

# Undergraduate Research Symposium May 17, 2013 Mary Gates Hall

## Online Proceedings

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### POSTER SESSION 2

Balcony, Easel 119

12:45 PM to 2:15 PM

#### **Intracellular Trafficking of Toll-Like Receptor 9 (TLR9) Ligands**

*Melanie Jean Coyne, Junior, Chemical Engineering*

*Mentor: Hong Shen, Chemical Engineering*

*Mentor: Helen Chen, chemical engineering*

With the proliferation of autoimmune diseases and cancer it is of increasing importance to discover new ways to utilize nanoparticles as carriers for the delivery of therapeutic agents. To achieve this aim, the trafficking of nanoparticles within dendritic cells must be better understood. When cells uptake foreign material, an innate immune response is triggered through the activation of pattern recognition receptors such as toll-like receptor 9 (TLR9). TLR9 ligands follow one of two pathways when introduced into a cell - one trafficking through early endosomes, the other through late endosomes. This research analyzes the intracellular trafficking of TLR9 ligands through the image analysis of dendritic cells. Using an imaging software, ImageJ, it is possible to plot the relative intensities of fluorescently labeled polystyrene nanoparticles coated with TLR9 ligands CpG 2216 or CpG 1826 as well as late endosomal markers Rab7 or LAMP2. By analyzing the co-localization of these intensity profiles, it can be determined if there is recruitment of the late endosomal marker to the endocytic vesicle of the nanoparticle. The recruitment analysis confirms which intracellular pathway is taken by these nanoparticles. A statistical analysis of a large sample size of nanoparticles will be performed. This research will shed light on how nanoparticles can be used as drug carriers by supplying critical information about the intracellular fate of nanoparticles coated with TLR9 ligands.

### POSTER SESSION 2

Balcony, Easel 114

12:45 PM to 2:15 PM

#### **Surface Energy of Graphene Determined by Intrinsic Friction Microscopy**

*Brad Anthony (Brad) Krajina, Senior, Chemical Engineering*

*Mentor: Rene Overney, Chemical Engineering*

The building material of graphite, a two-dimensional material of single atomic width, possesses remarkable electrical, thermal, and mechanical properties. Due to its exceptional properties, research in graphene is actively pursued for applications such as electronics, solar-cell technology, and sensing materials. A critical question is how graphene may be combined with other materials (e.g. polymers) to form unique hybrid materials with novel functional properties. Thereby of great importance is the surface energy of single layer to multilayer graphene. Following this, we are exploring the surface energy of few-atomic-layer graphene as a function of the number of atomic layers present. To this end, we prepared few-atomic-layer graphene materials through a simple technique involving cleaving bulk graphite with tape and transferring the cleaved material to a suitable substrate. Such materials can be readily identified under optical microscope and further characterized by atomic force microscopy (AFM) — a scanning probe technology that provides nano-scale information of materials by probing the surface with a tip of atomic-scale width. After initial topographical identification, the surface energy and friction values of graphene were determined using Intrinsic Friction Analysis (IFA). This technique analyzes energetically the thermally active adhesive modes of interactions between the probing tip and the graphene surface. With knowledge of the surface energy of the probe, the sample surface energy can be deconvoluted from the energy information. We have employed this technique on few-layer graphene materials of multiple thicknesses. Our results reveal an energy-friction iso-line that is representative for planar systems with thermally active internal modes that are restricted to vibrational modes. While we observe for decreasing thickness increasing friction forces, the surface energies are decreasing from bulk graphite of 63 mJ/m<sup>2</sup> to graphene of 48 mJ/m<sup>2</sup>.

### POSTER SESSION 2

Balcony, Easel 117

12:45 PM to 2:15 PM

#### **Molecular Simulations of Single-Chain Organic Photovoltaic Polymers in Various Environments**

*Melissa Gile, Senior, Chemical Engineering, Mathematics*

*Mentor: Jim Pfaendtner, Chemical Engineering*

The purpose of this study is to determine fundamental structure-solvent-property relationships in organic photo-

voltaic polymers (OPV's), with the overarching goal of increasing the efficiency of OPV's. A typical silicon-based photovoltaic plant outputs approximately 88,000 m<sup>2</sup> of photovoltaic cells each year- about the size of 16 football fields. On the other hand, an organic photovoltaic printer will produce the same area in up to 10 hours. OPV's are incredibly fast, cheap, and easy to produce relative to their inorganic counterparts, but fall short within the realm of efficiency; the 10% efficiency of OPV's can hardly rival the ~40% efficiency of inorganic photovoltaic technology. If the efficiency of OPV's can be increased, this will have a drastic impact on the competitive marketability of photovoltaic technology. This project aims at developing computational models to study the role of solvents in the self-assembly of polythiophenes during the printing process. These models are generated in GROMACS, a program that uses classical forces such as Coulombic or Van Der Waals forces, to predict how molecules will behave with time. This is problematic, however, for OPV's, as key interactions occur on the quantum level, and new classical force fields, which are computationally very efficient, need to be altered in order to accurately calculate these interactions. A force field is being developed and refined by comparing our computational results with experimental results from the Pozzo Research Group within the Department of Chemical Engineering. Once these results are reliably consistent with each other, we can begin running simulations and gathering data regarding how OPV's assemble in various environments. In particular, this poster explains a systematic methodology I have developed to use the GROMACS program to perform molecular dynamics (MD) simulations of single chain OPV's in various solvents as well as simulations of bulk OPV's in the melt state.

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## SESSION 2G

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### MICRO- AND NANO-MATERIALS IN ACTION

*Session Moderator: John Berg, Chemical Engineering*  
**242 MGH**

*3:45 PM to 5:15 PM*

\* Note: Titles in order of presentation.

#### **Rheology of Dense Calcium Carbonate Dispersions**

*Aaron Johnson, Senior, Chemical Engineering, Bioresource Science and Engineering*

*Mary Gates Scholar*

*Mentor: Kevin Hodgson, Bioresource Science & Engr.*

*Mentor: John Berg, Chemical Engineering*

From the fillers that give body to ordinary paper to the antacids that relieve indigestion, calcium carbonate suspensions play an important role in our day-to-day lives. It is often desirable to work with slurries that contain the high-

est possible fraction of solids. The goal of this research has been to investigate ways to improve the flow of high solids dispersions of calcium carbonate through the use of rheology modifiers. These are chemicals which, when added in small amounts, allow the dense slurries to flow as easily and smoothly as possible. Improving flow characteristics of high solids dispersions has a huge potential for reducing the amount of energy needed for various processes, such as pumping, coating and de-watering. One very promising modifier has been found to be sodium polyacrylate. Both traditional and new products, like nano-sized calcium carbonate particles, have shown significant improvements using this modifier. In this research, the rheological properties such as the viscosity function and the yield stress are determined as functions of additive amount, volume fraction of solids, and pH of the aqueous dispersion medium. All of these have been shown to important parameters in achieving optimum performance.

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## SESSION 2G

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### MICRO- AND NANO-MATERIALS IN ACTION

*Session Moderator: John Berg, Chemical Engineering*  
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*3:45 PM to 5:15 PM*

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#### **The Charging of Carbon Black Pigments in Apolar Media**

*Max Kaganyuk, Senior, Chemical Engineering*

*Mentor: John Berg, Chemical Engineering*

*Mentor: Matthew Gacek, Chemical Engineering*

Electrophoretic displays, such as the Kindle®, currently employ electrostatic effects in apolar media to create a paper-like display. In an electrophoretic display, images are comprised of black and white pixels generated by applying an electric field to reposition charged pigment particles. The optimization of this technology is limited due to the incomplete knowledge of the mechanism(s) by which particles acquire charge in these systems. My project explores the charging behavior of carbon black pigments dispersed in apolar media. Previous studies of mineral oxide particles have provided support for the theory of an acid-base charging mechanism for particles dispersed in apolar media with various charge stabilizing surfactants. My current work looks at the possible extension of the theory of an acid-base charging mechanism to carbon black pigments in apolar systems. I have investigated the charging behavior of four different carbon black pigments by measuring the electrophoretic mobility of each pigment dispersed in solutions of heptane, and a charge stabilizing surfactant at varying weight percentages. Three surfac-

tants were used for charge stabilization: Aerosol OT, SPAN 80 and OLOA 11000. Aerosol OT is a neutral surfactant in water, whereas SPAN 80 is acidic and OLOA 11000 is basic. The surface characteristics of each carbon black pigment were studied by Inverse Gas Chromatography (IGC) and X-ray Photoelectron Spectroscopy (XPS). The preliminary findings of my investigation show the sign of the charge for the carbon black pigments to be dependent on the charge stabilizing surfactant used.

### POSTER SESSION 3

Commons East, Easel 56

2:30 PM to 4:00 PM

#### Automated Protein Extraction and Analysis

Arrika LaSalle, Junior, Chemical Engineering, Biological Engineering, Montana State University

Howard Hughes Scholar, McNair Scholar

Mentor: Ed Dratz, Montana State University

Proteins usually contain many post-translational modifications in response to biological or environmental stimuli, which affect their activity, cellular localization, or protein partners. Mass spectral analysis is able to identify proteins and characterize post-translational modifications, but target proteins must first be isolated and extracted. Separation by two-dimensional polyacrylamide gel electrophoresis (2D-PAGE) is a powerful protein and protein isoform separation technique. An average of 40 protein isoforms from each eukaryotic gene may be visualized with fluorescent labeling, some of which are potential disease markers. They are often present in low abundance, making it challenging to recover them for mass spectral analysis. Current methods suffer from sample losses, contamination, and long, manual processes. Our protein extraction system will avoid these problems using automated electrokinetic extraction with in-line protein digestion and mass spectral analysis. Nanogram levels of fluorescently-labeled Bio-Rad proteins are separated by sodium dodecyl sulfate polyacrylamide gel electrophoresis. Target proteins are isolated and rapidly eluted directly from 2-D gel into our micro-capillary system using a high-voltage electric field. Proteins are digested in a microfluidic bioreactor, and peptides are deposited onto a trap column of a Chip LC and resolved for mass spectral analysis. The bioreactor and trap column will eventually be coupled with the extraction system using automated switching. Our micro-capillary system is high-throughput (~90% recovery of proteins), and 1-2 orders of magnitude faster than traditional electroelution processes. The principles of electrophoretic migration may be applied not only to separation of proteins onto gradient gels, but also to routine extraction and resolution of low-nanogram protein quantities directly from 2-D gel. Automation will decrease contamination by limiting the manual portion of the process to loading the gel onto the device, and may greatly

improve recovery of low-abundance proteins.

### POSTER SESSION 3

MGH 241, Easel 134

2:30 PM to 4:00 PM

#### Modeling $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3 - \delta$

—  $\delta$  (LSCF) with Nonlinear Electrochemical Impedance Spectroscopy

Stephanie Hare, Senior, Chemical Engineering

Mentor: Stuart Adler, Chemical Engineering

Solid Oxide Fuel Cells (SOFCs) are some of the most efficient fuel cells available, but their widespread use is limited by the high operating temperatures they require. New materials and characterization techniques are being investigated to reveal the properties of SOFC electrode materials to make them more feasible commercially. Electrochemical Impedance Spectroscopy (EIS) is a commonly-used analysis tool for the characterization of SOFCs. The technique measures the transient response of a SOFC electrode material by passing a sine wave current of specified frequency through the cell, and measuring the amplitude and phase of the cell voltage. When doing simple EIS, only the first harmonic of the response is analyzed, with higher order harmonics ignored. This is done using a linear approximation to describe the mass transfer and kinetics of the material, where these properties are non-linear when rigorously described. Recently workers have begun to explore the use of Nonlinear EIS (NLEIS). By including higher order harmonics, NLEIS seeks to glean significantly more information about the properties of fuel cell electrodes, allowing SOFCs to be more accurately modeled and their efficiency optimized. The goal of my project is to extend existing electrode response models to  $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$  (LSCF), a mixed-conducting cathode material of commercial interest. A successful model would have important implications in the alternative energy industry, and allow SOFCs to be a much more viable energy option in the future. My role in this research is to create SOFCs with LSCF as a cathode using simple ceramic firing and "screen printing" techniques to apply a thin electrode layer, and then run NLEIS in order to collect electrochemical data on the electrode. Once this is accomplished, it is expected that LSCF will behave as a combination of the previously studied materials LSC ( $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_3 - \delta$ ) and LSF ( $\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_3 - \delta$ ), however more testing must still be completed.

### POSTER SESSION 4

Commons East, Easel 58

4:15 PM to 5:45 PM

### **Mn:CuO Nanowires in Spintronic Devices**

*Arin Greenwood, Senior, Chemical Engineering*

*Amgen Scholar; NASA Space Grant Scholar*

*Mentor: Alec Pakhomov, Molecular & NanoTech User Facility (NTUF)*

*Mentor: Karl F. Bohringer, Electrical Engineering*

*Mentor: Paul Wallace, NanoTech User Facility*

Motivated by current interest in one-dimensional materials for their ideality and potential in the next generation of electronics, a device consisting of a microscopic four-point probe was developed with electron beam lithography (EBL) to investigate the conductance and resistivity of manganese-doped copper oxide (Mn:CuO) nanowires. Mn:CuO nanowires were chosen because they are known to be ferromagnetic and conductive below a critical temperature of 80K, while maintaining semiconductor properties and low resistance at room temperature. Nanowire samples were obtained from the Yang Group in Nanjing, China, and were deposited with ethanol onto silicon dioxide wafers to obtain a rough monolayer for easy isolation of individual nanowires. A pattern consisting of four contact lines was created with DesignCAD and conditions were optimized to obtain an adequate dose (charge/unit area). A subsequent process of precise alignment was performed to ensure complete overlap between the nanowire and pattern on a nanometer scale. With accurate alignment, the pattern was then etched onto a single nanowire, developed, and coated in a 50 nm thin film of gold to enable conduction between the nanowire and the four-point pattern. From this point, the current and voltage can be measured through the nanowire macroscopically. Consequently, the anisotropic resistivity of the material as well as gate voltage effects can be studied to verify the material's applicability to future spintronics devices such as field-effect transistors.