

Poster Session 2
10:00 – 11:15 pm
Sunday Nov 8, 2009

P2-1

Presenter: Amelia McNamara, Macalester College

Title: Model and Optimization of Organic Photovoltaic Cells

Advisor: Fadil Santosa, Director of the Institute for Mathematics and its Applications, University of Minnesota

Coauthors: Jordan Seeringz, Yi Zengx

This project focuses on optimizing the organic photovoltaic cell, an important topic in the energy industry which has not been well studied. We are especially interested in the optimization of the two active layers in the solar cell, the PEOPT polymer and the C60 (Fullerene) layer. Using a numerical scheme (the finite difference method) we solve the diffusion equation of excitons in the one dimensional case, and implement it with two different accepted models of energy dissipation. This allows us to compare the exciton density and u_x across the heterojunction between active layers which each model produces. Using our preferred model, we optimize the layer thicknesses of the two active layers, PEOPT and C60 and determined them to be 12 nm and 40 nm respectively. We extend our analysis to a two-dimensional case including a curved boundary at the donor-acceptor heterojunction, using the simpler model, and study the effect of such a boundary on the conversion efficiency.

P2-2

Presenter: Stephanie Lee, Macalester College

Title: High resolution spectroscopy of TaD and TaH

Advisor: Tom Varberg, Department of Chemistry, Macalester College

Coauthor: Casey Christopher

We have studied the 633 nm and 632 nm bands of tantalum hydride (TaH) and tantalum deuteride (TaD), respectively, by laser excitation spectroscopy. In each case the gas-phase molecules were prepared in a hollow tantalum cathode discharge source. In order to resolve the hyperfine structure arising from the tantalum and hydrogen nuclei, we recorded sub-Doppler spectra using the method of intermodulated fluorescence (IMF) spectroscopy. The appropriate Hamiltonian was used to complete a least-squares fit of the rotational and hyperfine data, resulting in an accurate set of molecular constants for TaH and TaD.

P2-3

Presenter: Spencer Bonnerup, Gustavus Adolphus College

Title: Photolysis of Imazethapyr on the Cuticle Wax of Corn (*Hyb jubilee*) and Soybeans (*Soya hispida*)

Advisor: Amanda Neinow, Department of Chemistry, Gustavus Adolphus College

Coauthors: Olson, Megan

Imazethapyr is an herbicide used commonly in Minnesota to control weeds in agricultural fields. The photolysis of imazethapyr yields products that haven't been studied extensively. To date, photolysis of imazethapyr has been studied only in water samples. However, the photolysis products that form likely depend on the matrix in which the herbicide is located. Thus, the purpose of this research is to develop a method that can detect changes in concentration of imazethapyr sorbed into/onto the cuticle wax of corn and soybeans (a more likely environmental matrix for this herbicide). In particular, the concentration of imazethapyr will be monitored as a function of irradiation time. The initial tests with the method will inform us whether the kinetics of the reaction is the same in water and plant matrices. After the method is developed, it will be used to detect, isolate, and identify the photolysis products. Ultimately, we hope to determine what effect the photolysis products have on the water and ecosystem that they enter.

P2-4

Presenters: Kirsten Indrelie and Jacob Wessels, Luther College

Title: The Role of Porphyrin Structure in Porphyrin-HSA Binding

Advisor: Olga Rinco, Department of Chemistry, Luther College

The efficacy of porphyrin binding to human serum albumin (HSA) is critical to clinical use in photodynamic therapy (PDT). Several porphyrins were utilized to measure the effect of porphyrin structure on its binding to HSA. Two categories of porphyrins were utilized: porphyrins with a hydrophobic and hydrophilic side: Protoporphyrin IX (PPIX), Protoporphyrin IX dimethylester (PPIXDE), and Chlorin e_6 (Ce6) and porphyrins with hydrophilic substituents on both sides: Hematoporphyrin IX (Hme), Hematoporphyrin IX dimethylester (HmeDE), and Deuteroporphyrin IX dimethylester (DPIXEG). The following methods were used for the analysis: Stern-Volmer quenching, fluorescence lifetimes, anisotropy, fluorescence binding, and homogeneous studies. The results indicate that PPIX, PPIXDE, and Ce6 bind to HSA efficiently, evidence that porphyrins bind strongly to HSA if they have a hydrophobic and hydrophilic side. Hme is thought to bind to HSA but likely to a lesser degree than the aforementioned three porphyrins. HmeDE and DPIXEG seem not to bind to HSA probably due to the lack of hydrophobic substituents.

P2-5

Presenter: Hannah Erickson, Macalester College

Title: 1,2,3-TRIAZOLE-DERIVED Pd(II)DICHLORO COMPLEXES

Advisor: Ronald Brisbois, Department of Chemistry, Macalester College

Huisgen's foundational investigations of the [3+2] dipolar cycloaddition between alkynes and azides (Huisgen *Pure Appl. Chem.* **1989**, *61*, 613) have been complemented and extended tremendously by the regiocontrolled, Cu^I-catalyzed modification reported in 2002 (Sharpless *et. al. Angew. Chem., Int. Ed.* **2002**, *41*, 2596; Meldal *et. al. J. Org. Chem.* **2002**, *67*, 3057). Due to simplicity, broad scope of application, high yields, and atom economy, Cu^I-catalyzed alkyne/azide "click chemistry" has impacted positively in all subdisciplines of chemistry that depend upon synthesis. The ability of the triazoles resulting from this reaction to subsequently act as ligands and complex with transition metals has previously been studied (Matano *et. al. Org. Let.* **2009**, *11*, 3338). We are intrigued by this research and sought to explore the potential of a variety of triazoles to act as ligands in a Pd complex.

P2-6

Presenter: Michael Mandel, Beloit College

Title: Circular Hydraulic Jump

Advisor: Paul Stanley, Department of Physics and Astronomy, Beloit College

The circular hydraulic jump is a common yet curious phenomenon characterized by the decompression of water in a radial pattern, as occurs when a falling stream of water encounters an obstacle. The circular hydraulic jump has been explored in application to several fields. In materials science, femtoliter scale "cups" have been designed and built from initially fluid metals such as gold and copper.(1) In the field of astronomy it is thought by some that the white hole, the supposed opposite end of a black hole, could operate on principles similar to the circular hydraulic jump.(2) It will surely be the case in the coming years that, as scientists continue to investigate circular hydraulic jump, many useful applications for this unusual phenomenon will be discovered. This research project has focused primarily on three topics in both experimental and theoretical aspects. The first is a theoretical investigation of the relationship of flow rate in the incident water and the radius of the jump created, followed by an experimental verification. The second topic is theoretical work done on patterns observed in the jump under certain conditions. The third topic is an investigation of the double jump, two successive sustained jumps, seen when a surfactant was added to the apparatus.

Currently, much of the research done in circular hydraulic jump is done with expensive and complicated equipment and techniques, such as laser dopler absorption spectroscopy or robotic apertures for the detection of liquid surface conduction. A side aim of this research is to demonstrate that much can be done in investigating the circular hydraulic jump without the aid of such equipment.

- (1) Mathur et. al., Phys. Rev. Lett. 98, 164502 (2007)
- (2) G.E. Volovik, JETP letters, volume 82, issue 10, pages 624-627, 2005

P2-7

Presenter: Jacki Werner, St. Olaf College

Title: Basal Reflectivity and Ice Velocity in the East Antarctic Ice Sheet

Advisor: Robert Jacobel, Department of Physics, St. Olaf College

Coauthors: Lapo, Karl and Olson, Jessica

The Center for Geophysical Studies in Ice and Climate (CEGSIC) at St. Olaf recently participated in the United States portion of the International Trans-Antarctic Scientific Expedition (US-ITASE), an international effort dedicated to understanding climate change and ice sheet stability in Antarctica. CEGSIC constructed a ground-based radar system to gather information about flow properties of the East Antarctic Ice Sheet by measuring the strength of radio echoes returned from the ice-bed interface. The presence of water at the basal boundary greatly enhances the reflectivity of radar signals, and water provides lubrication that can increase ice flow speeds. Radar data were acquired continuously along the 1700 Km US-ITASE traverse as a part of the International Polar Year and have been used to calculate values of relative basal reflectivity (a proxy for water content) from Taylor Dome, near the Antarctic coast, to South Pole Station in the interior. We then compared our results on basal conditions with ice surface velocities measured by satellite and found a strong correspondence between ice speed and basal reflectivity. While this result is not surprising, this is the first time remote sensing results have shown thawed bed conditions in association with high ice velocity outside a few specialized locations with subglacial lakes. This demonstrates that basal melting is widespread in East Antarctica and underscores the importance of water in controlling the motion of the largest ice sheet on earth.

P2-8

Presenters: Karl Lapo and Jessica Olson, St. Olaf College

Title: Basal Reflectivity beneath the East Antarctic Ice Sheet

Advisor: Robert Jacobel, Department of Physics, St. Olaf College

Coauthors: Jeff Stamp, Jacki Werner and Bern Youngblood

At the Center for Geophysical Studies of Ice and Climate (CEGSIC) at St. Olaf College we have constructed a ground-based radar system to gather information about flow properties of the East Antarctic Ice Sheet by measuring the strength of radio echoes returned from the ice-bed interface. Radar data were acquired continuously along the 1700 Km US-ITASE traverse as a part of the International Polar Year and have been used to calculate values of relative basal reflectivity from Taylor Dome, near the Antarctic coast, to South Pole Station in the interior. The amplitude of basal radar returns is determined primarily by water content at the ice-bed interface and wetness at the bed has been shown to greatly affect the speed of ice flow. In order to obtain a true picture of the basal conditions, we first needed to explore methods to correct the returned radar power for losses in the ice which depend on temperature and impurities and can vary from place to place. Our work shows that several different methods gave approximately the same result for attenuation and refinements in one of these have enabled us to produce a correction function that varies smoothly along the length of the traverse. The results show that the derived basal reflectivities can be fit by a double Gaussian model where the individual curves representing the wet and dry populations of basal echoes are separated by several standard deviations, providing a powerful tool for discerning wet from dry ice-bedrock interfaces.

P2-9

Presenter: Brad Frye, Carthage College

Title: Computational Fluid Dynamics Model of an Air Cyclone in Microgravity

Advisor: Kevin Crosby, Department of Physics, Carthage College

Air cyclones are a promising technology for first stage air filtration in future lunar habitats where lunar dust mitigation is a mission critical concern. Our experimental work with cyclones in microgravity as part of NASA's System Engineering Educational Discovery (SEED) program suggested that gravity does not play a significant

role in the operation of the air cyclone. If correct, this result paves the way for further study of cyclone filtration in microgravity.

Building on the SEED research, in this project we develop a computational fluid dynamics (CFD) model of the cyclone used in the experimental work in reduced gravity to address the following questions:

- How does collection efficiency scale with gravity?
- What are the dynamical forces acting on particles in an air cyclone?
- Can we understand our results in terms of these dynamical forces?

P2-10

Presenter: Gregory Hubers, Hope College

Title: Load-Induced Debonding of FRP Composites Applied to Reinforced Concrete

Advisor: Jeff Brown, Department of Engineering, Hope College

Coauthor: Joel Blok

Fiber-reinforced polymer (FRP) composites are widely used as a method of external reinforcement for damaged concrete structures. While composites have been demonstrated to significantly increase the strength of a damaged structural element, less is known about the long-term durability of FRP systems. This research investigated the effects of fatigue loading on FRP systems and utilized thermal imaging as a means for evaluating bond between the FRP composite and the concrete substrate. Twelve small-scale reinforced concrete (RC) beams were constructed and FRP was applied to the tension faces to simulate flexural strengthening. Cyclic loading was applied at various levels of the strengthened beam's monotonic load capacity and periodic infrared thermography inspections were performed. The condition of the bond was quantified through statistical analysis of the resulting phase images obtained at each load reversal increment. The relationship between bond condition and overall system performance was then investigated using a combination of deflection and strain data.

This material is based upon work supported by the National Science Foundation under NSF-REU Grant No. PHY-0452206, the Hope College Engineering Department, the Michigan Space Grant Consortium, the Florida Department of Transportation, and the University of Florida.

P2-11

Presenter: Hans Most, Macalester College

Title: M81 Group Dwarf Irregular Galaxy DDO 165. Connecting Recent Star Formation with ISM Structures and Kinematics

Advisor: John Cannon, Physics Department, Macalester College

Coauthors: Cook, D., Dolphin, A. E., Kennicutt, R. C., Jr., Lee, J., Skillman, E. D., Walter, F., Weisz, D. R.

We examine the process of "feedback" in the interstellar medium (ISM) of the M81 group dwarf irregular galaxy DDO 165. *VLA* HI imaging reveals a wealth of structure in the ISM, including a large central hole (~2.2 x 1.1 kpc), numerous smaller holes and shells, high-velocity gas throughout the disk, and a kinematically distinct northern region (Most et al. 2009). We extract spatially resolved recent star formation histories from *HST* imaging of this system, with particular focus on the regions showing these "feedback" signatures. Using improved estimates of the mass surface density, the disk scale height, and the HI volume density, we calculate that the energetics of these star formation events (some of which are temporally extended) are sufficient to create the observed structures in the ISM of DDO 165. As recently found for other systems, "feedback" plays an important role in the evolution of low-mass galaxies.

P2-12

Presenter: Eric Lauzon, Hope College

Title: The Preparation of Highly Conjugated Thiophenes for Use in Device Applications

Advisor: Elizabeth Sanford, Department of Chemistry, Hope College

Co-authors: Ketchum, Alex; Jeon, Ji-Min; Topp, Kaleb, Sanford, Elizabeth

Our work in the synthesis of new materials for device applications focuses on substituted poly(arylenevinylenes). Poly(arylenevinylenes) are a class of semiconducting polymers that can emit light through electroluminescence. In electroluminescence, light is emitted from a substance when it is excited by an electric field.

Poly(arylenevinylenes) are now used as components of organic light emitting diodes (OLED's) and light emitting electrochemical cells (LEC's). These technologies are used for molecular electronics including cutting edge displays. This poster describes the preparation of conjugated thiophene derivatives. The synthetic plan includes making core and end cap molecules that can be connected via carbon-carbon double bonds formed using a Wittig reaction. This methodology allows us to synthesize a family of materials, including both small molecules and polymers, for device testing.

P2-13

Presenter: Laura Macke, Macalester College

Title: Synthesis of Chemical Inducers of Dimerization (CIDs) for Use in the Yeast Three-Hybrid Assay

Advisors: Rebecca Hoye, Department of Chemistry and Paul Overvoorde, Department of Biology, Macalester College

Auxins are a class of plant hormones that control developmental events including cell division and elongation, tissue differentiation, root development, embryo polarization, tropic response to light and gravity, and apical dominance, but the biological pathways in which auxins control these processes are not well known. In high-throughput screens, various labs have identified a series of small molecules as potent inhibitors of auxin, which show consistent inhibition under a series of assays. At Macalester, we are working to develop the yeast 3-hybrid system (Y3H) as a tool screen out the protein(s) *in vitro* from the proteome of *Arabidopsis thaliana* interact with such small molecule auxin proxies. This involves working to expand the versatility of the Y3H system; the method has been used extensively for screening protein-RNA interactions but only recently has been used to extend utility to small molecule screening. More specifically, this project focuses on the organic synthesis of chemical inducers of dimerization (CIDs) essential the system.

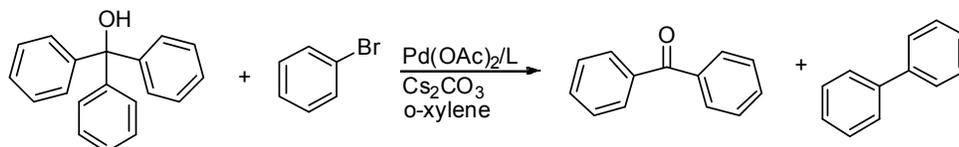
P2-14

Presenter: Valerie J. Winton, Hope College

Title: Investigation of Palladium-catalyzed C-C bond activation in tertiary alcohols

Advisor: Jeffrey B. Johnson, Department of Chemistry, Hope College

The activation and functionalization of carbon-carbon single bonds presents a significant challenge due to their thermodynamic and kinetic stability. Miura et al. have demonstrated the cleavage of carbon-carbon single bonds followed by functionalization through coupling with an aryl halide (*Journal of Organic Chemistry*, **2004**, *69*, 6942).



Carbon-carbon bond activation is proposed to occur via Pd-catalyzed β -aryl elimination of an aryl group from a tertiary alcohol. A series of differentially substituted tertiary alcohols was prepared and tested for relative reactivity in this transformation. Reactions examined the relative propensity to cleave groups containing differing hybridization, sterics, and electronic properties. Preliminary results suggest that steric effects dominate over electronics when comparing relative reaction rates. Further investigation promises to give insight into the process of selective carbon-carbon bond activation and the development of synthetic methods.

P2-15

Presenter: Allison Kennedy, Macalester College

Title: Rate of Capture of Dark Matter Particles

Advisor: Tonnis ter Veldhuis, Department of Physics, Macalester College

Nonbaryonic dark matter, specifically weakly interacting massive particles (WIMPs) can become bound within the Solar System due to three-body interactions with Jupiter and the Sun. Numerical simulation and analytical expressions were used to determine an average cross section for which a particle will become bound. This cross section of bound particles can be used as a step towards understanding the current dearth of WIMP detection by finding the WIMPs' rate of capture.

P2-16

Presenter: Sam Alvarado, Augustana College

Title: Synthesis of chelating phosphine-functionalized *n*-heterocyclic carbene ruthenium complexes

Advisor: Greg Domski, Department of Chemistry, Augustana College

We report the synthesis of novel phosphine-functionalized *n*-heterocyclic carbene ruthenium complexes. The synthesis was completed using air- and moisture-sensitive techniques, and chemical structures were verified by nuclear magnetic resonance (NMR) spectroscopy. Two of the complexes are binuclear pincer complexes, with the two metal centers linked by a phenyl group. These complexes will be used as catalysts for catalytic transfer hydrogenation reactions, where the binuclear design may increase the reaction rate as the result of a cooperational electrophilic effect.

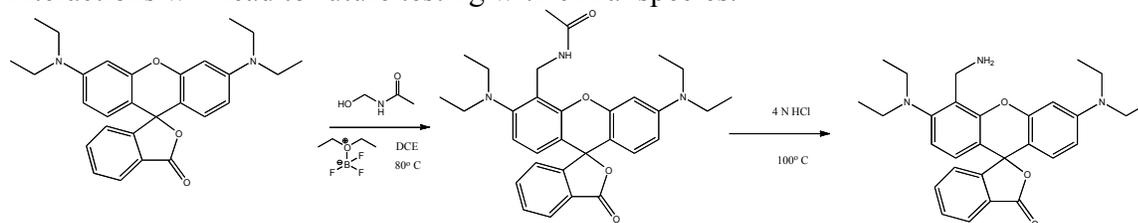
P2-17

Presenter: Mike Maher, Carthage College

Title: Formation of a Chiral Xanthene Dye and its Potential as an Enantioselective Sensor

Advisor: Clifton James Stephenson, Chemistry Department, Carthage College

Chiral enantiomers have different functions in chiral environments such as biological systems. Thus, chiral sensing is important and has many large applications in medical and pharmaceutical industries. Rhodamine B is a well-known dye that has a highly sensitive off/on mechanism, which allows it to exist in a closed, colorless lactone form and in an open, pink carboxylic acid form. It has previously been shown to have diastereomeric sensing abilities but its use as an enantioselective sensor has been largely unexplored. Rhodamine B is achiral, and in order to detect a chiral species, a chiral agent is needed. Via a Mannich reaction, we have synthesized a chiral rhodamine B derivative by adding an amidomethyl group to the 4-position. The closed form has a chiral center at C9, and the open form exhibits atropisomeric chirality, which allows our synthesized dye to be chiral in both forms. Further deprotection of the amide has left a tunable amine that can be modified for various sensing applications including potential enantiomeric detection. We have hypothesized that the aminomethyl group can support supramolecular bonding so that the off/on mechanism of the dye is not solely dependent on the pH of a solution. We are currently testing the chiral dye with achiral species to detect supramolecular interactions by creating titration curves with various acids and comparing them to titration curves of rhodamine B and with Rhodamine B and 1 equivalent of triethylamine. Confirmation of supramolecular interactions will lead to future testing with chiral species.



P2-18**Presenters:** Menyi Cao and Leah Chibwe, Colorado College**Title:** pH Selective PEBBLE Nano-Sensors for the Exploration of the Mechanisms of Bacteria/Eukaryotic Cell Interaction**Advisor:** Murphy Brasuel, Department of Chemistry, Colorado College**Coauthors:** Margaux Miller and Phoebe Lostroh

PEBBLEs (probes encapsulated by biologically localized embedding) are nanoparticle optodes used in the analysis of intracellular processes. In this project, we fabricated Oregon Green Q Dot PEBBLEs and used them to monitor the endosomal pH changes in the slime mould *Dictyostelium discoideum* that occur during chemotaxis stimulated by the cAMP (3'-5'-cyclic adenosine monophosphate). PEBBLEs were optimized for the pH range of 3 to 6, as this was the ideal range to monitor pH during cAMP release. It is known that some bacteria interfere with the normal function of eukaryotic ion channels. Changes in pH were measured with and without exposure to viable Salmonella to determine if Salmonella significantly interferes with the endosomal proton pumps.

P2-19**Presenter:** Tim Nagi, Hope College**Title:** Radiodating Streambed Sediment**Advisor:** Paul DeYoung, Department of Physics, Hope College**Coauthor:** Peaslee, Graham

The isotopic makeup of samples of streambed sediment collected in Wisconsin, varying in their original location, collection date, and depth, was analyzed using gamma-ray spectroscopy. The samples being analyzed were measured with high-purity germanium detectors in low background counting facilities. The goal of this project was to determine the ratio of the amount of sediment coming from surface sources (run-off) to the amount coming from underground sources (such as bank erosion). This was to be done by comparing the number of ^7Be atoms present at the time of sample collection to the number of supported ^{210}Pb atoms present at the time of sample collection. As part of finding these values, corrections are made for detector efficiency, attenuation, background radiation, elapsed time since collection, branching ratios and the presence of unsupported ^{210}Pb . Data collection and analysis is ongoing.

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