higher affinity for one of the polymer species over the other, the polymers self-assemble into nanostructures called micelles. However, this behavior is temperature-dependent. When the system reaches the critical micelle temperature, or CMT, the micelles become entropically unfavorable, and they break up into linear copolymers suspended in the solvent. In this study, we will investigate the CMTs of dilute solutions of polystyrene-b-polyisoprene (PS-PI) diblock copolymers, in the regime where we can assume very little interactions take place between the micelles. The PS-PI diblock samples are synthesized using a chain-growth polymerization mechanism called living anionic polymerization to have different polydispersities, i.e., different distributions of molecular weights. We will determine the CMTs of these PS-PI diblock samples by dynamic light scattering, from which we can monitor the size of the micelle aggregates formed in solution and pinpoint the temperature at which the micelles break down. We hypothesize that the polydispersities of these diblock copolymers will alter their CMTs.

28. **Hughes, Shantelle, Sonya Caston-Pierre, Ryan Gresback, Uwe Kortshagen**  
*Self-assembly of Germanium Nanoparticles*  
Home Institution: Jackson State University  
Sponsor: MRSEC  
Abstract: Recently, there has been significant interest in studying Germanium (Ge) nanoparticles for efficient solar cells. Rather than using silicon nanoparticles, Ge has better absorbence in the near IR and visible range of the solar spectrum. In order to enable good conductivities of self-assembled films of Ge nanoparticles the surface of Ge can be modified using selected monomers. My interest is in adhering propeonic acid (PA) onto the Ge surface to saturate surface electronic states and provide controlled interfaces between the Ge crystals. By using the carboxylic acids as functional groups on the Ge nanoparticles, the hydrophilic interaction will enable dispersion of the nanocrystals in polar solvents and attachment of the nanoparticles to hydrophilic surfaces. The passivated Ge particles will be characterized by TEM.
29. Kelly, Glenn, Matt Panzer, Bryan Boudouris, C. Daniel Frisbie
*Fabrication, Characterization, and Testing of an Alq3/NPB Organic Light-Emitting Diode*
Home Institution: University of Alabama
Sponsor: MRSEC
Abstract: Organic light-emitting diodes (OLEDs) have shown significant promise due to being brighter and using less power than traditional inorganic LEDs. To date, several companies have incorporated OLEDs into displays for consumer electronics. Typically, OLEDs incorporate at least two organic semiconductor layers; our objective to fabricate an OLED using Alq3 [Tris (8-Hydroxyquinoline) aluminum] as the emissive layer and NPB [6-Naphthylphenylbenzidine] as the hole-conducting layer. Thin films of these organic compounds were deposited onto a transparent electrode using vacuum thermal evaporation. Both optical microscopy and atomic force microscopy were used to characterize the organic surfaces. Finally, we applied a voltage to the device's electrodes to test its light-emitting capabilities. Results from all three stages have given us insight into the optimal design and fabrication techniques for these devices.

30. Larson-Mekler, Amanda, Masano Sugiyama, Victor Barocas
*Protein Crystal Growth of Triclinic Lysozyme in the Magnetic Field*
Home Institution: Simmons College
Sponsor: MRSEC
Abstract: Lysozyme can be crystallized in four different space groups: monoclinic, triclinic, orthorhombic, and tetragonal. The optimal growth conditions of triclinic lysozyme have not been determined and were investigated initially. Lysozyme crystals were grown in varying concentrations of precipitant, buffer, and protein. Once single crystals were obtained, they were diffracted in order to determine which concentrations produce the triclinic space group. The conditions that produced the highest quality and greatest volume of these crystals were then tested in a 9.4 Tesla magnet. The magnetic field facilitates the orientation of the macromolecule, thus larger crystals of higher purity grow. The magnetic field allows for more control over crystal growth and produces an ideal crystal for diffraction.

31. Leonard, Chris, Kent Mann
*Synthesis and Characterization of Anthracene -capped Oligothiophenes for Use in Thin-Film Transistors*
Home Institution: Gustavus Adolphus College
Sponsor: MRSEC
Abstract: Crystalline organic semiconductors may provide a cheaper alternative to silicon-based thin film transistors. To date, however, there has yet to be synthesized an organic material that can compare favorably to silicon’s conduction capabilities. Past research has shown that oligothiophenes are promising precursors to a slew of synthetic molecules capable of conducting charge in a thin film transistor. The purpose of this project is to synthesize anthracene-capped terthiophene using a Stille coupling method, characterize it using NMR, and cyclic voltammetry, and compare its electrical properties to previously synthesized terthiophene analogues as well as anthracene-capped bithiophene. Also, Anthracene-capped 3,3i dihexyl bithiophene was synthesized to improve the solubility of Anthracene-capped bithiophene, to allow for easier characterization. The expected results will show that the terthiophene analogue facilitates improved mobility over anthracene-capped bithiophene.
32. **Lin, Hui, Mamoun Bader, C. Daniel Frisbie**  
*Synthesis and Solid State Structures of New Organic Semiconductors*  
Home Institution: Pennsylvania State University  
Sponsor: MRSEC  
Abstract: My summer research plan includes the synthesis of new organic semiconductors using Knoevenagel condensation reactions of aromatic quinones with malononitrile. Based on previous experience in our group these targeted molecules are expected to have unique solid state structures and electrical properties conducive for favorable application as organic semiconductors. For instance we anticipate that the resulting materials would have low band gap, and form pi stacks with short intermolecular distances in the solid state.

33. **Malik, Ali, Sunny Choh, Chun Wang**  
*Synthesis of Cross-linked Hyaluronan Gels*  
Home Institution: Howard University  
Sponsor: MRSEC  
Abstract: Hyaluronan is a very important biomaterial which can be found mostly in the extracellular matrices, in the vitreous of the eye as well as in the sinovial joints. Its viscous hydophilic solutions possess high lubricity and also exhibit good shear properties. We are interested in producing a more robust form of this gel which will later be used in various tissue engineering and therapeutic applications. For this study, HA is modified with pendant amines (HA-NH2) through a carbodiimide-mediated reaction and further reacted with N-succinimidyl 3-(2-pyridyldithio)-propionate (SPDP). HA-PD, the resulting compound, can undergo various chemistries for modification and cross-linking. For this project, a disulfide exchange between the HA-PD and a molecule with free thiols will be performed to create a cross-linked hydrogel network. These modifications and cross-linking methods will be used to create hydrogels. Equilibrium and dynamic swelling experiments will then be performed to characterize these hydrogels.

34. **Martin, Hermanus, Charlie Blackwell, Yves Adjallah, James Kakalios**  
*Effects of Nanocrystals in Hydrogenated Amorphous Silicon Thin Films*  
Home Institution: Morehouse College  
Sponsor: MRSEC/IGERT  
Abstract: There has been a growing interest in the properties of mixed-phase materials consisting of hydrogenated amorphous silicon containing silicon nanocrystalline inclusions (a/nc-Si:H). Recent results suggest that these a/nc-Si:H films may possess superior electronic characteristics for photovoltaic applications. Prof. U. Kortshagen in the Dept. of Mechanical Engineering at the University of Minnesota has recently developed a dual chamber Plasma Enhanced Chemical Vapor Deposition system, whereby silicon nanocrystals are produced in one plasma system, which are then injected into a second plasma chamber, where a-Si:H is co-deposited using a silane plasma. This Co-Deposition system provides enhanced control over the nanocrystalline concentration (nanocrystal diameter of roughly 3-5 nm) while separately enabling the growth of a high quality amorphous silicon matrix. Kakalios’ lab has recently observed that these a/nc-Si:H films can display a non-trivial non-Ohmic current-voltage characteristic, where the deviation from Ohm’s law depends on the temperature and nanocrystalline concentration of the thin film mixed phase material.
35. Melby, Jacob, C. Daniel Frisbie  
*Fabrication and Characterization of Organic Thin Film Transistors (OTFTs)*  
Home Institution: University of Minnesota - Morris  
Sponsor: MRSEC/ITAMIT  
Abstract: There is a need to develop air stable organic semiconducting devices while also considering key performance parameters such as: on-to-off current ratio, field effect mobility, and threshold voltage. This research will focus on the fabrication and characterization of new p-channel OTFTs based on pentacene and novel thiophene-acene hybrid molecules. Highly crystalline thin films will be deposited from the vapor phase onto various gate/insulator substrates followed by deposition of metal electrodes. Thin film structure and morphology will be examined using X-ray diffraction and atomic force microscopy. The electrical properties of OTFTs will be observed using a top-contact transistor geometry and probe station. The connection between molecular/crystal structures and electronic properties provides a foundation for elucidating structure-property relationships and facilitates development of new organic semiconductors with enhanced transport properties.

36. Nelson, Erin, Jeff Roberts  
*Oxidation Kinetics of Silicon Nanoparticles*  
Home Institution: California Polytechnic State University  
Sponsor: MRSEC  
Abstract: Silicon nanoparticles are an important technology to develop because of siliconís low toxicity, high stability, and excellent semiconducting properties. Silicon is a reactive element that readily oxidizes in air. When silicon oxidizes, the crystalline particle core shrinks while the amorphous silicon dioxide on the outer layer of the particle grows. The differing size of the nanoparticles will alter the quantum confinement effects, such as light emission. Our study will focus on these particle changes. Fourier-transform infrared (FTIR) spectroscopy will be used to monitor native oxide formation on silicon nanoparticles. RF plasma will be used to generate silicon nanoparticles from silane gas. Particles will be subjected to wet and dry oxidation conditions after being subjected to temperatures ranging from 23 to 700 degrees Celsius.

37. Pendergraph, Samuel A., Zach Thompson, Frank Bates  
*The Effect of Curing Agents on Block Copolymer Modified Epoxies*  
Home Institution: University of Connecticut  
Sponsor: MRSEC  
Abstract: Self-assembling amphiphlic block copolymers can be used in a number of applications ranging from soaps and surfactants to vesicles in drug delivery. The ability to control the equilibrium morphologies of these polymers is an attractive feature in the aforementioned areas and has lead to extensive study. Recently, self-assembling block copolymers have been used to toughen epoxy thermosets. In this particular study, we are studying a three component epoxy system where the three components are the block copolymer, epoxy resin and the curing agent used to strengthen the resin cure. The epoxy and block copolymer will remain constant and the effect of varying curing agents will be evaluated.

38. Riedel, Theran, C. Daniel Frisbie  
*Synthesis and Photovoltaic Application of Polythiophenes*  
Home Institution: University of Wisconsin - Eau Claire  
Sponsor: MRSEC  
Abstract: Poly-(3-hexylthiophene) or P3HT is known to be a semiconductor that exhibits good behavior relative to other organic semiconductors, especially in the realm of organic based photovoltaic cells. However, it has limited potential for use due to the fact that it will degrade when exposed to air, so it
must be fabricated in an inert gas environment. The allure behind organic based semiconductors is that they have the potential to be far less expensive than the typical Silicon or other inorganic semiconductors. This is mainly due to the simplicity that is associated with their production. PQT-12, a poly-(3,3-dialkyl-quaterthiophene), has exhibited very good behavior compared to P3HT under normal atmospheric conditions, but has yet to be used in the photovoltaic realm.

39. Turner, Matthew, Thomas C. Marsh, C. Daniel Frisbie
   *In situ Self-assembly of a G-DNA Molecular Scaffold on Mica Using a Polymeric Template*
   
   Home Institution: University of St. Thomas
   Sponsor: MRSEC

   Abstract: Research on the structure and function of guanine rich nucleic acids has shown that multiple guanine repeats in a sequence enable these biopolymers to adopt a quadruple helical structure generally known as G-DNA. In the work described here, the DNA oligomer GGGTTG (Tet1.5) is used to create a self-assembling linear supramolecular structure termed a G-wire. The ability to grow G-wires on a substrate could be employed to make connections between nanoscale devices. Currently, the polymer poly-5-norbornene-2-carboxylic acid (D.P. 4000) with the amine-linked oligonucleotide GGGTTG at a frequency of 1 oligonucleotide to 10 carboxylic acid groups has been synthesized to serve as a rigid backbone for the self-assembly of G-wires. Atomic Force Microscopy is used to characterize polymer-templated self-assembly of G-wires on a mica substrate.

40. Bast, Erin, Betsy Edhlund, Matt Grandbois, Kristopher McNeill
   *Development of Singlet Oxygen Quantitation Methods by Flow Injection Analysis with Chemiluminescent Detection*
   
   Home Institution: Colby College
   Sponsor: Department of Chemistry - LANDO

   Abstract: Singlet oxygen (1O2), a reactive oxygen species photochemically generated in natural waters, can react with organic molecules, including several aquatic pollutants. Consequently, it is important to develop a selective and sensitive detection method for 1O2 to better understand its role in the environment. Trap-and-trigger chemiluminescent probes have been used to determine the concentration of 1O2 in dissolved organic matter of natural and simulated water systems. In this study, 3-(methoxytricyclo[3.3.1.13,7]decyldienemethyl)phenol reacts with 1O2 to form a dioxetane, which undergoes basic decomposition and quantifiable chemically induced electron exchange luminescence. Flow injection analysis is used to create a more efficient and accurate detection method.

41. Broschinski, Adam E., Jake L. Rafferty, J. Ilja Siepmann
   *A Program for Generating Initial Structures of Stationary Phases for Use in Simulations of Reversed Phase Liquid Chromatography Systems*
   
   Home Institution: West Virginia University Institute of Technology
   Sponsor: Department of Chemistry - LANDO

   Abstract: Reversed phase liquid chromatography (RPLC) is the method of choice for the separation of organic molecules. However, there is no general agreement about the retention mechanism on a molecular scale. In an effort to gain a better understanding of these separation processes, we are using particle-based simulations. The retentive phase of an RPLC system usually consists of long chain alkanes, typically 18 carbons in length, bound to silica support. Until now all simulation studies have focused on alkanes grafted to a planar silica support. In this research project, a general program was developed that allows for the generation of retentive phases on planar interfaces and for cylindrical pores. Furthermore, the program can also set up structures with end-capping of residual silanols on the silica substrate.
42. Carlson, Darrin, Dan Mullen, Rachel LaFond, George Barany
*A New Handle (BHL) for Synthesis of Peptide Hydrazides and Their Use in Chemical Ligation*
Home Institution: University of Minnesota - Twin Cities
Sponsor: Department of Chemistry - HEISIG
Abstract: A new Boc-hydrazide (BHL) handle was made for use in Fmoc-based peptide synthesis. This handle was prepared from commercially available tert-butyl carbazate, p-BAL linker and PEG-polystyrene resin. The BHL was used in the solid-phase peptide synthesis of two peptides, FYNRRRG1-NHNH2 and SFYNRRRG1-NHNH2, with good yield and crude purity. C-Terminal hydrazides are useful precursors for syntheses of C-terminal azides and for chemical ligations by coupling with aldehydes. We are exploring the use of C-terminal azides in native chemical ligation (NCL) and also attempting to circularize peptides that contain C-terminal hydrazides and N-terminal aldehydes.

43. Collins, Michael, Don G. Truhlar, Rosendo Valero
*Exploring Potential Energy Surfaces for Singlet Excited-State Cytosine Using Density Functional Theory*
Home Institution: Colby College
Sponsor: Department of Chemistry - LANDO
Abstract: Cytosine is one of five nucleobases which encode all genetic material for eukaryotic lifeforms. Due to exposure to ultraviolet radiation excited-state cytosine may fluoresce to produce another species, possibly fragmenting and damaging the genetic material. If the ground-state and excited-state potential energy surfaces (PES) form a conical intersection, a photostable non-radiative internal conversion may occur. This research investigates four isomers of cytosine at their first, second, and third excited states via computational methods. Gaussian03 and Turbomole were used for all calculations. After characterizing the electronic structure at the vertical excitation (absorption), the potential energy surface (PES) is mapped. Excited state minima and transition states are identified, pointing to likely pathways for non-radiative relaxations.

44. Curtis, Jane, Galen Sedo, Ken Leopold
*Microwave Spectroscopy of Open-Shell Complexes*
Home Institution: University of Minnesota
Sponsor: Department of Chemistry - LANDO
Abstract: Microwave spectroscopy has proven itself to be a valuable tool in the study of open-shell complexes. Recent modifications to the University of Minnesota’s Fourier Transform Microwave Spectrometer have made it possible to observe complexes containing the OH monomer, and investigations into two such systems are currently underway. The states in which the lone $\delta$ electron occupies the Px or Py orbital in the free OH monomer are degenerate, but upon complexation this degeneracy is lifted. Previous analysis of the OH-H2O spectra (1) has yielded information pertaining to the electron distribution, such as the orbital energy difference, hyperfine, and super-hyperfine constants. Similar investigation of OH-C2H2 will build upon this previous analysis. Attempts to observe the microwave spectrum of OH-C2H2 will be described.

45. **Dahlmann, Heidi, Aaron May, Thomas Hoye**  
*Magnesium Halide-Catalyzed Anti-Aldol Reactions: Lessons and Discoveries*  
Home Institution: Wisconsin Lutheran College  
Sponsor: Department of Chemistry - LANDO  
Abstract: The stereoselective aldol reaction is among the most important reactions in natural product synthesis. While several methods exist to obtain aldol adducts of high syn stereoselectivity, the methods for obtaining anti adducts remain scarce. One example of a highly anti-selective aldol reaction is between chiral N-acyloxazolidinones and aldehydes using catalytic magnesium halide and TMSCl with a suitable base.1 Although this chemistry is useful, its scope had previously been limited to non-enolizable aldehydes. During our investigation into generalizing this method to include enolizable aldehydes, we discovered a novel reaction in which an N-acyloxazolidinone is converted into an oxazoline via a magnesium iodide-catalyzed decarboxylation. Mechanistic details of the stereoselective anti-aldol reaction and magnesium iodide-catalyzed decarboxylation of N-acyloxazolidinones will be provided.  

46. **Downs, Karen, Aaron Massari**  
*Electrochemical Synthesis of Polyaniline and Substituted Polyaniline*  
Home Institution: Luther College  
Sponsor: Department of Chemistry - LANDO  
Abstract: The objective of this study is to electrochemically polymerize several derivatives of polyaniline (PANI). After synthesizing PANI using cyclic voltammetry, its properties were compared with those of cyano, chloro, and carboxyl substituted polyaniline. These substituted polymers were made successfully to varying degrees, with ortho-substitution favoring the polymerization reaction more than meta-substitution. Polymers were analyzed using UV-visible and IR spectroscopy. UV-Vis spectroscopy was useful in identifying the electronic transitions of the different oxidized states of each polymer, while IR spectroscopy was used to affirm the presence of different IR-active substituents. Many of the substituted polymers had limited growth patterns indicating a loss of electroactivity with increased film thicknesses.

47. **Fako, Valerie, Valerie Kramlinger, Gianluigi Veglia**  
*Overexpression, Purification and Characterization of SERCA Regulators for NMR Studies.*  
Home Institution: University of Illinois at Urbana-Champaign and University of Minnesota  
Sponsor: Department of Chemistry - LANDO and HEISIG  
Abstract: Pathophysiological regulation of calcium concentration in cardiac muscle is associated with many types of cardiomyopathies. Ca2+ATPase is located in the sarcoplasmic reticulum (SR) of myocytes and is responsible for pumping calcium into the lumen, directly leading to relaxation of cardiac muscle. Phospholamban (PLB), a 52-amino acid residue integral membrane protein, inhibits SERCA activity by lowering its affinity for calcium. Upon β-adrenergic stimulation, PLB is phosphorylated at Ser16 by Protein Kinase A (PKA) leading to a relief of SERCA inhibition resulting in calcium translocation into the SR lumen. Understanding these effects on a molecular level is critical to the understanding of the physiological and pathophysiological effects on the heart. For this reason, purification of PKA, SERCA, and PLB were carried out with the goal of studying the structure and dynamics of protein-protein interactions by solution and solid-state nuclear magnetic resonance.
48. Forsberg, Brady, Steven R. Kass
*Investigating Molecular Recognition: Synthesis/Application of Carcerands*
Home Institution: University of Wisconsin – Stevens Point
Sponsor: Department of Chemistry - LANDO
Abstract: Cram, Lehn and Peterson were awarded the Nobel Prize in 1987 for their studies in molecular recognition/host-guest chemistry. This work elaborates on the type of chemistry enacted by materials such as crown ethers, cavitands, and cryptands, which can be employed for use in accelerating the rates of many reactions. An example of this is the use of 18-crown-6 in the reaction of halogenonitrobenzenes with potassium thiophenoxide which leads to an acceleration of $1.4 \times 10^8$. This dramatic rate enhancement was accomplished by only a partial encapsulation of the K+. If one could entirely surround the cation and sever its connection to the counterion, much larger effects should be observed. Spherical cages known as carcerands provide a means to generate “naked” anions with extraordinary reactivity in solution. The synthesis and reactivity of such materials are unknown, so the goal of this project was to make a molecular ball with a cation trapped inside. Our synthetic efforts in this regard are presented.

49. Gebremichael, Eminet, Rajeswari Kasi, David Blank, Marc Hillmyer
*Plastic Solar Cells*
Home Institution: University of La Verne
Sponsor: Department of Chemistry - LANDO
Abstract: Solar cells based on the polymer poly(3-hexylthiophene), layered or blended with fullerene (C60), currently hold the record for efficiency in organic devices. In this particular research, an azide of poly(3-hexylthiophene) was successfully synthesized and subsequently linked to a C60 to form poly(3-hexylthiophene) azide-C60. The intermediary products and the final product were characterized by both 13C and 1H nuclear magnetic resonance spectroscopy, gel permeation chromatography and ultraviolet-visible spectroscopy. Femtosecond fluorescence upconversion measurements in isolated conditions indicated that there is no electron transfer between the polymer donor and the C60 acceptor. The lack of intramolecular charge separation following photoexcitation is a result of the large spatial separation of the poly(3-hexylthiophene) from the C60. Intermolecular electron transfer in thin films and efficiency of P3HTN3C60 in solar cell devices are currently being investigated.

50. Hinkle, Lindsay, Kari A. McGee, Kent R. Mann
*Synthesis and Characterization of Iridium (III) Complexes for the Detection of Oxygen*
Home Institution: Austin College
Sponsor: Department of Chemistry - LANDO
Abstract: Recently, there has been an increased interest in the development of oxygen sensors utilizing emissive transition metal complexes, especially those with predictable and consistent emission sites. The use of crystalline materials ensures this consistent emission site, and since void space can easily be created within these structures, oxygen can pass directly into the crystal lattice. Oxygen can thus reach the emissive metal site which can undergo emission quenching due to energy transfer to oxygen, allowing for the spectroscopic determination of oxygen concentration. Six iridium (III) complexes were synthesized with the general formula of $[\text{Ir}^{(\text{CN})2(L)\text{Cl}}$ or $[\text{Ir}^{(\text{CN})2(L')}2\text{Cl}]$, where $(\text{CN})$ is an orthometallating ligand, L is a bidentate phosphine or polypyridine, and $L'$ is an isocyanide. To increase the amount of space within the crystal, each chloride salt was metathesized to a tetrakis[3,5-bis(trifluoromethyl)phenyl] borate (TFPB) salt. Using TFPB generates void space due to poor anion packing and the fluorines allow for diffusion of oxygen into the crystal lattice. One particular complex, $[\text{Ir}(ppy)2(bpy)]$TFPB was further characterized using measurements of quantum yield, lifetime, and emission spectroscopy.
51. Hubers, Jeffrey, Brandie Kovaleski, Karin Musier-Forsyth
   *Mapping the Interaction of the HIV-1 Capsid Protein and lysyl-tRNA Synthetase using Covalent Crosslinking Studies*  
   Home Institution: University of Minnesota - Morris  
   Sponsor: Department of Chemistry - LANDO  
   Abstract: Human immunodeficiency virus type 1 (HIV-1) uses the host-cell tRNALys3 as the primer for reverse transcription. tRNALys3 is selectively packaged into assembling virions in a complex that includes other host-cell tRNALys isoacceptors and lysyl-tRNA synthetase (LysRS) as well as HIV Gag, HIV GagPol, and viral RNA. During packaging, the tRNALys/LysRS complex interacts with a Gag/GagPol complex, with LysRS interacting specifically with Gag and tRNALys interacting with GagPol. The regions critical for the LysRS/Gag interaction have been mapped to the C-terminal domain (CTD) of the CA region in Gag and motif 1 of LysRS (Kovaleski et al., 2006). Covalent crosslinking studies allow identification of proximal residues on closely interacting proteins. Using a Cys-specific homobifunctional crosslinker (bis-maleimidohexane) and a photoreactive heterobifunctional crosslinker (benzophenone-4-maleimide), studies were conducted to map specific residues involved in the CA/LysRS interaction. Using SDS-PAGE and western blot analysis, no significant CA/LysRS complex has been observed using either crosslinker, suggesting that the Cys residues on CA are not in close proximity to the LysRS/CA interaction site. However, both LysRS and CA formed homodimers using the benzophenone-4-maleimide crosslinker. Single Cys mutated forms of the CA protein were also generated for use in future crosslinking studies.

52. Kalstabakken, Kyle, Phillipe Buhlmann
   *Synthesis of Polymer-Anchorered Oligomeric Thioureas for Ion Detection*  
   Home Institution: University of Tulsa  
   Sponsor: Department of Chemistry - LANDO  
   Abstract: In an effort to develop an improved method of detecting chloride, phosphate and sulfate ions, polymer-anchored, oligomeric thioureas were constructed. The thioureas, which act as excellent hydrogen bond forming ionophores, are attached to amide resin beads. Chains of up to three thioureas are added to the beads through a reaction of an isothiocyanate and an anchored primary amine. Benzene spacers separate the thiourea monomers, supplying rigidity that should improve the ion binding selectivity. The synthesis of the oligomeric thioureas is described herein. The initial material, m-xylylene diamine, is monoprotected with a 9-fluorenymethyl carbamate (Fmoc) group. The remaining amino group is then converted to an isothiocyanate, which can be directly added to the polymer bead. This produces a thiourea monomer. The Fmoc protecting group can then be removed, providing an amino group for additional thioureas to be added using the same procedure. The oligomeric chain can then be capped through a reaction with phenyl isothiocyanate, creating the final thiourea.

53. Kucukdisli, Murat, Nicholas Zunker, Craig J. Forsyth
   *Synthesis of C31-C46 Domain of Phorboxazole*  
   Home Institution: Middle East Technical University, Ankara, Turkey  
   Sponsor: Department of Chemistry - LANDO  
   Abstract: Phorboxazole A and B, isolated from the sponge Phorbas sp., have been found to be potent cytostatic agents. This project is focused on the synthesis of the C31-C46 domain of a biologically active analog of Phorboxazole A. Synthesis of the C42-C46 building block involves a seven-step sequence from ( ) glycidol to synthesize a sulfone, which can be connected to an aldehyde at C41 through a modified Julia olefination.
54. Lanners, Jeff, Philippe Buhlmann
Potentiometric Measurements with Ionophore-Based Ion-Selective Microelectrodes Using a Unique Preconcentration Mode
Home Institution: University of Minnesota
Sponsor: Department of Chemistry - HEISIG
Abstract: Ion selective electrodes (ISEs) are sensors specially designed to select and detect one type of ion in a solution. Current research has led to the design and fabrication of electrodes that are much smaller than conventional ISEs. Potentiometric microelectrodes have several advantages over conventional ISEs, chief among them being the ability to measure in extremely small volumes. The electrodes used in this study are of the solid contact type, which distinguished them from normal ISEs that contain an inner filling solution. The solid contact makes these sensors not only more robust, but it also makes them amenable to microfabrication. The electrodes are created by electropolymerization of pyrrole on a gold electrode. The electrodes are then coated with an ion-selective membrane. In this series of experiments, a silver ion selective electrode was designed for the particular purpose of low detection limits. Unlike conventional electrodes, it contains two different ionophores. It was found to achieve a detection limit of 10E–8 M. This low detection limit was obtained by using a new preconcentration protocol that avoids the baseline drift problems typical for conventional potentiometric sensors.

55. Lindvall, Brian, Wayne Gladfelter
Zinc Oxide Nanoparticles
Home Institution: Century College
Sponsor: NSF/Lando/Renewable Energy
Abstract: In an effort to produce a more efficient solar cell, the Gladfelter research group has been working with Renewable Energy to make a transparent, conductive layer within the cell consisting of Zinc oxide. Our job in the lab has been to synthesize a precursor, bis-diisobutylamidozinc, and coat it with different ligands that correspond with various solvents. The solvent, along with the coated nanoparticles will be sprayed on to a substrate using an inkjet printer, and checked for conductivity. Our method of synthesis is important because it reduces the high cost of producing zinc oxide nanoparticles with a high vacuum system, and the expensive lithography step is replaced with an inexpensive inkjet printer.

56. Page, Sarah, Kris McNeill
Zinc-Cobalt Porphyrin Binding and Function in Dechlorination Reactions
Home Institution: University of Minnesota
Sponsor: Department of Chemistry - HEISIG
Abstract: Chlorovinyl compounds such as trichloroethylene (TCE) are common ground water contaminants. Zinc has been proven to dechlorinate these compounds, and has been used in water remediation. The rate of dechlorination can be increased by binding a catalyst to the zinc surface. Cobalt compounds, such as Vitamin B12 and other porphyrin model complexes like 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin cobalt (Co(TCPP)), have been shown to catalyze dechlorination. Co(TCPP) was studied to determine the degree to which it binds to zinc and the difference in the rate of catalyzed and non-catalyzed dechlorination. The products of the dechlorination reaction were also monitored and used as a diagnostic of the mechanism to determine the site of dechlorination.
57. Senkomago, Virginia, Shencheng Ge and Christy L. Haynes

Electrochemical Detection of Dopamine from Murine Retinal Amacrine Cells

Home Institution: Berea College
Sponsor: Department of Chemistry – LANDO

Abstract: Dopamine is a key neurotransmitter in the retina that is known to play a role in retinal light adaptation, the size of the receptive field and chromatic processing. The abnormal release of dopamine in the retina has been implicated in triggering retinal degeneration. The dopamine trigger hypothesis has not been tested due to insufficient analytical methods for intact cellular or whole retinal studies. Dopamine is an electroactive neurotransmitter; thus, single cell amperometry may be the appropriate tool to complete these studies. However, dopaminergic amacrine cells constitute a minute percentage of retinal cells and hence, are a challenge to culture for electrochemical studies. Several experiments were done to improve the protocol for culturing and isolating these cells. Firstly, the concentration and time for the dissociation of retinal cells with papain was adjusted. Secondly, retinal cells were plated on cover slips coated with an antibody to the extracellular loop of the dopamine transporter instead of poly-L-lysine. Both of these protocol changes increased the yield of intact dopaminergic amacrine cells. Carbon-fiber microelectrode amperometry was used to measure dopamine release from cells following stimulation with K+ enriched buffer. Further work is necessary to precisely analyze the characteristics of dopamine release from amacrine cells.

58. Smolensky, Eric, Robert Jilek, John Ellis

Syntheses of Unprecedented Low-Valent Titanium Species

Home Institution: University of Minnesota - Morris
Sponsor: Department of Chemistry - LANDO

Abstract: The preparation of subvalent polyarene transition metal complexes is a relatively new and poorly explored area of chemistry. The aim of this research is to synthesize a homoleptic polyarene titanium (II-) compound, namely [K(18-crown-6)]2[Ti(C14H10)3]. Further research involves the reactions of [Ti(C14H10)]2- with various other acceptor ligands; for example PF3, CO, pyrene, and ethylene. Characterization techniques, mainly NMR and IR, are used to structurally identify the products. The results suggest, with reasonable certainty, the successful synthesis of [K(18-crown-6)]2[Ti(C14H10)3] under moderate reaction conditions. Additionally, the spectra collected from the reactions with acceptor ligands indicate, in most cases, successful substitution reactions. Current and future work involves characterization of the products in the solid-state via X-ray diffraction and publication of the results in the Journal of the American Chemical Society or Angewandte Chemie.

59. Stracke, Jordan, Mark Distefano, Juhua Xu

Synthesis of Farnesyl Pyrophosphate Analogs for Affinity Chromatography and Photo Labeling

Home Institution: University of Minnesota
Sponsor: Department of Chemistry - LANDO

Abstract: Farnesyl pyrophosphate (FPP) is a biologically vital compound. It is a predecessor of cholesterol, hormones, rubber and many other natural products. Additionally, it is involved in many necessary protein interactions. We are interested in developing methods to purify enzymes which use FPP as a substrate. Affinity chromatography and photo labeling have been used in the isolation of many different types of enzymes. Here, these techniques have been utilized to create an affinity column and a photo label capable of selectively purifying and labeling enzymes which use FPP as a substrate. The affinity column consists of a non-hydrolysable FPP analog, farnesylmethylenephosphonophosphate, which is coupled to an Affi-Gel resin. This is a six step synthesis of which three steps have been completed to date. The photo labeling reagent, also an FPP analog, contains a benzophenone group attached to geranylmethylenephosphonophosphate through an ester linkage; the terminal phosphate group permits the incorporation of 32P which allows the reagent to selectively radiolabel isoprenoid
utilizing enzymes. The photo label synthesis involves five steps of which four have been completed to date.

60. Sutton, Sarah, Hao Luo, Yu Zhang, Peter W. Carr

Optimization of Reaction Catalysts and Solvents in the Silanization of Porous Silica in Preparing Stationary Phases for HPLC

Home Institution: St. Mary's College
Sponsor: Department of Chemistry - LANDO

Abstract: High Performance Liquid Chromatography (HPLC) is a technique heavily employed by the pharmaceutical industry to test the purity and stability of drugs and to separate biologically significant compounds, such as proteins and peptides. Stationary phases used in HPLC are primarily silica-based on account of their highly resolved peaks and their applicability to a wide range of solutes. Over the past several years, the Carr Lab has developed ultra-stable hyper-crosslinked silica-based phases using Friedel-Crafts chemistry. These highly crosslinked surface confined polymers are capable of withstanding high temperatures and acidic mobile phases which is advantageous to improving chromatographic efficiency and reducing analysis time. Our recent research has focused on optimizing the initial silanization step in the synthesis of this hyper-crosslinked phase. We have screened several combinations of reaction catalysts and solvents in terms of promoting the highest possible surface coverage of the Dimethyl Chloromethyl Phenylethyl Silane (DMCMPES) ligand while avoiding unwanted positive charge on the silica surface capable of ruining the retention of basic solutes. We have found that Dimethyl Formamide (DMF) promotes the highest ligand surface coverage (30% higher than with any other solvent) while still avoiding the generation of positive charge on the silica surface. These attributes are critical to optimum performance of the ultra-stable hyper-crosslinked silica-based phase.

1. Trammell, Brian C; Ma, Lianjia; Luo, Hao; Jin, Dihua; Hillmyer, Marc A.; Carr, Peter W. "Highly Cross-Linked Self-Assembled Monolayer Stationary Phases: An Approach to Greatly Enhancing the Low pH Stability of Silica-Based Stationary Phases." Analytical Chemistry. 74(18), 4634-4639 (2002).

61. Tanaka, Kari, R. Lee Penn

Reactivity of Ferrihydrite Nanoparticles

Home Institution: Macalester College
Sponsor: Department of Chemistry – LANDO

Abstract: Ferrihydrite is a poorly crystalline iron oxide that typically occurs in the 2-10 nm size range and is initially formed during precipitation of iron in soils and sediments. Ferrihydrite is metastable and serves as a precursor for transformation to more crystalline iron oxide phases such as goethite or hematite. Using surface-area normalized rates of reduction by hydroquinone, results demonstrate that, contrary to expectation, redox reactivity increases with increasing particle size. In addition, monitoring the rate at which ferrihydrite transforms to goethite by way of transmission electron microscopy (TEM) and small angle X-ray scattering (SAXS) demonstrates that growth rates increase with decreasing primary nanoparticle size. Finally, combining results from TEM with those from SAXS demonstrate that the latter method is an efficient means by which the formation of goethite from ferrihydrite can be quantified.

62. Voellinger, Kailey, Nicholas Lanzatella, Wayland E. Noland

Progress Towards Diels Alder Reactions of Tosylated 2-Vinylpyrroles

Home Institution: University of Minnesota
Sponsor: Department of Chemistry - LANDO

Abstract: The indole nucleus occurs frequently in nature and in many biologically active compounds. It is advantageous to study the synthesis of novel indole products, and new synthetic routes to the indole moiety. The potential for novel products to exhibit biological activity could be important in the
advancement of new pharmaceuticals. The novel products to be synthesized through Diels-Alder reactions between the diene N-tosyl-2-vinylpyrrole and variuosly substituted dienophiles such as maleamides and alkynes. Synthesis of N-tosyl-2-vinylpyrrole will be attempted using Wittig and Grignard Methods. The N-tosyl group, despite withdrawing electrons is potentially helpful in the Diels Alder reaction as it may prevent polymerization of the product and may help in crystallizing the final product. Detosylation and oxidation of the Diels Alder adducts results in both novel compounds and novel indole synthesis techniques.

63. Warner, Ellis, Andy Healy, David Blank
Photoionization of Isooctane
Home Institution: University of Minnesota – Twin Cities
Sponsor: Department of Chemistry - HEISIG
Abstract: Professor Blank, Sanford Lipsky, Andy Healy, and Ellis Warner are doing research involving the photoionization of isoctane utilizing 36-50 fs pulses of 400nm. We are then using a probe pulse in the 800nm- 1200nm range to detect and plot the electron decay in the liquid phase. I have been working with Andy Healy in setting up the laser and experiment this summer.
64. **Arola, Trina, William H. Ojala**  
*Intermolecular Interactions in Phenylhydrazone Crystals: Lewis Acid-Lewis Base vs. Hydrogen Bonding*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: We are working toward preparing new crystalline materials by co-crystallizing molecules we have designated “bridge-flipped isomers.” In these isomers, two major parts of the molecule are joined by a bridge of atoms; changing the bridge orientation relates one isomer to the other. We are currently examining phenylhydrazones, in which the bridge-flipped isomerism is Ar-NH-N=CH-Ar’ vs. Ar-CH=N-NH-Ar’ (where Ar = aryl). Co-crystallization would be facilitated if the bridge-flipped isomers were isostructural (same molecular packing arrangement). We are determining the solid-state structures of phenylhydrazones by single-crystal X-ray diffraction to identify isostructural bridge-flipped isomeric pairs for future co-crystallization experiments. Intermolecular interactions linking molecules into similar chains in the two solid isomers might encourage their isostructuralism, so we have prepared phenylhydrazones substituted with halogen atoms and nitrile groups to encourage intermolecular Lewis acid-Lewis base interactions. We find H-bonding between the bridge N-H and the nitrile group to be a competing and differentiating interaction.

65. **Athmann, Jon**, David Boyd, Jonathan Hennek  
*Synthesis and Characterization of Substituted Ruthenium Bipyridine Compounds*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: In an attempt to improve the efficiency of photovoltaic devices, a series of ruthenium bipyridine compounds have been prepared and characterized. The visible light absorbance of these ruthenium compounds can collect and deliver a larger portion of the energy available in the solar spectrum to a photovoltaic device if properly integrated into the device. The compounds studied include several that can be covalently linked to the metal oxide particles as part of the fabrication process. The synthesis and characterization of ligands and ruthenium compounds will be described.

66. **Balidemaj, Barjeta, William H. Ojala**  
*Intermolecular Interactions in Benzylideneaniline Crystals: A Comparison of a Fluorobenzylidene-Cyanoaniline to a Cyanobenzylidene-Fluoroaniline*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: The purpose of this study is to prepare crystalline benzylideneanilines and to determine their crystal structures by X-ray crystallography. An eventual goal is to co-crystallize benzylideneanilines that are “bridge-flipped” isomers of each other, isomers that differ only in the orientation of the –CH=N-bridge between the phenyl rings. We have been examining pairs of bridge-flipped isomers to determine whether they are isostructural, assuming identical molecular packing arrangements in their respective crystals, because these would tend to co-crystallize most readily. Lewis acid-Lewis base contacts between halogen atoms and nitrile groups on the benzylideneaniline molecules might encourage the isomers to pack in similar ways, so we have determined the crystal structures of two halogen/nitrile benzylideneanilines, 4-fluorobenzylidene-2-cyanoaniline and 2-cyanobenzylidene-4-fluoroaniline, to find out whether they are isostructural. We have determined that they are not. In this poster we describe these two different molecular packing arrangements.
67. Buck, Paul, Dwight R. Stoll, Xiaoli Wang, Peter W. Carr  
**Optimization of the First Dimension of a Two-Dimensional High Performance Liquid Chromatography System for the Analysis of Complex Biological Samples**  
Home Institution: St. Olaf College  
Sponsor: Department of Chemistry  
Abstract: Two dimensional High Performance Liquid Chromatography (2D-HPLC) is gaining attention from bio-scientists because of the dramatically improved resolving power of the technique compared to conventional one-dimensional separations. This added resolving power comes at the expense of greatly increased complexity of instrumentation and experimental conditions which makes it difficult to find the optimum separation conditions for a particular sample. In order for the second separation to resolve the highest number of peaks, the first dimension must be optimized to provide a broad range of peak elution times and a suitable gradient time, while keeping the eluent strength of the first dimension separation low relative to that used in the second dimension separation. Optimum conditions for such a system could be found by trial and error, but with virtually limitless possibilities, it is extremely unlikely that an acceptable set of conditions could be found within a practical time frame. We have used the Linear Solvent Strength Theory (LSST) of gradient elution and judiciously chosen solutes to model the separation of small molecules in biological samples. Using a Monte Carlo search algorithm several parameters such as gradient time, initial and final percent organic modifier, flow rate, column length and column inner diameter, can be varied simultaneously to find a set of optimal separation conditions.

68. Dickhudt, Tim, Tony Borgerding  
**Analyzing High Boiling Aromatic Compounds in Soil Samples Using GC-ArSLID**  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: The Aromatic Selective Laser Ionization Detector (GC-ArSLID) is an innovative way for analyzing aromatic compounds in that it is selective for only aromatics and no other compounds. We worked on maximizing its efficiency by adding various heating elements which was essential for being able to view higher boiling temperature compounds. This summer we have studied various soil samples as well as diesel fuel to see what kind of aromatic compounds can be found in our environment. Low boiling compounds such as toluene, xylene, cumene, various phenols, and halogenated benzene rings have been analyzed in concentrations as low as 1.6 x 10\(^{-6}\) M. Higher boiling compounds such as naphthalene, anthracene, benzanthracene, anthrone, fluorene, and acenaphthene have been analyzed in concentrations as low as 8.5 x 10\(^{-5}\) M. Extracts of soil and soot samples have been analyzed as well, indicating the presence of many aromatic compounds. Although we have not successfully identified any compounds in the samples, we have been able to identify how many rings compounds within these samples have.

69. Engebretson, Ann, Dan Besemann  
**Forensic Lipstick Analysis Using Chemical Fingerprinting via Gas Chromatography**  
Home Institution: Hamline University  
Sponsor: Hamline University Collaborative Research/Hamline University Mitsch Research Fund  
Abstract: Extractions of organic materials were done with acetone from a variety of common lipstick samples. Each extract was subsequently analyzed using gas chromatography with flame ionization detection (GC/FID). By identifying unique patterns in the chromatogram of each lipstick sample, class characteristics for each sample can be recognized and a searchable database of known samples of lipstick compiled. The ultimate goal being this assemblage of chromatograms of known lipstick samples to compare gathered unknown lipstick samples transferred from victim to perpetrator (or vice versa) at crime scenes assisting investigators in linking a suspect to crimes and/or victims.
70. **Haegle, Michelle, Ryan Haws, Daniel Besemann**  
*Analysis of O-H Stretch Frequencies in Methanol Clusters Using Density Functional Calculations*

Home Institution: Hamline University  
Sponsor: Hamline University Lund Fund  

Abstract: Using B3LYP/6-31+G* density functional calculations, our group analyzed the O-H stretch frequencies of more than 40 different hydrogen-bonded methanol clusters. Several trends were identified based on the size and shape of the cluster, as well as the position within the cluster. Results from this study will be used to interpret the vibrational spectra of liquid phase methanol solutions, furthering our understanding of hydrogen bonding in liquid environments.

71. **Heppner, David E., Benjamin F. Gherman, William B. Tolman, Christopher J. Cramer**  
*Modeling Dioxgen Activation in Active Site and Biomimetic Models for Dopamine β-Monooxygenase and Peptidylglycine α-Hydroxylating Monoxygenase*

Home Institution: University of Minnesota  
Sponsor: Department of Chemistry and Super Computing Institute/supported by The Arnold and Mabel Beckman Foundation (The Beckman Scholars Award)

Abstract: A variety of ligand sets have been constructed to model dioxygen binding to the copper site in dopamine β-monooxygenase (DBM) and peptidylglycine α-hydroxylating monoxygenase (PHM), whose active site, as characterized by X-ray crystallography, contains a η¹ Cu-O₂ adduct at the Cuβ site. Geometries and energies were calculated using density functional theory and multireference second-order perturbation theory methods. Anionic ligand sets stabilized η² dioxygen coordination to Cu and more peroxo-like character in the adducts with exergonic binding free energies that may indicate limited reactivity towards substrate. In contrast, neutral ligands, while also leading to energetically favorable free energies for oxygenation, favored formation of η¹ Cu-O₂ complexes like that seen in the crystal structure of the precatalytic oxygenated complex for PHM. This suggests that neutral biomimetic ligands may be necessary for the stabilization of η¹ dioxygen coordination. Additionally, the energetics of oxygenation as a function of ancillary ligand properties in stabilizing η¹ dioxygen coordination with the β-diketiminate model system have been examined. Pyridine ligands substituted at the para position preferentially stabilize η¹ dioxygen binding over η² as the electron donating character of the substituent is increased. Varying the steric bulk of cyclic ether ligands exhibits a similar influence. Finally, stabilizing η¹ dioxygen may be accomplished through use of ligands that can donate hydrogen bonds to the dioxygen moiety.


72. **Korte, Andrew, Kristine H. Wammer**  
*Analysis of Two Fluoroquinolone Antibiotics and their Environmental Photochemical Degradation*

Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  

Abstract: Two fluoroquinolone antibiotics, norfloxacin and ofloxacin, were examined to predict their respective photochemical fates in natural waters. Samples of norfloxacin and ofloxacin solutions in both
water obtained from Lake Josephine in St. Paul and deionized water adjusted to a similar pH (~8) were photolyzed under sunlight and analyzed by HPLC to determine concentrations at set time intervals. Photodegradation rates were rapid for both drugs, with a half-life of ~10 minutes for norfloxacin and ~40 minutes for ofloxacin at 50 uM concentrations and pH 8, with rates dropping sharply outside the pH range of 8–9. Degradation occurred more quickly in deionized water than natural water, indicating indirect processes likely will not significantly contribute to removal of the drugs in the environment. Rate was also found to be highly dependent upon concentration, with screening effects being seen at concentrations as low as 2 uM in the case of norfloxacin. Using degradation rates for solutions at a range of pH values and measured pKa values, decay constants were calculated for each of three species of norfloxacin allowing for the prediction of decay rate at the range of pHs relevant in natural waters.

73. Kramer, Ashley, Anthony Borgerding

*Analysis of Volatile Compounds of Diagnostic Interest using a Microdialysis Probe Extraction Technique*

Home Institution: University of St. Thomas
Sponsor: Department of Chemistry

Abstract: Our lab has had success using microdialysis sampling probes for volatile compound extraction from solutions into the gas phase as opposed to liquid dialysate extraction, which is more common. In our research volatile compounds were extracted from aqueous solutions through microdialysis probes using gas chromatography with a flame ionization detector (GC/FID). These compounds include acetone and dimethyl sulfide both showing a linear representation over a range of concentration (0.001-0.5% by weight for acetone and 10-200mM for dimethyl sulfide). Recently we have analyzed volatile compounds that are insoluble in water from organic solvent solutions using the microdialysis probes interfaced to a mass spectrometer (MS). We have obtained results for carbon disulfide (dissolved in methanol) over a concentration range of 10-200mM using this method of instrumentation and will also test isoprene and halothane. Our research lab is currently testing our probes on these volatile compounds (which can be found in human breath condensate) for the long-term goal of using microdialysis as an in-vivo method of study in biochemical systems such as different places in the human body.

74. Kuspa, Marika, William H. Ojala

*A Solid-State Comparison of Two “Bridge-Flipped” Benzylideneanilines*

Home Institution: University of St. Thomas
Sponsor: Department of Chemistry

Abstract: The purpose of our research is to crystallize organic compounds (specifically benzylideneanilines) and to determine their crystal structures by X-ray crystallography. The ultimate goal of this project is to determine the structures of a given benzylideneaniline and its “bridge-flipped” isomer (the isomer differing only in the orientation of the -CH=N- group between the phenyl rings) to determine whether the packing arrangements are similar enough (isostructural) to allow the compounds to be co-crystallized. The structure of 4-(N,N-dimethylamino)-N-(2-fluorobenzylidene)aniline (I) has been determined. The crystal structure has two molecules in the asymmetric unit in space group P2(1)2(1)2(1). The bridge-flipped isomer, 4-(((2-fluorophenyl)imino)methyl)-N,N-dimethylaniline (II), has been found by previous workers to crystallize in space group P2(1)/c. One of the molecules in the asymmetric unit of (I) has a torsional angle between the benzene rings of 2.48°, while the other molecule has an angle of 12.93° between the rings. The coordinates for (II) have not yet been published, so in future research its crystal structure will be re-determined and compared to that of (I). Because (I) and (II) crystallize in different space groups, it is unlikely that the two compounds will co-crystallize readily, but future seeding experiments may yet lead to co-crystallizable polymorphs.
75. Leeby, Katherine, Katherine Olson  
*Synthesis of Peroxyfluor-1 for Use in an ELISA Test with the Enzyme Alcohol Oxidase*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: The synthesis of Peroxyfluor-1 is a two-step reaction that involves multiple refluxes to achieve the final product. In place of these long refluxes the Biotage Initiator Microwave Synthesizer was hypothesized to produce the same results in a very short period of time. This was attempted for both steps but was found only to be successful for the second step. After synthesizing the Peroxyfluor-1 it was purified by column chromatography. Peroxyfluor-1 can be utilized to make a very sensitive ELISA test. Peroxyfluor-1 allows for colored samples to be tested as change in fluorescence is measured, instead of change in color. Alcohol Oxidase is an enzyme from Pichia pastoris that has the ability to convert alcohols into hydrogen peroxide. Hydrogen peroxide then converts the Peroxyfluor-1 into fluorescein, a highly fluorescent chemical. A competition ELISA can be set up with an analyte, such as estradiol, from the unquantified source and a known amount of the analyte linked to Alcohol Oxidase. The change in fluorescence can then be quantified to determine the concentration of the analyte in the unknown sample. Quantifying these unknown samples can be used to test for varied health conditions associated with changes in hormone levels.

76. Lundeen, Rachel, Kristine H. Wammer  
*Photochemical Behavior of Enrofloxacin in the Aqueous Environment*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: The fate and effects of fluoroquinolones (FQs), a type of antibacterial pharmaceutical, within aqueous environments is of growing concern. Environmental studies involving FQs are significant because these compounds are being detected in a wide range of field samples. The photolysis of enrofloxacin, an agricultural FQ, was studied in respect to the formation of photoproducts and rate of degradation (t1/2 ? 12 minutes) under environmentally-relevant conditions. Experiments showed a significant impact of pH on the rate of enrofloxacin degradation and indications of screening at concentrations of enrofloxacin as low as 1 µM. No rate enhancement was seen in experiments using natural water samples, indicating enrofloxacin has no indirect processes affecting photodegradation. A broad suite of photoproducts are observed when enrofloxacin is photolyzed, and bacterial growth studies done within our research group indicated that photolyzed enrofloxacin significantly inhibited growth due to the presence of these photoproducts. Recent research has indicated that ciprofloxacin, an FQ used primarily in human medicine, is a potential photoproduct of enrofloxacin photodegradation. LC-MS data suggests that ciprofloxacin is indeed a minor photoproduct of enrofloxacin in natural waters. Ongoing work is examining to what extent the antibacterial activity of the photoproducts can be attributed to the ciprofloxacin present.

77. Newman, Dana, William H. Ojala  
*Crystal Structure and Packing Arrangement Comparisons Between Bridge-Flipped Isomers: N-(para-Bromobenzylidene)aniline and N-Benzylidene-para-bromoaniline*  
Home Institution: University of St. Thomas  
Sponsor: Department of Chemistry  
Abstract: Our laboratory is currently attempting to co-crystallize organic “bridge-flipped” isomers, with hopes that this strategy can be used to synthesize new materials with applications in electronics, pharmaceuticals, circuitry, etc. Bridge-flipped isomers are compounds that differ from each other only in that the sequence of bridge atoms that connects the major structural components of the molecules is reversed from one isomer to the other. The likelihood of co-crystallization is increased if the individual crystalline compounds are isostructural with each other, meaning that they have the same molecular...
packing arrangement in the solid state. This research is focused on the synthesis and X-ray crystallographic analysis of benzylideneaniline bridge-flipped isomers, particularly on two compounds: N-(para-bromobenzylidene)aniline and N-benzylidene-para-bromoaniline. The crystal structures and packing arrangements of both compounds have been determined, and it has been found that these bridge-flipped isomers do not assume the same packing arrangement. Therefore, further computer analysis has been done in an effort to determine why the two compounds pack differently when the only molecular difference is the exchange of the –CH= and =N- positions within the bridge. This includes investigating potential halogen-halogen interactions, halogen-nitrogen contacts, and other contacts possibly involving the bridge atoms.

78. Presley, Tegan, Dan Besemann
Evaluation of Nonselective Transport Properties of an Amino Acid across Concentric Hollow-Fiber Membranes
Home Institution: Hamline University
Sponsor: Department of Chemistry
Abstract: A concentric hollow-fiber membrane apparatus for use in chemical separations was constructed. In addition to the selective permeability of the membrane, a selective carrier molecule may be suspended within membrane system. Tryptophan was used to test the nonselective transport properties of the system. It was determined that addition of a detergent to the feed increased the rate of diffusion across the membranes. Once optimized, this type of system may offer an efficient option for some large-scale chemical separations.

79. Schroeder, Jenna, Jacobson, K. Brook, Kristine H. Wammer
Analysis of the Antibacterial Activity of Tylosin and Enrofloxacin Photoproducts
Home Institution: University of St. Thomas
Sponsor: Department of Chemistry
Abstract: Enrofloxacin and tylosin are two antibacterial compounds used primarily for agricultural applications. Both have been found in natural waters at low concentrations. Both drugs are subject to photodegradation when exposed to natural sunlight. While attenuation by sunlight usually mitigates the environmental impacts of antibacterial compounds, problems may arise if the photoproducts themselves introduce additional antibacterial activity. In separate experiments the antibacterial activities of enrofloxacin and tylosin were compared to that of their photoproducts to determine whether the products presented any additional antibacterial activity against Escherichia coli DH5alpha. Enrofloxacin’s photoproducts greatly inhibited bacterial growth while tylosin’s main photoproduct (resulting from a photoisomerization) did not inhibit bacterial growth at all. These results indicate that photodegradation of tylosin will likely result in elimination of its potential to affect environmental microbial communities whereas assessment of enrofloxacin’s potential environmental impacts will likely need to include analysis of its photoproducts.

80. Welsch, Emily, Tim Murray, Craig Forsyth
Progress Toward the Total Synthesis of GEX1A
Home Institution: St. Olaf College
Sponsor: Department of Chemistry (Natural Product Organic Synthesis)
Abstract: My summer research has been focused on synthesizing the natural product GEX1A. GEX1Aís fascinating stereochemical properties and its biological significance have been the motivation behind this research. During the course of the summer, work has been completed toward the synthesis of two separate fragments of GEX1A. For the synthesis of the C1-C9 fragment, a Roush crotylation was performed to set two stereocenters. Also, modification of the previous route towards the C15-C19 fragment gained access to the desired aldehyde with improved efficiency via a Keck crotylation.
81. Ciriacks Klinker, Chanda, Michael T. Bowser

*Online Microdialysis-Capillary Electrophoresis Measurements in the Rat Striatum*

Home Institution: University of Minnesota
Sponsor: Department of Chemistry

Abstract: The need to measure chemical dynamics in the brain has motivated our lab to develop fast, efficient instrumentation capable of separating and quantitating numerous amino acids simultaneously. Amino acids are sampled from the striatum of an anesthetized rat using a 3mm microdialysis probe. Reverse microdialysis can also be used to deliver pharmacological agents to the striatum while simultaneously sampling the changes in neurochemicals. Dialysate is derivatized online and separated with high-speed capillary electrophoresis (CE). A flow-gated interface allows discrete volumes of derivatized dialysate to be injected into the separation capillary every 10-15s, thus giving us temporal resolutions that are significantly improved over those previously achieved. Fluorescence is detected in a sheath-flow cuvette by laser induced fluorescence. This system allows us to detect as small as an 8% change in concentration, which is another significant improvement over traditional methods. Specifically, we have been investigating D-serine and the NMDA receptor. Using reverse microdialysis, we have tested the effects of the non-NMDA receptor agonist kainic acid (KA), the NMDA receptor agonist NMDA, and their corresponding antagonists, CNQX and MK801. Changes in concentrations of glutamate, GABA, D-serine and L-serine were monitored. Application of KA resulted in increases in all amino acids monitored. However, the CNQX did not significantly block the effect of KA on D-serine. NMDA also induced increases in all amino acids monitored. This effect was attenuated by application of MK801.

82. Duckworth, Ben, Juhua Xu, Ayako Hosokawa, Zhiyuan Zhang, Mark Distefano

*Selective Labeling and Immobilization of Proteins*

Home Institution: University of Minnesota
Sponsor: Chemistry

Abstract: The emergence of the field of proteomics has required the need for new methods to both label and immobilize proteins in a site specific, covalent manner. To accomplish this, our laboratory utilizes an enzyme that specifically labels a tetrapeptide tag, genetically fused onto the C-terminus of a target protein, with an azide moiety. The protein-azide is then reacted with a fluorescent probe bearing an alkyne moiety using the Cu(I)-catalyzed [3+2] cycloaddition reaction. In addition, the azide-labeled protein can be immobilized onto alkyne-functionalized surfaces. The target protein was also labeled with the alkyne moiety and subsequently reacted with a probe/surface functionalized with an azide. It was found that less background, non-specific labeling occurred when the protein was enzymatically labeled with the alkyne and reacted with the azide probe. In addition to labeling proteins with fluorescent probes, this strategy was used to selectively dimerize proteins as well as label proteins with DNA. This approach has several advantages over other immobilization methods: the recognition tag is only four amino acids and does not require large fusion proteins, the target protein can be immobilized in pure form or in the presence of a complex mixture, and the target protein can be selectively labeled even in the presence of multiple cysteines. Therefore, this chemoenzymatic method should have broad applicability in proteomics and protein chemistry.

83. Eder, Angela, Edgar Arriaga

*Capillary Electrophoresis Monitors Enhancement in Reactive Oxygen Species Production upon Treatment with Doxorubicin*

Home Institution: University of Minnesota
Sponsor: Department of Chemistry

Abstract: Generation of reactive oxygen species (ROS) has been implicated in the onset of cardiotoxicity resulting from chemotherapy treatments incorporating doxorubicin (DOX). This study
investigated the role of DOX accumulation in the ROS production detected in individually electrophoresed organelles. While bulk measurements of ROS production in cells and organelles are not capable of discriminating between the effect of preparative procedures on measured ROS production, analysis of individually electrophoresed organelles demonstrated a difference in the measured ROS production as a result of various preparative procedures. Using capillary electrophoresis with dual laser-induced fluorescence detection, an increase in ROS production was observed in organelles isolated from cells treated with DOX compared to untreated controls. Two sub-populations of organelles containing both DOX and ROS were observed, one of which demonstrated a direct relationship between DOX uptake and subsequent ROS production, and a second one with low DOX uptake but large variation in ROS production.

84. Ergang, Nicholas, Justin C. Lytle, Kyu Tae Lee, Andreas Stein
Fabrication of a Three-Dimensionally Interpenetrating Electrochemical Cell System
Home Institution: University of Minnesota
Sponsor: Department of Chemistry
Abstract: We describe the first example of a three-dimensional solid-state interpenetrating electrochemical cell able to shuttle Li ions between two electrodes on a sub-micrometer lengthscale. A 3-D ordered macroporous (3DOM) carbon anode functioned as the foundation of the cell. It was fabricated via infiltration of a monolithic poly(methyl methacrylate) (PMMA) colloidal crystal template with a resorcinol-formaldehyde sol-gel precursor solution. A pinhole-free poly(phenylene oxide) (PPO) electrolyte was electrodeposited on the surface of the carbon anode. The remaining void space was filled with a V2O5-based cathode deposited via standard sol-gel techniques. The C/PPO/V2O5 composite was then lithiated and cycled.

85. Kovaleski, Brandie J., Robert Kennedy, Minh Hong, Karin Musier-Forsyth
Interaction Between HIV-1 GAG and Human Lysyl-tRNA Synthetase: A Novel Target for Anti-Retroviral Therapy
Home Institution: University of Minnesota
Sponsor: Department of Chemistry
Abstract: Human tRNA\textsubscript{Lys} is used as the primer for HIV reverse transcription. Both HIV Gag and GagPol are required for packaging of the tRNA into virions. Host cell lysyl-tRNA synthetase (LysRS) is also specifically packaged into HIV, suggesting a possible role for LysRS in tRNA packaging. Gag alone is sufficient for packaging of LysRS and these two proteins have been shown to interact in vitro using GST pull-down assays. Pull-down assays using truncated constructs have also revealed that residues important for homodimerization of Gag and LysRS are critical for the Gag/LysRS interaction. In this work, we report further in vitro characterization of the interaction between HIV Gag and human LysRS using affinity pull-down assays, fluorescence anisotropy measurements, and gel chromatography. An equilibrium binding constant of 310 ± 80 nM was measured for the Gag/LysRS interaction. We also show that capsid alone binds to LysRS with a similar affinity as full-length Gag. In addition, a truncated form of LysRS containing only the catalytic domain binds to capsid with a similar affinity as the full-length synthetase. Point mutations that disrupt the homodimerization of LysRS and Gag in vitro, do not affect their interaction. Taken together, these results suggest that dimerization of each protein per se is not required for the interaction, but that a similar, although probably not identical, interface may be used for the hetero-protein interaction. Gel chromatography studies also support the formation of a Gag/LysRS heterodimer. Current efforts are aimed at further characterization of the protein-protein interaction interface via NMR spectroscopy, and at the development of a high throughput assay for screening inhibitors of this novel target.
86. Labuza, Katherine, Peng Zhou, Ted Labuza
How Does the Loss of Moisture Affect the Textural Properties of Marshmallows?
Home Institution: University of Minnesota
Sponsor: Department of Food Science & Nutrition
Abstract: Marshmallows, a favorite of most children, have a general composition of sugar, protein (commonly gelatin), and water (Minifie, 1980). Researchers have suggested that unacceptable marshmallow texture (hardening) is caused by (1) protein-sugar reaction, (2) sugar crystallization, (3) collapse of the marshmallow structure with increasing density, (4) loss of moisture causing reduced plasticity, or (5) a combination of these factors. Jia (2004) suggested that marshmallows become stiff, hard, and unacceptable when their environmental storage condition is <61% relative humidity (RH) but his study did not evaluate whether moisture loss was the direct cause of marshmallow hardening. Therefore, this experiment was conducted to determine this effect. Commercially available marshmallows were stored for ~180 hours at five constant relative humidities and evaluated at several intervals during their storage. Measurements taken during the storage period included (1) weight change, (2) dimensional size (height and diameter) to calculate density, (3) instrumental elasticity texture values, (4) glass transition, (5) Degree of crystallinity by XDR, and (6) textural acceptability on a 1 to 5 point scale. Initially marshmallow at an aw ~0.6 are soft and above the Tg while textural unacceptability occurred during storage at 42% RH which is below the Tg line. This tactile unacceptability corresponded to about a 36% moisture loss without any change in density (dimensional size). In addition, the compression force measurements for the ~0%, 14% and 32% RH storage conditions were similar at the textural unacceptability value. There was no crystallization of sugar during storage for 1 1/2 years. Given these results and other data in the scientific literature, it was concluded that moisture loss reducing the plasticizing effect is the key factor for hardening of marshmallows.

87. McGee, Kari, Erica J. Marti, Kent R. Mann
Bis(acetylacetone) Complexes of Ruthenium and Iridium for Use in Environmental Sensors
Home Institution: University of Minnesota
Sponsor: Department of Chemistry
Abstract: Transition metal complexes have been explored for solid-state applications including solar cells, light-emitting diodes, and environmental sensors. Ruthenium(II) polypyridyl systems are particularly suited for these devices due to their desirable photochemical and redox properties. The focus of this research has been to control the solid-state properties of Ru systems by varying the ligands. Several Ru complexes with one polypyridine ligand and two substituted acetylacetone ligands have been investigated. The single crystal X-ray structures of these Ru complexes have revealed the presence of large voids within the crystalline lattice. Voids such as these can be occupied by smaller guest molecules, which alter the properties of the host molecule and allow the complex to behave as a sensor. Examination of the sensing ability of these complexes will be presented along with the investigation of analogous emissive Ir(III) systems.

88. Peterson, Alicia, Kristopher McNeill
Hydrodefluorination and Hydrodechlorination of Halogenated Ethylenes Using a Phosphino Rhodium Catalyst
Home Institution: University of Minnesota
Sponsor: Department of Chemistry
Abstract: Catalytic dehalogenation of fluorinated and chlorinated ethylenes by (PPh3)3RhCl is described. In the presence or the catalyst, C-F and C-Cl bonds are reduced by triethylsilane (Et3SiH) under ambient reaction conditions. Hydrodefluorination and hydrodechlorination reactions were monitored using a variety of NMR spectroscopic techniques including 1H, 19F and 31P NMR to determine product identity and kinetic parameters. These experiments give evidence for sequential
halogen removal. For example, trichloroethylene yields 1,1-dichloroethylene which then gives rise to vinyl chloride, which degrades into ethylene. The final dechlorination product, ethylene, subsequently dimerizes forming a series of butenes. As the number of halogens on the substrate decreases, the rate of the dehalogenation increases. It has also been shown that this catalytic system has a strong preference for sp2 over sp3 carbon halogen bonds.