



**ILLINOIS SCHOLARS
UNDERGRADUATE RESEARCH
POSTER EXPO**

APRIL 18, 2018 @ ILLINI UNION
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College of Engineering

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ISUR Scholars 2017-2018



Muneeb Ansari
Chem



Amber Boyce
ChemE



Patrick Burke
MechE



Hannah Chait
ChemE



Denzel Cruz
BioE



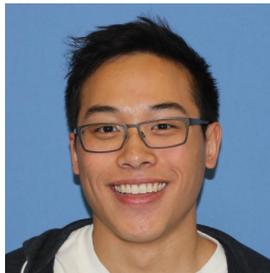
Emily Foley
MatSE



Nupoor Gandhi
CS



Marisa Gnadt
MechE



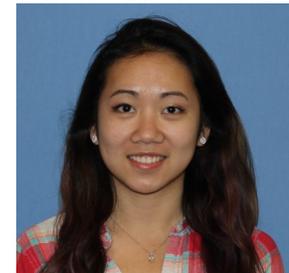
Than Huynh
BioE



Nicole Jugovich
ChemE



Andrew Kuznetsov
CS



Patricia Li
ChemE



Cynthia Liu
BioE



Jacob Maher
MatSE

Illinois Scholars Undergraduate Research (ISUR) Program

The College of Engineering Illinois Scholars Undergraduate Research (ISUR) program is for students looking for a structured two-semester research experience with a research learning community. The program facilitates opportunities to expand students' academic experience beyond the walls of the traditional classroom. Through the learning-by-apprenticeship model, students become familiar with research methodologies, develop their research skills, are exposed to what graduate school entails, and gain experience needed for graduate school acceptance or research in industry.

The goals of the program are to

- Introduce students to university research,
- Engage students in the College of Engineering and the research community, particularly through the learning-by-apprenticeship model; and
- Expose students to engineering research with focus on agricultural biotechnology, chemical solutions, electronics, semiconductor, information technology, energy, and other research.

Students in the program work closely with graduate student/postdoc mentors and faculty sponsors on research projects throughout the fall and spring semesters.

As part of the research learning community, new ISUR scholars enroll in a semester-long research apprenticeship class (ENG 199 UGR) in addition to the time spent on research. This course is designed to complement their research experience. Students learn about the basic elements of research, including the logical framework of research, forms of technical communication, and training of researchers. Students also gain an understanding of the research pursued at the university and the skills needed by researchers. A mixture of lectures, panel discussions, guest speakers, and interactive class discussions are used to cover the topics.

ISUR Contact Information:

Natasha Mamaril, PhD
Program Director
Coordinator of Undergraduate Research
nmamaril@illinois.edu
217.244.9995

ISUR General Email
isurprogram@illinois.edu
<http://isur.engineering.illinois.edu/>

College of Engineering
201 Engineering Hall
1308 W. Green Street, MC-272
Urbana, IL 61801

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A Novel Approach to Homogenous Catalysis using Encapsulation for Improved Efficiency

Muneeb Ansari¹, Dr. Damien Guironnet², Dr. José Andino-Martinez³

Research Sponsor: Shell Corporation

1. Undergraduate Scholar, School of Chemical Science
2. Faculty Advisor, Department of Chemical and Biomolecular Engineering
3. Faculty Advisor, School of Chemical Science

Homogenous catalysis can in some cases be negatively impacted if metal center active sites interact with one another. In order to prevent this situation, this study seeks to encapsulate individual catalysts within an elastomer made from hydrosilylation. First, the efficiency of the hydrosilylation reaction using different conditions to promote cross-linking densities was determined. Next, the ability for the newly formed gel to retain the encapsulated analyte was studied quantitatively.

Karstedt's Catalyst was used to create the gel by performing hydrosilylation reactions with poly(methylhydrosiloxane) and 2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane in the presence of hexanes. Encapsulation was attempted with PCP-iridium catalysts and later with anthracene to assess the size of the cavities. The ability for the analyte to remain encapsulated was studied by adding hexanes onto the gel. Vigorous shaking of the gel was carried out for a variety of periods. UV-Vis spectra of the supernatant hexanes allowed us to quantify the extraction.

Denser gels encapsulate the analyte more efficiently, but it is not clear how this will impact catalytic activity. Anthracene was not efficiently encapsulated seeing as 88% was extracted out of the gel. In a denser gel, less anthracene was extracted. The varying extents to which analyte is encapsulated suggest one can modify pore size and prevent extraction all together.

Future tests will determine if catalytic activity can occur while the catalyst is encapsulated and if the activity decreases significantly while encapsulated. These studies will determine the optimal gel density that prevents extraction while also allowing catalytic activity.

Fabricating a Hydrogel Platform for Enthesis Regeneration

Amber Boyce¹, Raul Sun Han², Dr. Brendan Harley³

Research Sponsor: Shell Corporation

1. Undergraduate Scholar, Department of Chemical and Biomolecular Engineering
2. Graduate Mentor, Department of Chemical and Biomolecular Engineering
3. Faculty Sponsor, Department of Chemical and Biomolecular Engineering

Tendon injuries, such as rotator cuff injuries, are increasingly common and require surgery, which has a high risk for re-failure. Re-failure is due to the surgical treatment's inability to regenerate the fibrocartilaginous transition from tendon to bone, or entheses. A collagen-glycosaminoglycan based tri-phasic scaffold was designed to emulate the native tendon-bone junction by having a compartment for pro-osteogenic and pro-tenogenic properties with a hydrogel between as the entheses. Hydrogels are ubiquitous in tissue engineering due to their physical and chemical properties. Using a photopolymerization reaction, human mesenchymal stem cells (hMSC) were encapsulated to gauge hMSC activity in the hydrogel. To promote cell growth, steps harmful to hMSCs during the gel formulation were minimized. Preliminary tests optimized the gel formulation, altering parameters such as PEG acrylate polymer weight%, photo initiator weight%, and UV lamp exposure time. Gel stiffness was measured with compression testing. Soluble TGF- β 1 was introduced to gels at a 10 ng/ μ L concentration, previously shown to induce chondrogenic differentiation. Over 21 days, metabolic activity, cell number and gene expression were measured with alamarBlue, Hoescht dye, and polymerase chain reaction (PCR) assays respectively. Results indicate a downregulation of metabolic activity and cell number in both the no growth factor and TGF- β 1 media conditions. Decreasing cell number could signify a lack of cell attachment and decreasing metabolic activity could be due to the decreasing cell number. Future work includes completion of the PCR assay to map out gene expression and investigation of other growth factors, TGF- β 3 and BMP-2, found in relevant literature.

Mitigation of Electromigration of Copper Interconnects via Graphene Passivation

Patrick Burke¹, Michael Cai Wang², SungWoo Nam³

Research Sponsor: Dow AgroSciences, Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Mechanical Science and Engineering
2. Graduate Mentor, Department of Mechanical Science and Engineering
3. Faculty Sponsor, Department of Mechanical Science and Engineering

As electronic devices densify, higher currents are pulled through the microscopic copper interconnects. A problem is the high current density supported by the interconnects. When the current density through a wire exceeds the carrying capacity the atoms disperse, causing a blow-out.

Graphene is a lightweight, mechanically strong, and electrically conductive material. Its direct passivation over these interconnects to reduce the current load experienced by the copper interconnects and prevent electromigration was investigated. Copper interconnects on the scale of microns were constructed to replicate these interconnects, connected on either side by copper electrodes. Nominal cross-sectional areas, resistivities, and current directly preceding blowout were recorded. More samples were produced, with graphene layered over these interconnects to mechanically restrain and electrically assist the channels. Graphene was synthesized through Chemical Vapor Deposition and eventually transferred from its copper substrate to a PMMA handle layer, then applied over the copper interconnects to passivate the interconnects.

From this data, we can conclude tentatively that there is a direct relationship between graphene passivation and enhanced electrical conductivity of the copper. Future work includes

Polymeric Micelles for Delivery of Immunomodulatory Factors

Hannah Chait¹, Aleczandria Tiffany², Dr. Brendan Harley³

Research Sponsor: Dow AgroSciences

1. Undergraduate Scholar, Department of Chemical and Biomolecular Engineering
2. Graduate Mentor, Department of Chemical and Biomolecular Engineering
3. Faculty Sponsor, Department of Chemical and Biomolecular Engineering

Craniofacial trauma accounts for 70% of reported injuries.¹ Craniofacial injuries caused by trauma (e.g. blunt force, explosives) have complex geometries and are often large. Better methods are needed to help regenerate the bone after serious trauma occurs. The Harley lab utilizes collagen-glycosaminoglycan scaffolds to regenerate bone. Incorporating growth factors into these scaffolds can further assist bone regeneration. Extended inflammatory response can be detrimental to healing, and my project this past year has focused on methods to reduce this extended inflammation. M1 macrophages are known to maintain inflammatory response while M2 macrophages reduce inflammation and promote healing. To mediate the polarization of M1 macrophages to M2 macrophages, we wanted to incorporate Interleukin 4 (IL-4) into the collagen scaffolds. The method of delivery we chose to explore was micelle encapsulation, and we focused heavily on micelle fabrication. In this work, micelles were fabricated from polylactide/poly(ethylene glycol)/polylactide (PLA-PEG-PLA) block-copolymer and chloroform using a double emulsion technique.² Micelles were loaded with model protein, bovine serum albumin (BSA), to study release and to troubleshoot our fabrication process. Microscopic imaging, confocal imaging, and scanning electron microscopy (SEM) were used to size and characterize the micelles. While this study shows promising evidence for micelles as a delivery vehicle for IL-4 to injury sites, further studies are needed to confirm and test their applicability.

(1) Jose, A., et al., *Management of maxillofacial trauma in emergency: An update of challenges and controversies*. Journal of Emergencies, Trauma, and Shock, 2016. 9(2): p. 73-80.

(2) Danafar, et. al. *Poly(lactide)/poly(ethylene glycol)/poly(lactide) triblock copolymer micelles as carrier for delivery of hydrophilic and hydrophobic drugs: a comparison study*. Pharm. Investigation. 2017.

Effect of Hyaluronan Transitions in the Tumor Microenvironment on Glioblastoma Invasion

Denzel Ryan Cruz¹, Emily Chen², Dr. Jann Sarkaria³, Dr. Brendan Harley⁴

Research Sponsor: Shell Corporation

1. Undergraduate Scholar, Department of Bioengineering
2. Graduate Mentor, Department of Chemical & Biomolecular Engineering
3. Collaborator, Mayo Clinic Cancer Center
4. Faculty Sponsor, Department of Chemical & Biomolecular Engineering

Glioblastoma (GBM, WHO grade IV astrocytoma) is the most common and aggressive form of brain cancer associated with rapid invasion and a short median survival rate (~15 months). The extracellular matrix is critical in GBM growth. Hyaluronic acid (HA), a major component in the native brain ECM and in GBM tumor microenvironment (TME), has been suggested to be a key contributor in its invasion and therapeutic outcomes. Throughout the GBM TME, not only do the HA presence and amount change but a variation in molecular weight (MW) has also been shown to contribute to GBM progression. Our lab utilizes a three-dimensional biomaterial hydrogel platform, which provides a GBM TME mimetic environment and allow the methodical examination of GBM *ex vivo*. Here, we report the relationship of the GBM invasive phenotype as a response to their TME composition. A family of methacrylamide-functionalized gelatin (GelMA) hydrogels with (15 w/w% of 10, 60, and 500 kDa HA) and without HA were made and seeded with patient derived xenograft (PDX) cells (in collaboration with Dr. Jann Sarkaria from Mayo Clinic). We therefore examined the cell responses when they are exposed to different TME, specifically invasion and invasion-related pathways. Here, protein expression of MAPK/ERK pathway (ERK & pERK) and matrix metalloproteinases (MMP-2 and MMP-9), which are known to promote GBM malignancy and invasion, were measured via Western blot. We also examined PI3K/AKT/mTOR pathway (pI3K & p-pI3K), which are associated with cell cycle and growth, to understand how HA MW influences GBM cell responses. In this work, we seek to provide new insight into how local HA content and MW contributes to GBM progression and potentially be a therapeutic target in the future.

Increasing the Electronic Conductivity of Li-Ion Battery Cathode Using Conversion Cathode-Metal Eutectic

Emily Foley¹, Julia Kohanek², Paul Braun³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Materials Science & Engineering
2. Graduate Mentor, Department of Materials Science & Engineering
3. Faculty Sponsor, Department of Materials Science & Engineering

Due to the increased interest in electric vehicles, there has been a push towards development of high capacity, fast-charging batteries. The limitation of improving batteries today is found specifically in the cathode, leading to an increased interest in alternative cathode materials. Conversion cathodes show a higher specific capacity than standard intercalation cathodes such

as the commonly used LCO. However, the systems exhibit low electrical conductivities on the order of 10^{-6} S cm^{-1} . Typically in order to increase the charging rate, a conductive additive (commonly carbon) is utilized. This addition though increases processing complexity and decreases energy density of the battery. To bypass this additional processing step and improve interface uniformity, a eutectic material composed of a conversion cathodic material and a metal is proposed to be used as the cathode within a Li-ion battery.

The present study has focused on developing and analyzing two eutectic systems: AgCl/Ag and AgCl/Cu. Both systems were prepared with ~ 10 wt% metal and held at 650°C for 5 hours. The formation of a eutectic phase was confirmed via scanning electron microscopy and electron dispersion spectroscopy. Half-cell tests are being conducted against Li-metal currently in order to observe the effectiveness of this novel cathode. Both coin cell and Swagelok configurations utilizing a 1 M LiPF_6 in 1:1:1 EC:DMC:EMC electrolyte solution are being tested. Results from this testing will elucidate whether the metallic phase can provide an electronically conductive network without affecting the conversion cathode phase operation.

Multi-dimensional Features for Prediction with Tweets

Nupoor Gandhi¹, Alex Morales², ChengXiang Zhai³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Computer Science
2. Graduate Mentor, Department of Computer Science
3. Faculty Sponsor, Department of Computer Science

With the rise of opioid abuse in the US, there has been a growth of overlapping hotspots for overdose-related and HIV-related deaths in Springfield, Boston, Fall River, New Bedford, and parts of Cape Cod. With a large part of population, including rural communities, active on social media, it is crucial that we leverage the predictive power of social media as a preventive measure.

We explore the predictive power of micro-blogging social media website Twitter with respect to HIV new diagnosis rates per county. While trending work in Twitter NLP has focused on primarily text-based features, we show that multi-dimensional feature construction can significantly improve the predictive power of topic features alone with respect STI's. By multi-dimensional features, we mean leveraging not only the topical features (text) of a corpus, but also location-based information (counties) about the tweets in feature-construction. We hypothesized that counties in the same geographic region have similar topical distribution, so we constructed additional smoothing features and slang-based features to reflect regional colloquialisms. We develop novel text-location-based smoothing features to predict new diagnoses of HIV. We found that these location-based features significantly improved the features generated by our baseline LDA topic model, reflecting the geographic distinction better than exclusively text-based analysis.

A New Method to Measure Rate of Evaporation of Droplets for Different Temperatures

Marisa Gnadt¹, Alperen Ahmet Gunay², Nenad Miljkovic³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Mechanical Science and Engineering
2. Graduate Mentor, Department of Mechanical Science and Engineering
3. Faculty Sponsor, Department of Mechanical Science and Engineering

Evaporation is an important process in processes such as condensers and heat exchangers. This is due to the prevalence of heat exchange between droplets and their surroundings. The traditional method involves time interval measurements of the size of the droplet, which can be inaccurate because of the difficulty of having a small enough time interval. In this study, we instead used a method where a droplet that is spatially steady due to deposition of smaller microdroplets at a constant rate is measured while it is evaporating. Varying temperatures were used as in real life applications a steady temperature is unrealistic. Also, materials of varying functionalities were used to study the effects of different contact angles. We showed that increasing surface temperature and relative humidity of the environment led to higher evaporation rates. In the future, this research can lead to more accurate measurements that will benefit other studies.

The Incredulity of Contemporary Cardiologists: Integrated Imaging as a Marker for Diagnosing PAD in Preclinical Models

Than Huynh¹, Jamila Hedhli², Lawrence W. Dobrucki³

Research Sponsor: Dow AgroSciences

1. Undergraduate Scholar, Department of Bioengineering
2. Graduate Mentor, Department of Bioengineering
3. Faculty Sponsor, Department of Bioengineering

One in twenty Americans over the age of 50 has peripheral artery disease (PAD). This debilitating circulatory condition displays symptoms such as pain or cramping in the legs and is physiologically caused by narrowing blood vessels reducing blood flow to the limbs. Although common, PAD is often underdiagnosed in a clinical setting leading to inappropriate courses of treatment and worsening morbidity. Contemporary modes of assessing PAD lack a reliable approach to allow a primary care clinician to examine peripheral vasculature and the expression levels of various genes.

In this study, we employed an integrated multimodal approach with SPECT imaging using two molecular probes targeted at HIF-1 α and $\alpha v\beta 3$, as well as label-free imaging modalities (a novel high-sensitivity ultrasonic Power Doppler methodology, laser speckle contrast, and photoacoustic imaging) to assess the effects of PAD on perfusion, tissue oxygenation and angiogenesis. We found that while deep muscle mass took on the order of a week to show signs of blood perfusion recovery, the superficial tissue layer began to recover within a single day. We also showed that within the ischemic muscle mass, blood oxygenation begins to recover

early, even before blood perfusion shows significant signs of recovery. Finally, we found HIF-1 α activation precedes α V β 3 activation, agreeing with its known function as a global regulator of the hypoxia response. The combination of these techniques offers an unprecedented perspective to distinguishing between various stages of PAD and ultimately, an earlier more confident diagnosis.

Controlling Crystal Formation in Organic Semiconductors

Nicole Jugovich¹, Hyunjoong Chung², Ying Diao³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Chemical & Biomolecular Engineering
2. Graduate Mentor, Department of Chemical & Biomolecular Engineering
3. Faculty Sponsor, Department of Chemical & Biomolecular Engineering

The objective of this project was to optimize the single crystal fabrication process using simple dropcasting to control crystal formation. Previous studies have explored this topic, but the central problems of controlling the dimensions and nucleation density of the crystal still remained.

Two high-performing organic semiconductor systems were studied: 6,13 Bis (triisopropylsilylethynyl) pentacene (TIPS pentacene) with a decane solvent and ditert-butyl [1] benzothieno[3,2- b][1]benzothiophene (ditBU-BTBT) with a tetralin solvent. Some advantages of organic electronics over their traditional inorganic counterparts include their low cost and flexibility.

This project placed more emphasis on single crystals instead of thin films as previously studied. Crystal behavior was monitored as contact angle and concentration were varied. Three different substrates were used to manipulate the contact angle: bare (low), OTS (medium), and HTMS (high). To prepare a sample, a drop of solution of desired concentration was placed on an appropriate substrate. Microscope images of various samples were analyzed after the solvent evaporated to specifically determine how changing these parameters affects crystallization. Additional high speed camera timelapses were performed to characterize the nucleation and growth process.

The crystal formation mechanism must be studied more in-depth before these organic crystals can be used in electronic devices on a large scale. Crystal research's potential benefits include improving the quality of organic electronics and the discovery of inexpensive, efficient ways to create these materials.

Future work will focus on further quantifying the effect of contact angle and concentration, in addition to using other methods to observe the flow within the droplet.

Understanding Human Sorting

Andrew Kuznetsov¹, Aditya Parameswaran²

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Computer Science
2. Faculty Mentor, Department of Computer Science

To economically address our world's exponential increase in unstructured data, companies employ a combination of human judgement and automated techniques (specifically, machine learning) to label, classify, sort, and structure collected data. The key issue with crowdsourcing, however, is that humans often take time to respond, make mistakes, and need to be compensated monetarily. This study, part of on-going work, examines naive sorting behavior under a variety of conditions and interface interactions with the goal of formulating a comprehensive model for crowd-worker sorting performance, effort, and error. The research team developed a highly-customizable sorting web interface, which was used to collect experimental data on Amazon Mechanical Turk. In these trials, sorting behavior was compared with traditional sorting algorithms - revealing that non-expert sorting behavior natively gravitates toward certain algorithms depending on the magnitude of worker effort required to execute each, and is sensitive to the original order of items, difficulty in performing pairwise comparisons, and transitivity. Future work includes developing novel interface interactions that adapt to dataset content, as well as automated interventions for the prevention of inefficient sorting patterns.

Biomaterial Models of the Tumor Margins in Glioblastoma

Patricia Li¹, Sara Pedron Haba², Dr. Brendan Harley³

Research Sponsor: Shell Corporation

1. Undergraduate Scholar, Department of Chemical Biomolecular Engineering
2. Research Scientist Mentor, Carl R Woese Institute for Genomic Biology
3. Faculty Sponsor, Department of Chemical and Biomolecular Engineering

The purpose of this research is to create hydrogels to imitate the spatially-heterogeneous tumor microenvironment to help with understanding glioblastoma (GBM), the most aggressive form of brain cancer. This is done by optimizing the culture of primary tumor cells within the hydrogel platforms. These gelatin-based platforms contain hyaluronic acid (HA) gradients to analyze how cells are influenced by HA, which is the main component of the brain extracellular matrix. The cells are characterized based on the transcriptomics and RNA sequencing is a precise way of analyzing profiles on gene expression. This relies on very pure and clean RNA from cells, which is difficult to acquire due to RNA degradation and the heterogeneity of the primary cell samples. As a result, the current focus is on the establishment of a reproducible protocol to extract RNA from tumor tissue mimics that is valid for RNA sequencing. Patient-derived samples (expanded in orthotopic mouse model, provided by Mayo Clinic) were encapsulated in gelatin hydrogels with different concentrations of hyaluronic acid through a linear gradient. Subsequently, the different sections of the cell-cultured hydrogel gradients,

containing different concentration of HA, are prepared for RNA extraction and quantification. The RNA is extracted from spatially graded hydrogels and analyzed by Agilent Bioanalyzer (Roy J Carver Biotechnology Center). The reproducibility of the process and integrity of the samples was assessed by looking for consistent clean results from the RNA ribosomal ratio. Clean results had high RNA integrity numbers (usually around 8.0) on a scale of 1-10. By replacing the use of the bead beater instrument with a mortar and pestle system (keeping low temperature), adding DNAase (clean interfering DNA), and keeping the cells in ice throughout the process, the RNA degradation decreased. Results indicated that it was possible to reach the 8.3 RNA Integrity Number (RIN) throughout the sample gradient. Future work will target the elimination of nucleotides interference and the reproducibility along different patient-derived GBM tumor cell samples.

Development of an Electrical Differential Counter-based Immunosensor for the Detection of Sepsis Biomarkers

Cynthia Liu¹, Jacob Berger², Enrique Valera³, Rashid Bashir⁴

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Bioengineering
2. Graduate Mentor, Department of Bioengineering
3. Postdoctoral Associate, Department of Bioengineering
4. Faculty Sponsor, Department of Bioengineering

A potentially fatal complication, sepsis is an inflammatory response cascade that leads to fever, increased heart and respiration rate, blood clots, and sometimes multiple organ failure. Annually, more than 1.5 million in the United States alone are diagnosed with sepsis; of them, 250,000 die. Sepsis is the leading cause of hospitalization and hospital readmission, costing \$24 billion a year. A major contributor to the prevalence and mortality of sepsis is its generalized and rapidly escalating nature, which makes it difficult for sepsis to be diagnosed in a timely matter and drastically increases mortality. An estimated 80% of sepsis deaths are preventable if they are caught early in the disease progression, during the hyper-inflammatory initial phase of the disease. To this end, we have developed a rapid point-of-care device for the detection of cell and protein biomarkers associated with the initial stages of sepsis. Our previous experiments have validated its accuracy in quantifying levels of leukocytes, CD4/CD8 cells^{1, 2}, and CD64 expression on neutrophils. Here, we adapt this point of care technology to analyze sepsis-associated protein biomarkers IL-6 and PCT. Technological validation of the immunoassay and preliminary results are presented.

The chief components of this device are PDMS microfluidic channels and a differential counting chip containing two electrode pairs and a capture chamber. A sandwich immunoassay for the target protein was implemented on the surface of micro beads, which are then passed through an entrance counter to assess the initial substance levels that enter the capture chamber. Antigen bound beads are captured on pillars in the capture chamber, and do not pass through the exit counter with the empty bead complexes. The differential measurement between the entrance and exit levels determines the percentage of capture and therefore the concentration of

the protein of interest. The electrodes and PDMS molds for channels and chambers are constructed using traditional lithographic techniques. The on-chip quantification of these proteins was validated using plasma from whole blood obtained from potentially septic patients at the Carle Foundation Hospital Intensive Care Unit, as well as using spiked samples. The measurement of protein levels in buffer and blood were compared to clinical gold standards, and show good correlation. The immunosensor accurately detected IL-6 levels with a limit of detection of 127 pg/mL and a EC50 of 734.4 +/- 0.2 pg/mL.

Our on-chip experiments with various proteins have established that the speed of the immunoassay is limited by diffusion, otherwise known as the rate of antibody binding. We seek to overcome this barrier by using magnetic beads and inducing mixing using alternating magnetic fields.

- 1) N. N. Watkins et al., *Sci Transl Med*, 2013, 5, 214ra170.
- 2) U. Hassan et al., *Nature Protocols*, 2016, 11(4), 714-726

Rejuvenation in Metallic Glasses through Ultrafast Heating

Jacob Maher¹, Dan Rosenthal², Professor Robert Maass³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Materials Science and Engineering
2. Undergraduate Mentor, Department of Materials Science and Engineering
3. Faculty Sponsor, Department of Materials Science and Engineering

One of the limitations of applications for metallic glasses is the degradation of thermo-mechanical properties as a function of time and temperature, known as aging. Rejuvenation is a process of reconfiguring the amorphous structure in a favorable way, which reverses the process of aging and increases the enthalpy stored in the alloy. Previous research has developed multiple methods to impose rejuvenation into a metallic glass such as cyclic loading, plastic deformation, shot peening, and annealing.

Whilst traditional thermal protocols lead to aging of metallic glasses, we explore in this work rejuvenation via ultrafast heating of a metallic glass. We are able to rejuvenate vitreloy 106a samples by rapidly heating just below the crystallization temperature followed by cooling. We manipulate the heating rate of vitreloy 106a samples through capacitive discharge heating. A voltage on the order of 200 volts is discharged. A MACOR heat sink is attached to the sample to influence the cooling rate after discharging. Too slow of a heating or cooling rate results in crystallization of the system, which is undesirable. High speed pyrometry is used to record temperature profiles of the samples under argon and high vacuum conditions. XRD data is collected to provide insight into crystallinity.

Temperature evolutions are plotted against time in order to reveal heating rate, cooling rate, and glass transition temperature. Future work will involve DSC to unveil the enthalpic relationships towards heating and cooling patterns generated through capacitive discharge heating.

Design of an Autonomous Large Drone Swarm

Raimon Roglans¹, Grace Gao²

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Aerospace Engineering
2. Faculty Mentor, Department of Aerospace Engineering

Unmanned Aerial Vehicles, or drones, are now common commodities in both academic and commercial organizations. In research settings, many labs are studying different methods of autonomous movement and collective action; meanwhile commercially, drones are used globally for conservation of endangered populations and critical ecosystems and construction management and maintenance. Here, a platform is proposed, designed, and built for a large drone which can be easily scaled to become a swarm that can also organize autonomously.

The primary components in need of development were an electronics payload that could control the individual drone and act as a relay between the rest of the swarm and the user of the system. There was also a need to develop a robust mechanical system that could bear the electronics payload, but minimize weight and mechanical failures. A critical component of earlier iterations of this drone, the Illinois Big Quad Rotor (iBQR), was the variety of electronic components that allowed the iBQR to function. Previous iterations of the iBQR had these components more loosely joined and this presented constraints and restrictions on the abilities of the iBQR, so a PCB was designed which created a uniform integrated component for all the electronics the iBQR used. The mechanical systems had components that relied on aluminum and the payload container constrained the materials that would be carried as well as adding unnecessary weight. Creating carbon fiber components to replace certain aluminum components as well as a modular system for storing the payload allowed for a lighter and better drone.

Concluding these improvements on this iteration of the iBQR allows for a test bed for first an individual autonomous drone, and eventually a swarm of such drones working in tandem.

Chiral Measurements of D-Aspartate in the Pancreas

Jack H Schnieders¹, Amit V Patel², Cindy Lee, Stanislav S Rubakhin, and Jonathan V Sweedler³

Research Sponsor: Shell Corporation

1. Undergraduate Scholar, Department of Chemical and Biomolecular Engineering
2. Graduate Mentor, Department of Chemistry
3. Faculty Sponsor, Department of Chemistry

The islets of Langerhans are small cell clusters in the mammalian pancreas. Immunostaining the islets revealed high concentrations of D-aspartate (D-Asp) and glucagon in alpha cells, and of D-alanine (D-Ala) and insulin in beta cells. It was discovered that beta cells release D-Ala with insulin in high glucose concentrations, indicating they could be co-localized in the same

granules. The purpose of this study is to determine whether D-Asp is released similarly with glucagon from alpha cells in low glucose concentrations. Characterizing D-amino acids in the islets will yield information on their potential usage as pancreatic signaling molecules which may help develop diabetes therapies. This study is being conducted by two different methods.

The first method uses capillary electrophoresis (CE) with laser-induced fluorescence (LIF). CE separates species based on charge, viscosity and size, and the aspartate enantiomers are resolved by incorporating chiral additives into the buffer. All species are reacted with a fluorogenic tag to allow their relative concentration to be determined by LIF. The D-Asp peak is identified on the complex electropherograms by standard addition and enzyme treatment experiments.

The second method employs high pressure liquid chromatography (HPLC) with mass spectrometry (MS). HPLC separates species based on interactions with the stationary phase and a chiral column separates the aspartate enantiomers. Effluent is vaporized and run through a triple quadrupole MS. Relative abundance is only recorded for molecules whose parent ion and fragment masses match the molecule of interest. Data is charted against time to produce an extracted ion mass chromatogram.

Fabrication of Perovskite Solar Cells Via Flow-Limited Field-Injection Electrostatic Spraying

John Simonaitis¹, Professor Kevin (Kyekyoon) Kim²

Research Sponsor: Semiconductor Research Corporation/Intel,
Office of Undergraduate Research, Kim Funds

1. Undergraduate Scholar, Department of Electrical and Computer Engineering
2. Faculty Sponsor, Department of Electrical and Computer Engineering

In the last decade, lead halide perovskite solar cells have taken the photovoltaics community by storm, increasing to over 22% efficiency at an unprecedented rate while offering low-cost fabrication from earth-abundant materials. However, several key issues remain, one of the most significant being scalability due to the slow processing, large thermal budget, and/or non-scalability of current techniques. In this work, we report an inexpensive, low-temperature (~70°C), and fast (~15 minute) method of spraying and converting perovskite solar cells all in a single step without the use of flash-annealing. With this technology, known as Flow-Limited Field-Injection Electrostatic Spraying, we achieved high device efficiencies with a standard FTO/TiO₂/Perovskite/Spiro-MeO-Tad/Gold architecture.

Mineralized Collagen-Amnion Scaffolds for Repair of Craniomaxillofacial Bone Defects

Simona Slater¹, Marley Dewey², Dr. Brendan Harley³

Research Sponsor: John Deere

1. Undergraduate Scholar, Department of Chemical and Biomolecular Engineering
2. Graduate Mentor, Department of Materials Science and Engineering
3. Faculty Sponsor, Department of Chemical and Biomolecular Engineering

Craniomaxillofacial Defects (CMF) are critically sized defects of the skull which cannot heal naturally. A tissue engineering approach to treatment enables a more custom solution that is less invasive. Specifically, the study combines amniotic membrane (AM) and mineralized collagen in a suspension to form a scaffold. A 5:1 ratio suspension of mineralized collagen to amnion was homogenized, then poured into molds and set by freeze drying. A variety of tests are performed on the mineralized collagen AM scaffold, using mineralized collagen scaffolds as a control. First, mechanical strength testing and Environmental Scanning Electron Microscopy (ESEM) imaging were studied. Mineralized collagen-AM demonstrated a higher Young's Modulus, maximum collapsed stress, and collapsed strain. When comparing strain verses stress, the mineralized collage-AM exhibited greater endurance. ESEM revealed a visual integration of the AM into the scaffold. Next, porcine adipose derived stem cells (pASCs) were seeded in both types of scaffolds and cultured in normal growth media and high inflammatory growth media. Tests were performed to study cell viability through investigating cell number and metabolic activity. The mineralized collagen-AM scaffold was found to maintain a cell population and minimize the effects of inflammatory media. The results are evident from minimal differences in cell population in the mineralized collagen-AM samples with inflammatory and normal growth media. Analysis of gene expression, pore size, mineralization, and protein activity is ongoing. From current data, AM scaffolds successfully combined healing characteristics of mineralized collagen and immunomodulatory properties of amniotic membrane to provide a platform aiding osteogenesis and minimizing inflammation.

Accelerated Molecular Dynamics Study of Dislocation Climb in Nickel

Lauren Smith¹, Anne Marie Tan², Dallas Trinkle³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Materials Science and Engineering
2. Graduate Mentor, Department of Materials Science and Engineering
3. Faculty Sponsor, Department of Materials Science and Engineering

The nickel-based turbine blades of an airplane engine are exposed to extremely high temperatures and stresses. Under these conditions, line defects in the crystalline structure called dislocations can absorb vacancies and undergo a process known as dislocation climb, which is a key mechanism underlying creep behavior in metals. Therefore, a detailed understanding of dislocation climb is important in order to accurately predict safe operating conditions for turbine blade materials. A key mechanism driving dislocation climb is the absorption of vacancies by

steps on dislocation lines known as jogs. We simulate this process in pure nickel using accelerated molecular dynamics, specifically the ParSplice method. ParSplice runs many simulations in parallel, and then pieces these together to create one long trajectory. Through these simulations, we can understand the mechanisms for dislocation climb and the rates at which it occurs. Using molecular statics, we determined the energy barriers for vacancy hops in and around the jog as well as the binding energies between the vacancy and the dislocation line. Dynamic simulations reveal the preferred pathways for vacancy migration towards the jog as well as the rates of vacancy absorption at the jog. These results give important insights into the atomistic mechanisms of dislocation climb in addition to the rates of climb at high temperatures.

EPen: A Handheld Device for Measuring the Stiffness of Soft Tissue

Robert Stavins¹, Anthony Fan², M Taher Saif³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Mechanical Science and Engineering
2. Graduate Mentor, Department of Mechanical Science and Engineering
3. Faculty Sponsor, Department of Mechanical Science and Engineering

Progress has been made over the last two decades in measuring the elastic modulus of hard materials at macro, micro, and nano, scales. An unmet need is measuring the modulus of soft materials like, cell culture substrates, in-situ tissues for disease diagnosis, and scaffolds for tissue engineering, in their native environment. Methods to measure modulus must satisfy two conditions: (1) the instrument must reach the site of the materials, and (2) be able to quickly measure the materials' mechanical properties before they change with time. The objective of my research is to develop a new device for stiffness sensing that is more affordable, portable than current technologies like atomic force microscopy and nanoindentation. The method uses two well established theories of mechanics. First, buckling of a long slender bar; a bar subjected to an axial compressive force, P , at the ends buckles when the force exceeds a critical threshold, P_{cr} . When $P > P_{cr}$, the bar continues to buckle with small force increase. Thus, P_{cr} can be considered the force supported by the bar at any time post-buckling. Second, Hertz contact theory; a hard sphere in contact with an elastic material subjected to a compressive force deforms the material or indents it. To measure stiffness, one must measure force and displacement. The device makes use of a gold/palladium coated glass fiber and a movable piston that controls the flexible length of the fiber. The load at which fiber buckling happens determines the indentation force and the buckling displacement can then be measured electronically.

The Missing Link between Acoustic Stealth and Poroelasticity

Greg Stroot¹, Mattia Gazzola²

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Mechanical Science and Engineering
2. Faculty Sponsor, Department of Mechanical Science and Engineering

The primary focus of this paper is to understand the mechanisms behind the impressive acoustic stealth of the owl. This is done through the use of computational fluid dynamics, computational aeroacoustics, and stochastic optimization. Specifically, for this presentation, results are presented on the validation of the libAcoustics computational aeroacoustics library of OpenFOAM. Such results allow for further computations to be run with assurance that the data is correct.

Cycle Testing of NaNO₃ for Solar Thermal Energy Storage

Rachel Tham¹, Dr. Matthew Alonso², Dr. Bruce Litchfield³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Agricultural and Biological Engineering
2. Graduate Mentor, Department of Agricultural and Biological Engineering
3. Faculty Sponsor, Department of Agricultural and Biological Engineering

With three billion people cooking powered by wood, animal dung, and charcoal, these fuels' emissions cause over four million premature deaths a year, in addition to negatively impacting the environment. Further, many developing communities are forced to spend one-quarter of their income on household fuels. Solar energy, in the form of a Sun Bucket, can provide a solution and do so in a culturally appropriate manner. It is crucial to understand the heating properties of candidate thermal storage material used within a Sun Bucket and how long these materials can be used to store energy. This project addresses this issue by determining whether the thermal storage capacity of candidate materials degrades or decrease over time. This work describes the testing method and thermal storage capacity of NaNO₃ over 370 cycles. Results and further work will determine if there is a statistically significant degradation in the thermal storage capacity of NaNO₃.

Graph Theory-Based Gluing Formulae for Quantum Mechanics and Electronic Structure Calculations

Michael Toriyama¹, Ivan Contreras²

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Materials Science and Engineering and Department of Mathematics
2. Faculty Mentor, Department of Mathematics

Recent insights have suggested that spectral graph theory supplies a combinatorial interpretation of how a quantum system's state evolves with time, following the locality principle of quantum mechanics. A graph is defined by the possible positions that a particle can exist in three dimensions, as well as a discrete Laplacian matrix governing the particle's dynamics towards equilibrium. In the present study, we prove several theorems regarding the matrix that show how the discrete energy levels of this particle changes as the topology of its space (i.e. the graph) evolves. From these, we provide an algorithm that computes the energy levels when two graphs are glued, which represents an event where the particle suddenly exists in a larger space. Such formulae suggest a robust graph-theoretic method for computing electronic structures of matter, where the space in which the particle resides can be made larger with no significant increases in computational cost.

Negative Thermal Expansion in Anisotropic Oxides

Whitney Tso¹, Scott McCormack², Prof. Waltraud Kriven³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Materials Science and Engineering
2. Graduate Mentor, Department of Materials Science and Engineering
3. Faculty Sponsor, Department of Materials Science and Engineering

Thermal expansion is an important property that describes how the dimensions of a material changes with change in temperature. It is expected that a material would expand when upon heating, similar to how a gas expands during heating. However, there have been studies on materials with negative thermal expansion recently. This means that a material actually contracts upon heating. This is extremely useful as these materials can be used to tailor the thermal expansion coefficients of a composite materials by adjusting the ratio between the matrix phase and reinforcement phase. This study shows that the overall volume of the anisotropic oxide ($\text{Yb}_2\text{W}_3\text{O}_{12}$) is negative. Interestingly, the volume contraction is not uniform. This lack of uniformity results in strain within the material on heating. To better understand how the dimensions of the anisotropic material changes as a function of temperature, phase information of $\text{Yb}_2\text{W}_3\text{O}_{12}$ are collected using synchrotron X-ray diffraction and a quadrupole lamp furnace up to 1500 °C. The X-ray diffraction data was analyzed using the Reitveld refinement method in the software package GSAS-II to extract the volume, lattice parameter, and thermal expansion as a function of temperature.

Universal, Green Chemistry Approach to Synthesizing Functional Theranostic Gold Nanoparticles

Rachele Wen¹, Aaron Schwartz-Duval², Dipanjan Pan³

Research Sponsor: Dow AgroSciences

1. Undergraduate Scholar, Department of Bioengineering
2. Graduate Mentor, Department of Bioengineering
3. Faculty Sponsor, Department of Bioengineering

Cancer is a genetic disease characterized by cell abnormalities. Gold nanoparticles (GNPs) can combat cancer by acting as an early diagnostic and/or therapeutic. GNPs are ideal for cancer applications since they are bioinert, unique in their optical properties, used in photothermal ablative therapy, and suitable for various imaging techniques (infrared, computed tomography, fluorescence, photoacoustic). To make the GNPs specifically targetable to cancer, they can be combined with cancer specific proteins, functionalizing them. Current synthesis methods to prepare functionalized GNPs (fGNPs) rely on heating, pH changes, and synthetic materials. These methods can degrade or modify targeting-protein characteristics.

Here we have developed a single-step synthesis of fGNPs using nicotinamide adenine dinucleotide (NADH), a coenzyme in all cellular life involved with redox metabolism, as a reducing agent. Our synthesis method, involves the direct addition of NADH to ionic gold (Au^{3+}) in the presence of fetal bovine serum (FBS), our model protein. We have optimized this synthesis for protein adhesion to the GNPs and to maintain protein integrity. With this method, fGNPs can be synthesized in a single-step without degrading the protein. GNP formation was confirmed using ultraviolet-visible light spectroscopy and transmission electron microscopy imaging. Interactions between GNPs and proteins were characterized using SDS-PAGE.

In the future, we plan on using homotypic adhesion to target cancerous cells by using our synthesis method to functionalize GNPs with membrane extracted from cancer cells. The fGNPs can then be targeted back to the membrane source and detected using imaging techniques to identify the location of cancerous cells.

Adaptation of a Smartphone Spectrometer system to analyze light-scattering properties

Elizabeth Woodburn¹, Kenneth D. Long², Prof. Brian T. Cunningham³

Research Sponsor: Semiconductor Research Corporation/Intel

1. Undergraduate Scholar, Department of Bioengineering
2. Graduate Mentor, Department of Bioengineering
3. Faculty Sponsor, Department of Electrical and Computer Engineering, and Department of Bioengineering

Increases in the availability and usage of point-of-care testing have been facilitated by the development of devices that allow for simple, low-cost measurement of biological samples. The aim of this project was to adapt the TRI-analyzer device to analyze the light-scattering properties of urinary dipsticks to detect abnormal analyte concentrations.

White balance settings and the spectral region of interest for color differentiation were optimized using measurements from strips of colored paper. Readings were then taken from dipsticks saturated with water under a variety of conditions to determine sources of variation between readings. Solutions of lithium acetoacetate, to represent the most common urinary ketone of acetoacetic acid, were prepared at several concentrations to match the reference color ranges provided to read the strips. Three strips were dipped into each of the concentrations and evaluated in the cradle when they were fully dry (roughly 40 minutes after sample application, to minimize evaporation error). The limit of detection was estimated to be approximately 3.5 mg/dL, which is lower than the minimum concentration detectable by human visual analysis.

Demonstrating that the strips retain their diagnostic value when read well after the target time of 15s, despite changing in color, has significant potential value to apply to the next phase of the project. Current work is focused on expanding the existing platform and test procedures to facilitate the analysis of dipsticks that detect a total of ten analytes in urine.

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Raimon Roglans
Aero



Jack Schnieders
ChemE



John Simonaitis
EE



Simona Slater
ChemE



Lauren Smith
MatSE



Robert Stavins
MechE



Greg Stroot
MechE



Rachel Tham
ABE



Michael Toriyama
MatSE



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MatSE



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