2019 SUMMER

UNDERGRADUATE RESEARCH SYMPOSIUM

WEDNESDAY, JULY 24

9:30am - 11:45am

Jordan Hall of Science Galleria

ROSTER OF STUDENT RESEARCHERS

#	STUDENT RESEARCHER	PROJECT TITLE	ADVISOR	DEPARTMENT
1	Nicole Aggarwal	Composition of Online Racism: Decoding Racist Internet Memes	Dr. Susan Alexander	Sociology
2	Adriana Archilla Fraticelli	Controlling Lymphatic Tube Formation Using Synthetic Hydrogels	Dr. Donny Hanjaya-Putra	Aerospace and Mechanical Engineering
3	Grace Arntz	Stability of a Thorium Metal Organic Framework in Extreme Conditions	Dr. Peter C. Burns	Chemistry and Biochemistry
4	Lindsay Baca	Factors of Psychosocial Risk as Moderators for Father Involvement	Dr. Julia Braungart-Rieker	Psychology
5	Kyle Barrentine	The Adjustment of Network Size Among Depressed Persons with Too Large of a Social Network	Dr. David Hachen	Sociology
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8	Joseph Brennan	Improving process-guided deep learning approach to lake temperature estimation with data assimilation techniques		
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43	Stephen Koch	Fabrication of Ductile yet Tough Polymer Composites	Dr. Tengfei Luo	Aerospace and Mechanical Engineering
44	Ebrima Komma	Solvent-in-Salt Liquid Crystalline Electrolytes for next- generation rechargeable batteries	Dr. Jennifer Schaefer	Chemical and Biomolecular Engineering

45	Katie La Costa	Dynamic Peptide-based Nanomaterials for Enzyme Targeted Drug Delivery	Dr. Matthew Webber	Chemical and Biomolecular Engineering
46	Zijuan Liang	Fabrication of Gold Nanoplates Using Substrate-immobolized Seeds Lined with Planar Defects via a Directed-Shock wave	Dr. Svetlana Neretina	Aerospace and Mechanical Engineering
47	Mary Manley	Microbial contamination of Ayurvedic medications collected in Nepal	Dr. Reena Lamicchane-khadka	Biological Sciences
48	Alondra Marrero	Biosorption of Rare Earth Elements through Cell Surface Display of Lanthanide Binding Proteins	Dr. Na Wei	Civil and Environmental Engineering and Earth Sciences
49	Hannah McGinness	Preparation of semi-Interpenetrating Network (s-IPN) Membranes Based on Matrimid® Polyimide and Celazole® Polybenzimidazole (PBI) for Gas Separation Applications	Dr. Ruilan Guo	Chemical and Biomolecular Engineering
50	Sanesha McPherson	Solving semidefinite programs using Bertini and Matlab	Dr. Jonathan Hauenstein	Applied and Computational Mathematics and Statistics
51	Erick J. Mendez	Tuning a Hydrogen Bonding Network to Control the Phase, Dynamic and Electrochemical Behavior of Redox-active Deep Eutectic Solvents	Dr. Edward Maginn	Chemical and Biomolecular Engineering
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54	Akil Mondie	Exploring Substituent Effects on Friedel-Crafts Hydroxyalkylation via Hammett plot projection	Dr. Haifeng Gao	Chemistry and Biochemsitry
55	Dalia Mota	Tracking in Indiana's Schools	Dr. William Carbonaro, Dr. Amy Langenkamp	Sociology
56	Samirah Muhammad	Cucurbituril Functionalized Absorptive Membranes for The Detection of Fentanyl in Water	Dr. William Phillip	Chemical and Biomolecular Engineering
57	Linda Nwumeh	Dialogue Structure Patterns Predictive of Success in a Communicative Search Task	Dr. Kathleen Eberhard	Psychology
58	Emmanuel Okafor	Prototype Implementation of Frequency domain diffuse optical spectroscopy using a multi-phase approach.	Dr. Thomas O'Sullivan	Electrical Engineering
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62	Kimberly Riordan	Synthesis Toward a Trigonal Pyramidal Sulfur Radical Supported by a Triarylborane Framework	Dr. Emily Tsui	Chemistry and Biochemistry
63	Jessica Saeli	Lost in Translation: Love, Sex, and Death in the Autobiography of Nikolai Berdyaev	Dr. Ann Astell	Theology
64	Danielle Sanchez	Selma: Sisters and Saints	Dr. David Clairmont	Theology
65	Gabriella Sanford	Advanced Wireless Communications for Drone Swarms	Dr. J. Nicholas Laneman	Electrical Engineering

66	Zachary Schoon	RadioHound: A low cost spectrum sensor	Dr. Bertrand Hochwald	Aerospace and Mechanical Engineering
67	Charles Sleeper	Parallelization of NLP Applications for Genocide Prediction	Dr. Paul Brenner	Center for Research Computing
68	Josemaria S. Soriano	Ionothermal Synthesis of Actinide-Based Metal Organic Frameworks and Clusters	Dr. Peter C. Burns, PhD	Chemistry and Biochemistry
69	Joy Thompson	Experimental and Computational Insights on Ethylene Oligomerization by Oxide-Supported Group 4 Metal Hydrides	Dr. Jason Hicks, Dr. William Schneider	Chemical and Biomolecular Engineering
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74	Stephanie Wallace	Magneto-silica nanoparticles (MagSiNs) for combinatorial chemotherapeutics and gene delivery against metastatic cancers	Dr. Prakash Nallathamby	Aerospace and Mechanical Engineering
75	Manchen Wen	Modeling Migration on a Global Scale	Dr. Paul Brenner	Computer Science and Engineering
76	Hang Xie	Sentiment Analysis on Global News	Dr. Paul Brenner	Computer Science and Engineering
77	Ruyu Zhou	Modeling Migration on a Global Scale	Dr. Paul Brenner	Computer Science and Engineering

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Composition of Online Racism: Decoding Racist Internet Memes

Nicole Aggarwal
Sociology
Saint Mary's College

Faculty Advisor: Dr. Susan Alexander

This research analyzes the composition of online racism expressed through racist Internet memes. Internet memes, an offspring of participatory media platforms, are defined as an image accompanied by a caption, most often one across the top and bottom. Based upon Hall's (1972) "encoding-decoding model," this research study focuses solely on the decoding process, analyzing potential viewer interpretations and possible social effects. There is no way to know whether an Internet meme is an original, who first created it, or where it truly originated from; this research does not look at the encoding process or the intentions of meme creators. Using keyword phrase searches on Google and two user-created meme websites, a sample of 300 racist Internet memes was compiled.

This research found thirteen different racial themes: Stereotypes, Embodied Racism, Exaggeration, Inferiorization, Dehumanization, Minimization or Denial of Racism, Exclusion, Popular Figures, Mocking or Parody, Criminality, Explicit Language, White Superiority, and Colorblind Racism. Overall, the data suggests that racist ideologies created and diffused online through racist internet memes are more explicitly racist than previous literature has suggested. Across all categories, racist internet memes disproportionately target black individuals compared to any other racial group. In regards to the frequency of themes, stereotyping occurs the most often across all racial groups. Although stereotyping was the most prominent, other racial themes targeted specific populations. For instance, Asians were more frequently mocked while Blacks were always the subject of racist memes featuring criminality.

This study sheds light on the possible dangers of online spheres containing explicitly racist ideologies. More importantly, in relation to the decoding, these racist online artifacts can be potentially harmful for both viewers and victims. The racial groups targeted in these racist memes may internalize this online content. On the other hand, these racist ideologies expressed through memes may reinforce racist beliefs within particular viewers or encourage adoption to those who may have never considered them. If racist content, as described in racist internet memes, can continue to circulate in online platforms, users can create or perpetuate explicitly racist ideologies while escaping the tangible limitations and sanctions of the offline world.

Controlling Lymphatic Tube Formation Using Synthetic Hydrogels

Adriana Archilla Fraticelli
Aerospace and Mechanical Engineering
College of Engineering

Faculty Advisor: Dr. Donny Hanjaya-Putra
Grad Student or Postdoctoral Mentor: Laura Alderfer

Approximately 250 million people worldwide suffer from lymphedema, a life-long disease that causes swelling due to abnormal lymphatic vessel development or disorders. Lymphangiogenesis, the formation of new lymphatic vessels from pre-existing ones, has been hypothesized to be the first long-term treatment option for lymphedema, which can arise from multiple diseases or cancers. Here, we utilize hyaluronic acid (HA) hydrogels to investigate mechanical and biomechanical cues that regulate lymphangiogenesis. Using different substrate stiffnesses as mechanical stimuli and a supplemental growth factor as biochemical stimuli, lymphatic endothelial cell (LEC) growth and migration is promoted, causing lymphatic vessel formation. The best tube formation has been found to occur in the softest substrate at the highest concentration of supplemental growth factor supplied. Real-Time PCR analysis suggests several genes, associated with matrix remodeling and cell migration, are directly linked to these findings and may be the underlying mechanism of improved lymphatic vessel development. Collectively, investigating the molecular controls of lymphangiogenesis and regulating LEC behavior will allow us to create an implantable gel to promote lymphatic vessel formation as a therapeutic option.

Stability of a Thorium Metal Organic Framework in Extreme Conditions

Grace Arntz
Chemistry and Biochemistry
College of Science

Faculty Advisor: Dr. Peter C. Burns
Grad Student or Postdoctoral Mentor: Sara Gilson
Other Contributors: Patrick Julien

A tetravalent thorium metal organic framework (Th-MOF) was synthesized solvothermally. The crystals were studied using single crystal X-ray diffraction, powder X-ray diffraction (PXRD), Raman spectroscopy, and Fourier transform infrared spectroscopy (FTIR). The stability of the Th-MOF was examined under several different conditions: standard atmospheric conditions, gamma-irradiation study, and low-pH. Results indicated that the Th-MOF crystals were stable outside of the mother solution for at least 48 hours before they began to degrade, as indicated by Raman and FTIR spectroscopies. The post-irradiation PXRD, FTIR, and Raman data demonstrated good radiation resistance when exposed to a 1 MGy dose of gamma radiation. The crystals were also soaked in 5 M nitric acid and retained crystallinity suggesting resistance to low pH.

Factors of Psychosocial Risk as Moderators for Father Involvement

Lindsay Baca
Psychology
College of Arts and Letters

Faculty Advisor: Dr. Julia Braungart-Rieker

A critical question applying to intervention research is understanding the extent to which families benefit from the respective project's goals. It has been previously understood that participants in more disadvantaged circumstances reflect poorer intervention outcomes compared to their counterparts facing less life adversity (Lundahl, Risser, & Lovejoy, 2006; Reyno & McGrath, 2006). The present study sought to examine the degree to which psychosocial risk (e.g., mental health, relational stress, insufficient income) moderated (increased or decreased) the effects of a parenting and couples intervention to promote father involvement and family functioning. Our longitudinal study includes 400 mothers and fathers (current N = ~125, 26% minority status) who completed measures of stress, depression, marital conflict, and parent involvement over four time points during infancy. Parents were also randomly assigned to family-based interventions to promote parenting and reduce family conflict. Utilizing father questionnaire data, we performed 9 multiple regression analyses that resulted in one significant interaction effect between dysphoric symptoms and conflict intervention efforts. This indicates that intervention efforts were more effective in promoting father involvement for fathers with more depressive symptoms suggesting the need to target depressed fathers for family interventions. While only three additional psychosocial risks (e.g., parental stress, parent report of negative infant temperament, minority status) proved marginally significant ($p < 0.1$) in these preliminary analyses, we were also able to conclude that the utter participation in the sensitivity and conflict intervention group has a significant effect on father involvement across the sample.

The Adjustment of Network Size Among Depressed Persons with Too Large of a Social Network

Kyle Barrentine
Sociology
College of Arts and Letters

Faculty Advisor: Dr. David Hachen

This poster tests a dynamic model of the relationship between the size of a person's social network and depression. Data was collected during the multi-year NetHealth study about college student's social networks (obtained from text and calling records) and their mental health (obtained from periodic surveys). While prior research has shown that people with larger networks are less depressed, we investigate whether having too large of network can increase depression. The model stipulates that people have an expected network size based on their personality, their extraversion level. We expect deviations from expected network size to be problematic and associated with depression. We then expect an adjustment in network size. Depressed individuals with too large a network will experience a decline in their network size to levels that they can manage better. As a result their depression levels will decline as the size of their network gets closer to the size expected by their personality. We test these hypotheses with NetHealth data on depression and network size at two time points, Spring 2015 (their second semester) and Fall 2016 (their third semester). Results indicate that depressed individuals with too large of a network experience a decline in their network size and as a result their depression levels. Depression acts as a mechanism that brings a person's network size closer to the size they can manage given their personality. When individuals exceed their capacity to manage their network, they tend to move closer to their expected network size and as a result their depression levels decrease.

Synthesis and measurement of charge switching in mixed-valence molecules

Grant Barthelems
Electrical Engineering
College of Engineering

Faculty Advisor: Dr. Greg Snider
Grad Student or Postdoctoral Mentor: Matthew Filmer
Other Contributors: Dr. Emily Tsui, Alexei Orlov

As the longevity of Moore's law is in question and limits on heat dissipation force design compromises, such as multi-core processors and dark silicon, new options for computing must be explored. One promising model is molecular based computing, in which one of the first steps is to measure the movement of a single localized electron within a molecule. To do this, a highly sensitive electrometer, such as a modified single electron transistor, must be designed and tested. In this case, the experimental procedure for testing these nanoscale devices is arduous and time consuming as it requires hours of preliminary room temperature tests and then possibly days to achieve the cryogenic conditions needed to test the devices. Thus, in order to make progress more efficiently, automated testing systems must be designed. First, replacing the manual control of the thermal switches within the cryogenic chamber with a motorized system was necessary to allow the different steps of the cooling process to be performed without a user physically present. This system involved designing a mount for a motor and four magnetic sensors, interfacing with them through a microcontroller, and designing a program to track position and correctly command the motor to move as needed. The next step is to address electrical testing. With many pads per die leading to many different devices, automated room temperature testing would significantly speed up the process. This was accomplished by fabricating and debugging a previously designed custom switch matrix and computer program which can quickly route test signals to various devices within a die, eliminating as much as two hours of testing time per die. Lastly, in order to produce the precise tunnel junctions within the electrometers consistently, the use of super-smooth high entropy materials is desired. To do this the lithography and etch steps to a fabrication process were developed and tested.

WiFi Leaf Detection System

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Every fall many places in the US are faced with the management of fallen leaves. In several cities, including the area around the University of Notre Dame, the local municipality is in charge of leaf pick up and disposal to prevent people from simply burning leaves and polluting the air. The issue then lies in knowing the best time to go around and collect leaves. Currently, city vehicles are scheduled to pass through neighborhoods, possibly wasting resources if no/few leaves are there for pick up, or one has to schedule a pick up. So what if there was a way to automatically know when to go around and collect leaves?

We know that leaves can weaken the strength of WiFi signals. But how reliably could WiFi be used to sense leaves or the lack of leaves on trees? This research was motivated by the following questions: Can one efficiently infer the impact of leaves on WiFi with captures of data packets transmitted over WiFi to possibly determine the most efficient time for leaf pick up? Are packet captures too noisy? Are there enough packets?

Currently, for this research, captures of unencrypted data packets have been collected with Wireshark, an open-source packet capture and analysis software, on a Raspberry Pi in multiple locations and on multiple WiFi channels. And code has been written to read the packet captures and analyze the information within the files, specifically the access points, signal strength, and number of packets.

Improving process-guided deep learning approach to lake temperature estimation with data assimilation techniques

Joseph Brennan

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Lake water temperature is a master ecological variable, controlling biogeochemical rates and dictating suitable habitat for fishes. Accurate water temperate prediction in these bodies of water is crucial to inform scientists and natural resource managers how lake contributions to global biogeochemical cycles and their ability to support inland fisheries may change in the future. Process-based models, which rely heavily on scientific theory and focus on physical consistency, have been the classical choice for predicting lake temperatures. However, they often ignore valuable water temperature observations which have been collected by various agencies throughout the past four decades. In contrast, deep learning models rely completely on observations while ignoring physical theories altogether, which can produce predictions that are inconsistent with physical laws. New methods to combine both approaches, called process-guided deep learning (PGDL), leverage the strengths of both scientific theory and temperature observations to improve lake water temperature predictions. In this analysis, we advance the PGDL method further by introducing data assimilation techniques into PGDL, which accounts for uncertainty in both process model structure and temperature observations, thereby producing estimates of water temperature that are closest to true temperature. We demonstrate the utility of this method by applying the modeling technique to Lake Mendota, a well-studied lake in Wisconsin, USA.

Construction of a POMDP Learning Model for Human Robot Collaboration

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The collaboration of humans and robots in the industrial and home environment is essential to the progression of modern robotics. The implementation of a vector auto regressive partially observable Markov decision process (VAR-POMDP) allows humans and robots to collaborate on high level objectives with precision and accuracy. The undergraduate research experience in human robot collaboration is tasked with the implementation of this model in a low-cost personal robot. Creating a system for tracking a unique stochastic (human) model is integral for providing meaningful data to the robotic control system. The VAR-POMDP learning model is recognized for its ability to accurately predict the stochastic actions of a human contained within a predefined environment. Distinct from prior work the proposed demonstration does not predefine human states or transition states in order to show the flexibility of the proposed VAR-POMDP model in many unique situations. A Bayesian non-parametric learning model is implemented in the construction of the demonstration to define potential human states through observable data collected within the operating environment. The states defined by the Bayesian learning model are multiplied by the predefined discretized states of the robotic environment to create a set of all perceivable states. These states form the foundations for a state transition matrix which is used to predict human behavior. The successful implementation of this demonstration has advanced the validity of the proposed VAR-POMPD model. The further implementation of this model in the fields of assisted living and driver assistance systems will induce innovation and advancements.

Sorting Ontologically Narrowed NLP Edited Text with a Scientific Workflow

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“Pace non trovo. Et non ó da far guerra.”

“I find no Peace. But I don’t want war.”

–Petrarch Sonnet 134

Although genocides are rare, their occurrences will always shock and forever leave a devastating, irrevocable impact on the world. Nevertheless, we believe no level of catastrophe goes without warning. Furthermore, this project aims to outline these warnings by mining through stockpiles of news articles in search of possible triggering events. With the help of Information Retrieval (IR), Natural Language Processing with Stanford CoreNLP, and sentence classification with PETRARCH all embedded in the SONNET pipeline, our hope is to use Event Coincidence Analysis (ECA) to predict the potential causes of these mass atrocities and contribute our findings toward future prevention efforts.

Before conducting event coincidence analysis on a batch of news articles, they must undergo a series of annotations, a filter, and an event coder. The SONNET pipeline begins with retrieving millions of documents from the LexisNexis database in an unfiltered XML format. These documents are then loaded into a specific country subdirectory of a library where they will be referenced multiple times for element/attribute extraction during the preparation phase of SONNET. The first of those extractions is the raw text element of each article to be passed into Stanford CoreNLP. Each of these documents possesses a unique ID that the SONNET pipeline utilizes to ensure that every attribute extracted follows the correct document. Next, the raw text elements are parsed and annotated through CoreNLP and emitted as XML files. These files are then filtered and passed through a Python based XML annotator. The annotator then extracts a second round of attributes, the date and source name, from the original documents. Once those attributes are appended to the tagged and filtered XML files, they are placed in a library for PETRARCH to read and code events. After PETRARCH finds the events using the CAMEO dictionaries, all of the event data is compiled and formatted for ECA.

Data mining procedures can vary broadly for political science research. Our initial attempts with this particular project depended solely on human ability. Subsequently, two specific problems have risen from this approach. First, when the number of articles

exceeded a certain threshold (i.e.: 300+ articles) to get a larger scope of information, the task became decreasingly feasible for a human coder. Second, due to varying levels of interpretation among multiple human coders, a manual approach has led to discrepancies among individual data points, resulting in low inter-coder reliability, and possibly inaccurate data analysis. Utilizing an automated workflow resolves both of these issues by absorbing a large threshold of reading material through parallelization and increasing inter-coder reliability through Natural Language Processing and coding ontology. This workflow will greatly assist political scientists seeking to integrate more software into their text mining projects.

Dual-Polarized Monopulse Radar

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Monopulse antennas are used in radar to track targets and are also used passively in radio astronomy and in electronic support measures (ESM). In radar applications, monopulse radar is favored for its ratio-based processing—which offers some resilience to jamming—and it conventionally involves single-polarization implementations. Dual-polarized monopulse concepts, however, are beginning to appear in literature, primarily as a means to augment the monopulse radar's ability to counter jamming. One example is the paper by Zhang and Pan ("Adaptive Countering Technique for Angle Deception Based on Dual Polarization Radar Seeker") which deals with monopulse methods enabled by dual-polarization radar architectures to counter angle jamming. Our goal in the summer research project was to work with data associated with a fabricated monopulse antenna in various tasks, including: 1) synthesizing monopulse antenna patterns; 2) implementing monopulse signal processing techniques; 3) modeling and analyzing system responses to simplistic target scenarios, and finally, including dual-polarized methods discussed in literature that aim to improve jamming-resilience.

To work towards these goals, antenna pattern modeling based on recently fabricated dual-polarized monopulse antennas was achieved using an electromagnetic modeling tool called FEKO. The resulting antenna pattern characterizations were exported to MATLAB where sum and difference antenna patterns based on linear combinations of element patterns were synthesized and compared with the FEKO estimates. Additionally, monopulse radar signal processing algorithms were implemented and applied to simplistic single- and two-target scenarios. Plans are to integrate methods from literature to investigate performance in the presence of jamming.

Improving Hands-On Implementation of Collaborative Intelligent Radio Systems for Congested Wireless Environments

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Current pedagogical techniques of understanding communication systems and hands-on implementations of radio systems are on the decline as more teaching institutions begin to hide key elements of communication systems. One such key element would be the physical radio path which upconverts and down converts a radio signal. The importance of student's comprehension of these key elements will give them the insight to diagnose and find solutions to problems that lay at the core of communications systems. The goal of this project is to devise curriculum and a laboratory setup that is low-cost and packaged to be accessible to academic and government institutions. The research this summer is determining and testing the laboratory setup and materials for the course which consists of a radio path and an ADALM 2000, which is a device that is able to send and receive signals among other features. My role is to utilize On-Off Keying (OOK) modulation to modulate a signal and send it out through an ADALM 2000, then receive a signal through the ADALM 2000, and demodulate it in order to get my original signal that was sent out. This will allow the students to see their signal being sent out and received which will improve the students understanding of how radio systems work. This combined with the theory and laboratories of the course will improve the student's comprehension of an overall communication system.

Adiabatic Circuit Simulation

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Heat dissipation is a major limiting factor in modern computing. Reversible logic is a method of low energy computation that minimizes heat generation by following Landauer's Principle. This states that there is no fundamental lower limit to the energy dissipated when performing reversible operations. Thus, by creating a circuit that performs computations reversibly, we can reduce the heat dissipation. Such a circuit is known as a reversible circuit, which should be run adiabatically to minimize losses.

Our implementation of reversible logic involved 3 logic levels: "1", "0", "NULL". The default logic level is the "NULL" state, logic values will always return to this state. Sharp jumps in potential differences dissipate a lot of energy. In order to prevent sharp jumps, Bennett clocking can be implemented. This involves using ramping "power clocks" and saves energy by avoiding abrupt transitions in the voltage. Bennett clocking involves using a multiple phase clock, with one phase for each level of logical depth in the circuit. The clock phases ramp up successively from lowest logic level to highest, and then ramp down in reverse order. This produces a reversible operation, with ramps that ensure that the costly sharp jumps in potential do not occur.

Automated design tools do not exist for adiabatic circuits, so the physical design must be created by hand. Then a circuit schematic can be generated, which can be used in a simulation using Verilog. This is in reverse order compared with conventional circuit design, due to the lack of design tools. Generating Verilog code from adiabatic circuits is a major advantage since Verilog allows for us to easily simulate circuits to ensure they function as expected. However, when designing adiabatic circuits, the simulation, and verification via Verilog required several steps. The simulations were successful, allowing for the verification that the circuit had the correct output, and that it operated adiabatically.

Development a Flowing Thin-Film Plasma-Liquid System

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The study of plasma-liquid systems is a growing field with a wealth of applications including wastewater treatment, pollutant removal, nanoparticle processing, and medical therapy. These applications hinge on the unique chemistry driven by plasma-liquid systems, which can simultaneously induce reductive and oxidative reactions. Recent experiments processing potassium ferricyanide in a plasma electrolytic cell however, observed a significantly lower faradaic efficiency, the ratio of product molecules to incident electrons, than predicted. This reduced value is consistent with a reaction limited by reactant depletion at the plasma-liquid interface. To mitigate this effect, the aim of this work is to construct a microfluidic flowing thin-film plasma system to examine the effects of transport on plasma-liquid reactions and faradaic efficiency. A microfluidic system was constructed out of polycarbonate and characterized under different flow, plasma, and solution conditions. These findings show that there is an optimal balance of these three parameters in order to achieve a stable flowing plasma-liquid system.

Augmenting Drones Used in Emergency Response

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Drones can be used to enhance emergency response efforts in fire-fighting and river rescue by assisting in diverse tasks and reducing the exposure of human beings to dangerous situations. For instance, fire-fighters currently use manually operated drones to inspect the outside of facilities and difficult to reach areas, and to collect video or sample information from the site of an accident. This project aims to augment manually operated drones with semi-autonomous ones.

To operate autonomously, drones need to communicate with each other over a network. I therefore explored vertex centric frameworks for graph processing (Think Like A Vertex), communication between drones in military applications, Ad hoc On Demand Distance Vector (AODV) routing protocols and Python sockets programming for networking. In AODV, when needed, each node notes a change in neighbourhood topology, and discovers the next hop node in a route using routing tables, the source node's IP address, and the destination address. Broadcasting is achieved by flooding with control packets for route discovery so that, data packets are sent along the discovered route. I developed a prototype for communication between nodes or drones in a graph and implemented a shortest path algorithm in Python for physically separated and moving nodes. The algorithm is a modification of the existing AODV algorithm and has been tested across a network of Raspberry Pi computers.

I visited with fire-fighters to learn about their daily work, experience with their current drones and to identify areas that need improvement. Some of the challenges for drone users are getting a reliable connection to the Wi-Fi network, making plans to bring drones down safely if a component fails, and collision detection and avoidance. I wrote programs to collect and process information about peripherals connected to nodes and attributes of each node. The main results are the prototype, Python programs and user feedback that I wrote for drones.

Analyzing Throughput and Consistency within the Work Queue Distributed Computing System

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Distributed computing systems enable users to design and execute high-throughput workflows by utilizing a large number of resources within computer clusters, clouds and grids. Work Queue is one such distributed system framework. Work Queue's master-worker structure allows users to create a high-throughput application at the "master" machine, and connect "worker" nodes to execute concurrent tasks within the cluster. Using Parsl, a parallel programming Python library developed at the University of Chicago, users can easily write programs that utilize Work Queue to perform their tasks concurrently. Parsl's intuitive syntax of creating Python "apps," or functions, that are run in parallel provides a simplistic approach to user-end distributed computing.

Our research began by examining the Work Queue "executor" for Parsl, the Python module that integrates Work Queue's framework with the Parsl library. In comparison to other Parsl executors, we initially discovered that the Work Queue executor experienced much lower throughput for Parsl tasks. Due to the structure of Work Queue, which uses files to pass data and communicate between processes, the serialization and deserialization of information for each Parsl task became very expensive. After exploring several alternative serialization techniques in Python, we discovered that transferring function information as source code drastically decreased the overall time of writing to and reading from files. As a result, we found that overall throughput on the Work Queue executor could be increased from .5 tasks per second to over 130 tasks per second.

We continued our research by exploring the question of environmental consistency in a distributed system. Due to the heterogeneous nature of these distributed systems, distributed workflows often struggle to maintain consistent runtime environments for their tasks, especially with heavily environment-dependent languages such as Python. The language requires a specific interpreter as well as the necessary module dependencies in order to run its programs, thus making it difficult to maintain consistency between different machines. As a result, tasks within a distributed environment cannot be guaranteed of successful execution due to the possible absence of the necessary dependencies, and certain machines might even be rendered unusable due to their environment configuration, greatly diminishing the total amount of resources available.

A common solution to the problem of Python dependencies is to use virtual environments. Virtual environments create an isolated configuration within the overall machine, and

contain the necessary dependencies that allow the application to work. Environment management systems such as Conda provide simple tools that can be utilized to create and maintain these virtual environments for Python applications. Our research found that these virtual environments provide a great tool to maintain homogeneity between different nodes of a distributed system. Using a parsing algorithm to determine a function's module dependencies, we are able to install the necessary modules into the environment, package it, and send it to a worker machine where the task environment is established. Our study has also created a simple-to-install package containing all of the tools necessary to run Work Queue, using the Conda package management system.

The Path Toward Resilient and Self-Sufficient Refugee-Host Integrated Communities

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Kenya hosts a growing population of nearly 500,000 refugees. Dadaab camp in Garissa county (southeastern Kenya) and the Kakuma camp and Kalobeyei integrated settlements in Turkana county (northwestern Kenya) are the most prominent refugee complexes in the country and home to refugees mainly from South Sudan and Somalia.

Refugees residing in these three camps depend almost entirely on international assistance for their survival. Host governments and donors are urging a shift to increase the self-sufficiency and resilience of refugee populations. Self-sufficient persons lead productive and independent lives while contributing to the broader community; in other words, a self-sufficient refugee would be free from dependence on humanitarian assistance. Likewise, resilience is the ability to manage adversity and change without compromising current and future well-being.

This comprehensive desk review includes an analysis of the past, ongoing, and planned approaches to building resilient and self-sufficient refugee-host integrated communities in Garissa and Turkana counties in Kenya. Further, this desk review consolidated reports from USAID, WFP, The World Bank, UNHCR, and other humanitarian/aid organizations. The findings of this desk review suggest that there is a significant gap between the goal of "inclusion of refugees" and the planned activities proposed by various organizations. However, newly proposed projects such as KISEDP and CRRF may represent an innovative approach for supporting refugees' development and overall resilience.

Above all, this desk review serves as a framework for the field data collection commissioned by USAID/Kenya that will take place this fall by Dr. Oka and his research team. The fieldwork, alongside this desk review, will provide a nuanced and policy-impactful understanding of the complex pathways and barriers to building resilience and self-sufficiency in refugee-host integrated communities.

Spectroscopic Photoresponse System for Measurement of Semiconductor Heterostructure Band-Offsets

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Polarizable materials including ionic polymers and ferroelectrics are being used as dielectrics in capacitors, and gate oxides in transistors for analog memory for machine learning and in new types of circuits mimicking neural signaling. In these applications, the barrier heights presented to electrons in metal-oxide-semiconductor (MOS) structures are key design parameters and are not well known. Our aim this summer has been to configure a measurement system that can dynamically control the energy of incident photons impinging on a semiconductor device and record a photoresponse (e.g. photocurrent, photovoltage, photocapacitance) as a function of applied bias. In a MOS structure there is an energetic barrier to block electron flow across the oxide. Electrons can be excited over the barrier if light with an energy exceeding the barrier is absorbed by the electron. In the presence of an internal or external electric field the electron can flow across the barrier and current can then be detected. By spectroscopically controlling the incident illumination, the onset of this current increase can be used to determine the barrier height. In the case of a ferroelectric or ionic polymer the barrier can be changed depending on the polarization. While this effect has been predicted, this has not been directly measured.

A measurement system has been configured consisting of an Energetiq Laser Driven Light Source, Newport Monochromator, Newport Filter Wheel, Thorlabs optical fibers, Thorlabs detectors, and Keithley sourcemeter. The laser injects light into the monochromator which is then set to a certain diffraction grating and a known wavelength of light is output. This light then travels through the filter wheel blocking all higher order harmonics of light. Coupling this light with an appropriate optical fiber allows for up to 2x10^-5 W of power to be focused on a device. The system has been demonstrated to show detector response in the range from 6.2ev to 0.7eV (200 nm to 1800 nm). Further, a process for fabrication of MOS structures has been designed and a three-level photomask set for fabrication of devices has been designed. Both FET and IPE structures with Corbino disc geometry were added to the mask. The Corbino disc geometry allows measurement of photocurrent in lateral structures without the need for device isolation. Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy/ Atomic Force Microscopy (SEM/AFM) test structures were also added to the mask.

The spectroscopic photoresponse system will not only be fundamental in measurement of the barrier height in ionic polymers and ferroelectric MOS structures, but it also will be made available to other interested users at Notre Dame.

Developing New Infrared Spectroscopy Techniques for Catalytic Reactions

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Infrared (IR) spectroscopy is an important characterization tool for catalysis research that allows for the direct measurement of surface-bound species and leads to enhanced understanding of reaction mechanisms. Here we report on our recent work in developing new IR capabilities for studying catalytic reactions. In particular, we have built an in situ transmission cell to make quantifiable surface measurements and a plasma modified diffuse reflectance IR spectroscopy (DRIFTS) cell to study the effects of nonthermal plasma on surface species. To benchmark these new systems, experiments studying CO adsorption on various metals and CO hydrogenation within an unmodified DRIFTS cell were done. CO adsorption on metal surfaces is a well-characterized system making it a useful testcase for developing new techniques. Previous studies from our group have demonstrated the enhanced activity within catalytic reactions from the presence of a nonthermal plasma, though the mechanism behind this enhancement is unknown. Through the plasma modified DRIFTS cell we will be able to replicate these experiments and develop insight into the mechanism behind the enhancement of the surface-level catalysis being carried out. The last device we have begun building is an IR transmission cell. This cell will provide us with a means to quantify surface species present in our catalytic reactions in the IR, something that the DRFITS cell is unfortunately unable to do due to its inability to fully collect and send the light transmitted from the sample to the detector. The development of these techniques will ultimately allow us to carry out more detailed and quantifiable catalytic reaction studies and expand the range of conditions we are able to perform measurements under.

Ni_2P and Fe_2P Catalysts Synthesis and Characterization

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The dehydrogenation process of converting alkanes to alkenes is important in CISTAR's efforts to turn small carbon chains into longer ones. In order to do this many other materials have been used as catalysts, such as platinum tin. The tin in platinum tin helps separate the platinum atoms, making the catalyst more selective to the desired products. Phosphorus in metal phosphides can act similarly to tin in platinum tin by helping to separate the metal atoms. We looked at two metal phosphide catalysts, Ni_2P and Fe_2P which are cheaper than platinum tin and have not been investigated as much for this chemistry. We simulated potential crystalline structures of the Ni_2P and Fe_2P catalysts using density functional theory calculations which showed us the equilibrium lattice constants having the lowest amount of energy. The calculated lattice constants matched known lattice constants of the catalysts. To synthesize the metal phosphides we used the process of temperature programmed reduction (TPR). We then used powder X-ray diffraction (XRD) to find the crystalline structures of the catalysts we synthesized. We found that the crystalline structures of our synthesized catalysts matched the known XRD patterns for Ni_2P and Fe_2P, indicating we synthesized the Ni_2P and Fe_2P phases of these materials.

How Halide Composition Influences Temperature-Dependent Perovskite Solar Cell Properties

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Global energy demand is expected to more than double in the next 30 years. To avoid the most harmful impacts of climate change, renewable energy must play a pivotal role in powering our future. Solar energy is a desirable solution as the amount of energy from the Sun that hits the Earth in one hour is more than the world consumes in a year. Recently the field of solar energy (photovoltaics) has benefitted from the discovery of a new class of highly efficient, low-cost light absorbing materials called perovskites, which can be utilized in solar cells. These perovskites are named as such due to their chemical formula ABX3, where A is a cation, B is a metal, and X is a halide anion such as bromide or iodide. The perovskite composition can be easily tuned by adjusting the halide component, which changes the perovskite's ability to absorb light, enhances its ability to carry charges, and increases its stability against moisture. To date, the highest perovskite solar cell efficiencies reported utilize a mixed halide composition (with bromide, iodide). In addition to these beneficial properties, perovskites also exhibit an unusual property: the ability of the material to absorb light is highly dependent on temperature. This means that in the operating range of a solar cell (typically 0-100°C) its performance will also be highly temperature-dependent. It is thus crucial that we understand how perovskite solar cell operating efficiency changes with temperature to predict its overall performance in the field. In this study, the influence of the halide composition on the temperature-dependent light absorbing properties of the prototypical perovskite methylammonium lead halide (MAPbX3) is investigated for the full range of halide ratios. Additionally, solar cells utilizing these compositions have been tested at room (23°C) and high (100°C) temperatures to investigate the impact of temperature-dependent light absorption on the real-world parameters that affect solar cells. Future directions include investigating the mechanism of how temperature affects the movement of charge (electrons) within perovskites at various temperatures to provide a deeper explanation of our results. This study will elucidate the extent that halide composition influences perovskite solar cells and will allow for better prediction of solar cell efficiencies operating under real-world conditions.

CANO's Effect on Disadvantaged Communities: Evidence of Domestic Violence Perpetuation

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The majority of acts of violence against women, including homicides, are committed by intimate partners or ex-partners. Domestic violence imposes a burden on society by reducing victims' physical and psychological wellbeing as well as their productivity in the labor market. Previous research has uncovered some of the factors that affect domestic violence, including women's potential wages relative to men, unilateral divorce laws and emotional cues. However, the relationship between housing security, homelessness and domestic violence has not been well disentangled. Domestic violence can be a cause of homelessness but also a consequence, if for example fear of homelessness reduces a victim's ability to escape the abusive situation or to report incidents to the police. In this project, we estimate the causal impact of local nuisance laws on reporting of domestic violence and eviction rates. Criminal activity nuisance ordinances (CANOs) penalize property owners when certain types of activity occur on or near their property, reported primarily through 911 calls to a residence. A large body of qualitative research links CANOs directly to tenant eviction. This eviction threat may create a strong disincentive for tenants to call for police assistance, even when their own physical safety is at risk. Our analysis examines the first order effect of CANOs on eviction risk, the mention of domestic violence in CANOs on eviction rates, and the effect of CANOs on intimate partner violence reporting rates. Our data include police-reported municipal level crime incidents, municipal level evictions data, and CANO legislation for cities and towns in Ohio collected from municipal websites or municipal town hall offices.

Simulating The Effects of Climate Change on SRP Load in a Midwestern Agricultural Watershed

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Nutrients in agricultural runoff have been identified as an important cause of eutrophication in large downstream water bodies such as the Great Lakes and the Gulf of Mexico, where harmful algal blooms and hypoxia have caused major impacts to both human systems and natural ecosystems. Global climate models project strong seasonal changes in precipitation and air temperature (T) patterns over the Midwest and Great Lakes region in the coming decades. For Indiana (IN), winter and spring precipitation are projected to increase by 25-30%, and temperatures are projected to increase by about 5.5 °C by the 2080s for the RCP 8.5 emissions scenario for the ensemble mean. With climate warming, precipitation falling as rain is expected to increase, whereas precipitation falling as snow is projected to decrease. In IN the ratio of precipitation as snow to precipitation as rain is projected to decrease by approximately 50% with warming. These shifts in the hydrologic cycle have been shown to increase winter and spring runoff and flooding in many areas of the Midwest and Great Lakes region. Increases in high flows are, in turn, expected to increase turbidity and nutrient concentrations in streams, especially in winter, when loss of snow cover will expose bare soils more frequently in a warmer future.

Scientists use process-based hydrologic models such as the Soil Water Accounting Tool (SWAT) or statistical models like linear regression to determine the level of the environmental impact that runoff has on water quality for both historical and future conditions. The goal of this study was: a) to evaluate the performance of predictive models of SRP load, and b) to determine the expected nutrient load for a future climate scenario for the 2080s. The study was carried out using data collected for the Shatto Ditch, a small agricultural watershed in Indiana. First a linear regression model was fit between daily-time-step streamflow simulated by a calibrated SWAT model and observed/modeled Soluble Reactive Phosphorus (SRP) load for 2007-2013 interpolated from grab samples using the LoadFlex model. The regression model was then compared to the SWAT simulations for SRP load for the same time period. The results show that the regression model has somewhat higher skill in predicting SRP load (NSE = 0.384) than calibrated SWAT simulations (NSE = 0.341). Based on this assessment we used projected future streamflow from SWAT as inputs to the regression model to predict future SRP load for the RCP8.5 scenario for the 2080s. In response to climate change, average monthly nutrient load in the Shatto ditch is shown to increase in cool season (nov-apr)

and decrease in warm season (may-oct), with an annual total increase of SRP load of about six percent.

Assessing the Relationship Between Spousal Attachment and Parenting Stress

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The role of attachment remains pertinent throughout the lifespan, providing a framework for relationships formed in childhood and adulthood. Individually, secure attachment improves one's ability to emotionally self-regulate (Cassidy & Shaver, 2016). Within partnerships, secure attachment promotes a strong foundation of trust, emotional support and reliability between partners. Parenting stress, or the stress that arises when the demands of parenting exceed the resources available, affects both the individual, their partner, and their children (Sanner, 2017). There is an abundance of research on the negative effects between parent-child attachment and parenting stress, but very little has been done to analyze the relationship between spousal attachment and parenting stress. Because secure attachment provides emotional support and regulation, it was hypothesized that securely attached couples would report lower levels of parenting stress. Participants included ~200 couples with an infant who completed self-reports using the Parenting Stress Index (PSI) (Abidin, 2012) and Spousal Attachment Style Questionnaire (SASQ) (Becker et. al, 1997). Both mothers ($r(201)= -0.343^{***}$) and fathers ($r(195)= -0.338^{***}$) with higher levels of secure attachment to their spouse reported lower levels of parenting stress. In contrast, parents reporting higher levels of fearful attachment or preoccupied attachment to their partner reported higher levels of parenting stress (correlations ranged from -0.338 to 0.385)***.

Polymer Membranes with Tunable Microporosity for Gas Separations

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Grad Student or Postdoctoral Mentor: Tanner Corrado

The market for membrane-based technology for gas separations is expanding rapidly as membranes achieve higher levels of permeability and selectivity. Iptycene-based polymer membranes are drawing special attention for their ability to achieve desired combinations of permeability/selectivity, while also demonstrating remarkable resilience to the problems of physical aging and plasticization. The hierarchical molecular structure of the pentiptycene unit (the iptycene unit focused on in this study) adds configuration-based free volume to the polymer, while pentiptycene also allows for the tunable creation of rigid ladder-like polymers, due to inflexible bonding, which also impede tight chain packing, enabling high gas permeability. This strategic building of the polymer is the foundation of the longevity of its internal free volume, which helps maintain its high gas permeability via hindering membrane densification over time. Additionally, bulky substituent groups added on the center ring also help the polymer chain keep its initial shape, while also allowing for tunable selectivity depending on the size and nature of the substituent group. This poster focuses on the design and creation of a series of pentiptycene-based ladder polymers, emphasizing methods and efforts to optimize reaction conditions to improve yields and purity, which is important for the formation of solution-processable, high molecular weight polymers. Challenges in the synthesis of the pentiptycene monomers were approached with a methodical examination of the reaction conditions and purifications. Furthermore, optimization of polymer synthesis reactions was studied using the PIM-1 polymer synthesis as PIM-1 is used in the copolymer with pentiptycene and has similar behavior. Film casting conditions were also experimented with in efforts to reproduce consistent, defect-free thin polymer films for testing. Finally, the addition of a bulky, branched isopropoxy substituent group to the center ring was performed in order to better understand its effects on polymer solubility, microstructure, and gas transport performance vs. a linear substituent group attached to the same location. Through optimization of reactions, time and effort is continually saved as yields increase, and higher molecular weight polymers are more feasible as purity of the pentiptycene monomer increases. Additionally, tuning of the polymerization procedures led to enhanced polymer solubility and better control over the molecular weight. This poster presentation will cover the design process of the pentiptycene copolymers, the optimization of the reaction procedures, and characterization of the final membranes.

How Teacher Support Affects Math Attitudes and Active Procrastination in High Achieving Students

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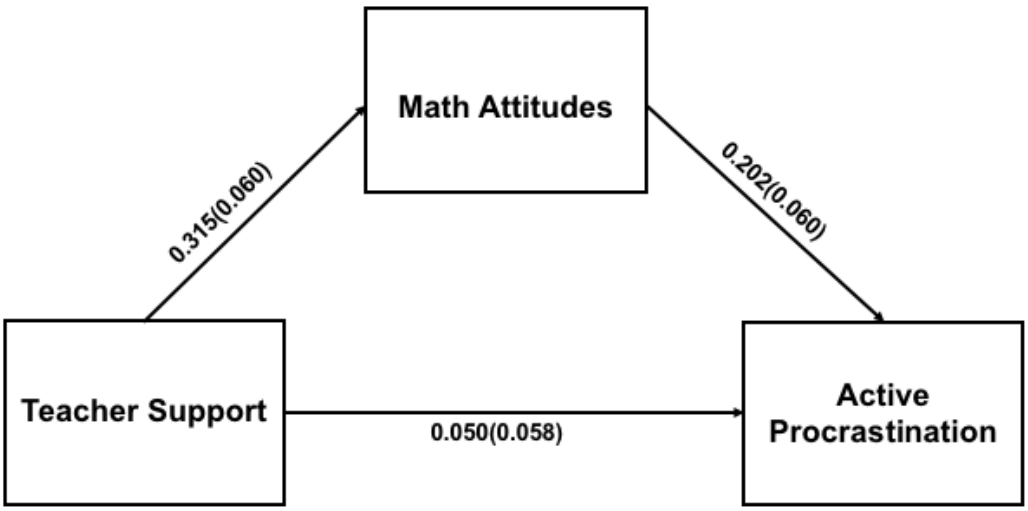
Past research has shown that teachers are important in the development of positive attitudes towards math, which includes boosting self-confidence in their ability to perform in mathematics (de Lourdes Mata, Monteiro, & Peixoto, 2012). Interestingly, some research has shown that among high-achieving students, greater confidence in their ability to succeed, however, is positively associated with active procrastination, which is procrastinating deliberately due to preference for working under pressure (Schraw, Wadkins, & Olafson, 2007). These constructs are important to look at together as no research has looked at the link between teacher support, math attitudes, and active procrastination in high-achieving students. The current study aims to create a mediation model in which teacher support impacts active procrastination with math attitudes as the mediator in high-achieving students. Participants included 319 high school students enrolled in an AP Statistics course (mean age = 16.92, SD = 0.92, 56% female). Math attitudes were measured with a shortened version of the Attitudes Towards Math Inventory (Lim & Chapman, 2012). Active procrastination was measured with the New Scale of Active Procrastination (Choi & Moran, 2010); on this scale, a higher score represents a more positive attitude towards mathematics. Teacher support was measured with a researcher developed scale based on a previous collection of teacher support data (Klem & Connell, 2004). Analysis examined the indirect effect of teacher support on active procrastination mediated by math attitudes. Teacher support had a direct effect on math attitudes ($\beta = 0.180$, $z = 2.977$, $p = .003$). Math attitudes had a direct effect on active procrastination ($\beta = 0.304$, $z = 5.033$, $p = .000$). Teacher support had no direct effect on active procrastination but did have an indirect effect via math attitudes ($\beta = 0.055$, $z = 2.563$, $p = .010$). These findings could be due to teacher support improving self-confidence which increases the use of the work-under-pressure strategy in high achieving students. Future studies could look at how effective active procrastination is for learning and understanding mathematics as opposed to just performance in mathematics.

Table 1

Standardized regression coefficients and standard errors for direct and indirect paths

Paths	Standardized Coefficients (SE)
Indirect Effects	
Teacher Support → Math Attitudes → Active Procrastination	0.064(0.021)*
Direct Effects	
Teacher Support → Active Procrastination	0.050(0.058)
Teacher Support → Math Attitudes	0.315(0.060)***
Math Attitudes → Active Procrastination	0.202(0.060)**
Total Effect	0.114(.056)

* p < .01, ** p < .003, *** p < .000



Hydrothermal Synthesis of Uranyl-based Metal Organic Frameworks

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Metal Organic Frameworks (MOFs) are coordination polymers consisting of metal ions or metal clusters coordinated to organic ligands to form two or three-dimensional structures. MOFs develop features, such as porosity and large surface areas, from metal-ligand interactions while keeping the electrooptical properties of the metal center and the ligands. This characteristic, along with having simple syntheses, makes MOFs suitable for diverse applications. In the context of coordination chemistry, d- and 4f-block metals are usually chosen for the synthesis of MOFs but MOFs using actinides have also been reported in the literature. For instance, [(Th2F5)(NC7H5O4)2(H2O)][NO3] , and (UO2)3(v-BTC)2(H2O)4 contain thorium and uranium, respectively. Herein, the synthesis and structure of three uranyl-based MOFs, Ba(UO2)2(PO3CH2CO2)2 (BaUC2P1) tetragonal I-4c2, Pb(UO2)2(PO3CH2CO2)2 (PbUC2P1) tetragonal I-4c2, and Pb(UO2)2[PO3(CH2)2CO2]2 (PbUC3P1) monoclinic C2/c are presented. The first two MOFs are isostructural except for the change of counter cation. The third compound has the same overall topology of the first two but with a bent coordination.

Participatory Design Activities To Support The Holistic Review Process For Undergraduate Admissions

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Holistic admissions is a complex and subjective decision-making domain in which application readers attempt to identify students who are both capable of succeeding at a university or college and that fit the needs of the institution. A common part of the process is “committee review” where admissions officers discuss the merits of an applicant, especially those that are not a clear admit or reject decision. In this meeting, an admissions officer is typically responsible for “representing” that applicant for the rest of the committee and arguing for admission as the committee works collaboratively to reach the final recommendation. From prior studies, we suspected that sensemaking and narrative visualization techniques might be appropriate in support of collecting and presenting evidence during the committee meeting. Thus, we conducted a series of participatory design workshops with admissions officers at the University of Notre Dame to better understand the challenges and opportunities in collecting and presenting evidence in a typical holistic admissions “committee meeting”. Based on those workshops, we present designs ideas in support of collaborative decision making and storytelling in the holistic admissions domain. Our findings stand to inform the design of software tools in support of collaborative review processes in general and holistic admissions process in particular.

Adverse childhood experiences and economic opportunity.

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Other Contributors: Katie Hieatt

This research examines the association between childhood trauma and the economic outcomes of adults. Current research documents that adults that experienced trauma during childhood tend to have a variety of poor health outcomes and a higher degree of risk-taking behavior. One shortcoming of this research is that typically, data sets that collect information on adverse childhood events (ACE) collect no other information about childhood conditions. As child trauma tends to be correlated with parental education and income, the lack of information about these childhood conditions represents a potential omitted variable bias in regression models. Our work aims to examine the role that these missing variables play in current research. We will do so by utilizing data from the 1994 National Longitudinal Study of Adolescent to Adult Health (Add Health), a longitudinal sample of students that were 7-12 year of age during the 1994-95 school year. A sample of the original respondents are surveyed every few years and currently, data is available for Wave IV when the respondents were 24-32. Add Health is unique in that detailed data about the respondent's childhood environment was collected while in Wave III and Wave IV, ACE-type questions were also asked. With this data, I estimate models similar to that in the literature where health outcomes are regressed on basic demographic controls and ACE-type indicators. We then can add in the variable that describe the respondent's childhood environment such as parental education and income. The change in the coefficients on the ACE-type variables between these two models indicates the degree of omitted variables bias in other research that is present when one does not consider these childhood economic status variables. A better understanding of these correlations could deliver significant benefits to society by the development of public policy that improves the quality of life of those experiencing unfortunate circumstances early in life.

Improving the Longevity of Lithium Metal Batteries

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Lithium metal has extremely high potential as an anode material for high energy and rechargeable batteries. This is due to lithium's high theoretical capacity and low redox potential, but challenges exist in successfully implementing lithium metal in batteries commercially. Lithium metal batteries struggle to cycle in the long term because of the formation of an inhomogeneous solid electrolyte interphase layer (SEI) on the surface of the lithium. This layer causes the lithium to deposit dendritically and as these dendrites grow, the battery eventually short circuits. Through the production of lithium symmetric cells, I have observed how increased water content in an electrolyte helps form a better SEI. Since the dried electrolyte forms a worse SEI on its own, I am studying the use of an artificial SEI in the form of a coating on the separator and comparing the data to the control. This intentional, regulated SEI gives the lithium metal a uniform surface to plate in charge and discharge cycles, thus improving the longevity of the cell.

The analysis of Nepali pharmaceuticals using paper-based analytical devices and Raman Spectroscopy

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Effective pharmaceuticals make up the backbone of proper healthcare systems. People are put at an unjust risk when medications are compromised, which can occur in both developed and developing countries. In order to ensure adequate healthcare for all, inexpensive, rapid, easy to use, and scalable devices are being developed to test for substandard, spurious; falsely labelled, falsified and counterfeit (SSFFC) medical products. The purpose of this project was to assess the quality of Nepali pharmaceuticals utilizing yeast based paper-based analytical devices (BioPADs) and Raman Spectroscopy to detect prednisone or prednisolone in allopathic (pharmaceutical) and ayurvedic (holistic healing system) medicines. Samples, collected during the summer of 2018 by Heather Shepherd ('19), were subjected to BioPAD testing. Preliminary testing suggested a number of the ayurvedic medicines may contain prednisone, though further development of the BioPAD is required. Collecting during the summer of 2019, following the World Health Organization (WHO) sampling guidelines, resulted in a total of 135 allopathic and 114 ayurvedic samples collected from four regions of Nepal: the Kathmandu Valley, Pokhara, South, and Southwest. Testing of the 2019 allopathic samples from the Southwest region using Raman Spectroscopy indicated ~80% of the tablets contained prednisolone. The lack of prednisone or prednisolone suggests that the API may be either too low for detection, or not present at all. Further testing with a quantitative method, liquid chromatography mass spectrometry, is planned to validate the qualitative BioPAD and Raman results.

High-Throughput Polymer Membranes as Platforms for Tailored Chemical Functionality

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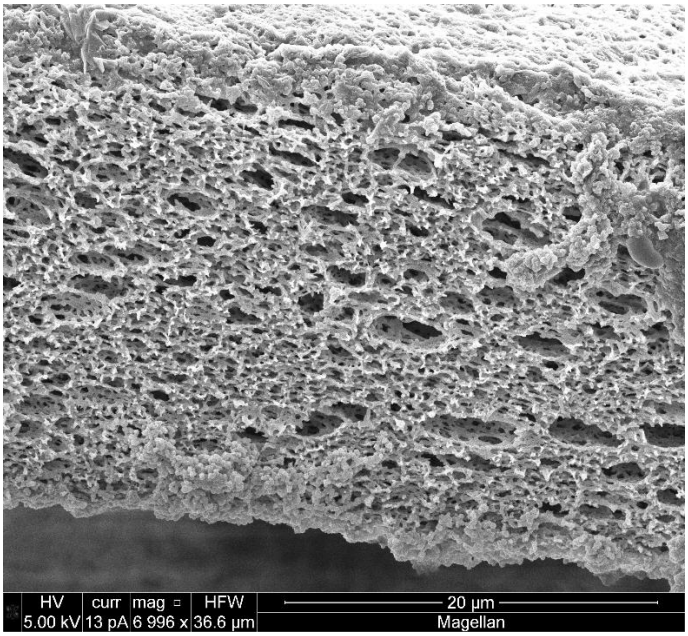
The surface-segregation and vapor-induced phase separation (SVIPS) membrane casting process provides a platform for producing polymer membranes that are tailored for a multitude of flow-through applications. Perhaps the most important feature of this platform is the inter-connected pore structure present in the membrane that the process yields. The bicontinuous pores allow for a high throughput (~7000 L m–2 h–1 bar–1), while also greatly reducing mass transfer resistances between target particles and the pore walls of the membrane (Figure 1). Maximizing the interactions between target solutes and pore walls is important because the SVIPS process allows for chemical functionalities along the pore walls to be tailored in a controlled manner. Polymer functionalities have thus far been preserved through the casting process, while the location of the tailored moieties in the pores allows for further chemical functionalization after casting as well. Therefore, this platform can utilize a multitude of functionalities to efficiently perform filtrations, separations, and reactions.



Generation of Plasma Activated Water (PAW) using Mechanical Actuation of Piezoelectric Crystals

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Grad Student or Postdoctoral Mentor: Jinyu Yang

A hand-cranked system for piezoelectric actuation was developed to observe plasma-surface interactions with water. Piezoelectric spark igniters were implemented into a constant-torque producing system for pseudo-transient sparking. The discharge current generated by the applied piezoelectric spark igniters was measured to be approximately 409.9 mA during a time of 90 ns. The pH of water was observed to decrease drastically from 7 to approximately 2 with an activation time of 5 minutes. This decrease in pH is believed to occur due to plasma interactions with nitrogen concentrations present in air. Sodium perchlorate and sodium chloride were used to increase the conductivity of the solution, and nitrate concentrations from a small volume of sodium perchlorate solution were measured after 5 minutes of plasma exposure. Nitrate concentrations were measured to be approximately 1.5-2.5 mg/l. These values were promising when compared to concentrations recorded using other forms of plasma generation. The findings from this study have strong implications in the field of plasma agriculture due to the potential of plasma activated water for enhancing plant growth.

Self-Esteem Levels by Race, Gender, and Network: Students of Color on a Majority White Campus

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Using a dataset collected at the University of Notre Dame regarding social networks and health data, this research focuses on the intersections of race, gender, self-esteem, and racial homophily, or similarity of one's social network to one's own self on a majority White campus. Based upon previous research, people of color progress through what is referred to as Cultural and/or Racial Identity Development in which they develop their own identity in an environment where they are the racial "outsider" (Allen, 1992; Coard, Breland, & Raskin, 2001). As people of color progress through the phases of this model, their comfort with their skin color fluctuates. This phenomenon, when applied to this dataset, shows the same sensation in the self-esteem levels of students of color. In the early waves of the survey, self-esteem is low, then rises, then falls, reflecting this exact pattern. Overall, the self-esteem levels of people of color and women were lower than those of Whites and men. Social network composition also impact self-esteem levels.

Black networks, in general, consist of more cross-racial ties and are larger than White networks (Cazenave, & Straus, 2017). Same-race friends are also very important to the support systems of Blacks (Ueno, 2009). When projected onto the data, It was found that the more racially homophilous, or similar, one's network is, the higher the self-esteem, reflecting the need for same-race social ties. This finding can also be projected onto gender as it was found that the higher the proportion of females in a social network, the higher self-esteem.

This research highlights the lasting effects of racism and sexism, as students of color and women were shown to have lower self-esteem overall. The need for same-race and same-gender relationships possibly reflects the necessity of a support system of similarity in a place where students of color and women are viewed as the "other." Within a majority White university, the self-esteem of students of color rely on a growth period as well as support from those in their networks to become accustomed to and develop their own identity.

HEMT-High Linearity GaN Transistor

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Grad Student or Postdoctoral Mentor: Nivedhita Venkatesan

In the world of wireless communication, HEMT's(High Electron Mobility Transistors) play a critical role in the recent development. Because of the unique property of high power, high frequency, and high gain, it makes a great candidate for military and commercial wireless applications. For cellar station application, GaN transistor device is more efficient at higher frequency with broader bandwidth than the Si LDMOS(Silicon laterally diffused metal oxide semiconductor device). Which in terms, give us a higher data transfer rate. For military applications(Radar), Because of the higher bandgap of Gallium Nitride semiconductor material, GaN HEMT is the perfect replacement for the GaAs pHEMTs as it could achieve higher power, higher frequency, and higher bandwidth at the same time.

The goal of our research is to develop a GaN device model as an amplifier that will be able to satisfy our ever advancing technology needs in the next few decades. As of now, we are in the early development phase where we model our device in the Synopsys Technology Computer Aided Design (TCAD) and optimize it in the Advance Design System(ADS)for higher gain, OIP3, and IIP3 value. My task in the research includes doing analytical Figures of Merit for the model device and experimenting Low Pull simulation as an alternate, more efficient way to get load impedance from the model, which speed up the research progress.

Applying Event Coincidence Analysis to Predict Triggers of Mass Atrocities

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Event coincidence analysis (ECA) is a powerful statistical technique which is specifically attuned to the relationships between series of rare events over time. ECA enables researchers to identify the strength, directionality, and time lag of the relationships between these occurrences within an interval of time. This analysis applies ECA to an examination of potential rare event triggers to mass atrocities that have been identified via the SONNET pipeline. This software encodes the syntactical elements of sentences to be passed through Petrarch which then locates trigger identifiers. In this initial analysis, we utilize the LexisNexis news article database to retrieve articles which have been tagged for potential triggering events, such as coups, by human coders to validate this newly developed pipeline for event coding. Our aim is to use the software to better understand the precursors to mass atrocities in order to inform prevention efforts.

Software-Defined Antennas with Phase-Change Materials

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Reconfigurable antennas have become increasingly relevant for wideband spectrum operations as the frequency of distributed circuits corresponds to their physical geometry. Currently, advanced RF ICs enable extremely wideband radios, but lack corresponding antennas and other distributed structures. Reconfigurable distributed circuits have been realized with switch networks (e.g., antenna array, switch matrix) which limits flexibility. Another method to achieve reconfigurability in such distributed structures is with spatial patterning of phase change materials such as vanadium dioxide(VO2). These materials exhibit spatially dependent conductivity between that of an insulator and a metal depending on the local temperature of the medium. By incorporating a micro-heater-array below a film of VO2 conductive circuits can be “drawn” or programmed. However, the conductivity of VO2 in its metallic state is 105 S/m (107 S/m for metals). By incorporating metallic inclusions into the VO2 film, the loss can be reduced to acceptable levels.

In addition to being thermally activated, VO2 can be field activated--that is, by placing an electric field across the material which is beyond some critical switching field, the VO2 can be induced into its metallic state. While the critical field is fixed for the material, the corresponding critical voltage depends upon electrode geometry. In this work, we propose to engineer metallic inclusions with varying radii of curvature and gaps in order to make a settable critical voltage. In such a way a single analog voltage varied from, e.g., 0V to 10V could be used to program the length of an antenna depending on which band radio must operate. We refer to this as a software-defined antenna.

We examined the electric field between two conducting spheres as a way to set the switch point. Theoretical analysis and ANSYS HFSS full-wave electromagnetic simulations were used to quantify the field between the combination of electrode designs. Generally, the peak electric field is inversely proportional to the radius of curvature and gap size. Based upon these results, we designed a programmable antenna with intermittent electrodes of progressively higher critical voltages. In such a way, a low control voltage results in a short antenna (high frequency) and as the control voltage is increased it switches the next (longer) electrode into its metallic state thereby increasing the length of the antenna. We compare the performance of this programmable antenna to a conventional fixed antenna. Gain and input match are shown to be tunable over a wide operating frequency range while the fixed antenna has a single operating band. Future work will aim to develop a prototype based upon this preliminary design.

Triple Point Enhancement of Thermally-driven Plasma Generation

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Grad Student or Postdoctoral Mentor: Jinyu Yang
Other Contributors: Seong-Kyun Im

Traditional methods of generating non-equilibrium gas discharges have involved using electrodes at hundreds to thousands of volts, but by taking advantage of the material properties of non-centrosymmetric crystals, a plasma can be generated with alternative sources of energy such as vibration or heat. In this study, a lithium tantalate pyroelectric crystal was thermally cycled with a resistance heater to produce an atmospheric pressure gas discharge. Due to the intrinsic properties of the crystal, a change in temperature with respect to time creates a significant electric potential at the crystal surface, leading to the breakdown of the nearby air molecules and the formation of plasma. A copper plate parallel to the crystal and a picoammeter were used to determine the current of the plasma. By coating the pyroelectric crystal with a pattern of silver paint, “triple points” were created that significantly enhanced the resultant current of the discharge, which was found to be on the order of 1-2 nA for an unmodified crystal, and on the order of 30 nA for the painted pyroelectric. Time-integrated visualization showed the formation of surface discharges on both crystals during the thermal cycling. With further study, substantial discharges could be generated without the need for a power supply, and potentially lead to the development of portable plasma devices, air and water purification via waste heat capture, or surface modification.

Dysphoria and Well-Being in Daily Life: Constructing Valid Short Forms for Ecological Momentary Assessment Studies

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Daily life studies are a growing area of research due to their ability to provide important details about symptoms of disorders as they are occurring in natural contexts. Daily life studies utilize methods of collecting data that involve self-report assessments occurring several times a day in natural settings, as opposed to traditional methods of collecting data at a single point in time in a laboratory; this is often referred to as Ecological Momentary Assessment (EMA). However, there are only vaguely established guidelines for creating and analyzing valid self-report measures that are specifically meant for daily life studies. This project is the first stage of creating and testing the validity of two modified short forms, each consisting of a total of three items, that will be standardized for EMA usage. More specifically, the Dysphoria and Well-Being scales from the expanded version of the Inventory for Anxiety and Depression Symptoms (IDAS-II; Watson et al., 2012), were empirically analyzed using large aggregated data sets. This was done via a two-stage process that allowed for 1) the identification of the most representative items from each scale using both factor analyses and internal consistency analyses, and 2) looking at content and item correlations as guidance for the selection of two additional non-redundant items for each scale. The process of creating these scales, as well as the upcoming process of testing them, will be used to inform future scale creations and promote ecologically sound methods of data collection for daily life studies.

Poster #40

Video Games as Escape in a Crisis of Masculinity

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In Manhood in America: A Cultural History (2018) Kimmel describes American manhood as rooted in the ideal of the “Self-Made Man,” in which masculinity is entirely dependent upon one’s work in the public sphere (p.13). Economic and social changes in American society have led to recurrent “crisis of masculinity,” as men are no longer able to achieve “self made” manhood. Kimmel finds that men cope with such crises by escaping to homosocial fantasies, such as the frontier, 19th century fraternal orders, sports, and the sexual fantasies of Playboy. Today, certain genres of video games are found to be prominent homosocial escapist media (see: Vanderhoef, 2013; Ecklund, 2012; Blackburn & Sharrer, 2019). Drawing on regional sales data of 16,598 video games, I compare the means of genre sales between North America, with a self-made man model of masculinity, and Japan, with a softer version of masculinity, to determine if North America has higher sales of genres associated with escapism and exclusion. Further, Using a sample of the highest selling games from the highest selling genres in North America, I conduct a content analysis of 25 official game and sales websites coding for themes from the historical escapist products described by Kimmel (2018). The findings suggest that video game sales in North America are positively associated with genres most associated with masculinity, and the highest selling games within these genres exhibit escapist themes, especially escaping to homosocial fraternities and sports. This research supports a contemporary crisis of masculinity in America is occurring as a result of rapid social and economic change and men’s continued use of escapist media to recreate the past.

Development of Eu(III) Complex Coatings with Oxygen-Sensitised Luminescence

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Grad Student or Postdoctoral Mentor: Daiki Kurihara

Photochemical sensor technologies have applications as diverse as measuring breath alcohol levels, tracing the spread of cancer cells and heavy metal detection.Changing conditions in the sensor molecules' microscopic environment are detected macroscopically by observing some change in the colour or intensity of the light absorbed or emitted by the material.

Fluorophores whose emission is quenched by the presence of oxygen have found applications in aerospace engineering. Higher partial pressures of oxygen (corresponding to higher total air pressure) yield lower intensity emission. If a layer of such a molecule can be absorbed onto a surface, the pressure distribution across that surface can be measured by observation of the varying intensity of the pyrene's emission across the surface. This is referred to as a Pressure Sensitive Paint, or PSP.

In order to obtain similar information about an object in motion, a second dye whose emission is not heavily pressure dependence is required. This dye acts as a reference dye to compensate for the fact that observed light intensity depends on the distance between the source and the observer. This type of 2-dye paint is referred to as a two-colour PSP.

Discussed here is the potential application of sensitised Europium complexes as the signal dye in a two-colour PSP. The normally pressure-independent emission of Eu(III) complexes can be sensitised to changes in pressure by the addition of a pyrene-derivative molecule which is strongly quenched by oxygen. It is suggested that a pressure-dependence in the characteristic strong, sharp emission peak of Europium complexes would be favourable for two-colour PSP applications.

Characterizing Information Leakage in Low Power Wireless Modules

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Faculty Advisor: Dr. Siddharth Joshi
Grad Student or Postdoctoral Mentor: Mark Horeni

Many Bluetooth chips are vulnerable to wireless attacks because the digital logic and radio transceiver are on the same integrated circuit, causing them to be too close to each other. The digital circuit performs cryptographic tasks and the radio transceiver broadcasts the signal. The closeness of the two allows information from the digital circuit to leak electromagnetically into the radio transceiver and be transmitted as noise in the Bluetooth signal. After enough data is collected an algorithm called correlation radio analysis (CRA) can decrypt the keys. Due to the variability of silicon in the fabrication process it is not likely that a CRA trained on one chip will work on many other chips. Our research set out to train a convolutional neural network (CNN) using the same data collected for CRA to create a more generalized algorithm. Data was collected wirelessly with a software defined radio (SDR) while the Bluetooth chip was continuously broadcasting and encrypting a plaintext message. The keys stayed the same while the plaint text changed. An SDR equipped with a well working CNN could be placed in a room discreetly and decrypt Bluetooth signals.

Fabrication of Ductile yet Tough Polymer Composites

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Grad Student or Postdoctoral Mentor: Yungsong Pang
Other Contributors: William Cumberland, Liu Jianuo

In this work, we demonstrate a molecularly aligned, graphene reinforced polyethylene (PE) and polydimethylsiloxane (PDMS) composite substrate that exhibits very high flexibility, stretchability and strength. A process for creating high-strength PDMS-PE composites through corona treatment bonding and stretching is described. During this process, the PE and PDMS are treated with silane coupling agents, which increase the bonding affinity of both materials. The PE and PDMS are then laminated together in a stretching device, producing a composite that is able to be stretched up to a point but also has high tensile strength. This process is applied in order to create flexible electronics with greater tensile strength and durability than pure-PDMS based electronics. Different composition ratios between the PE and PDMS have been investigated, as well as different mixing ratios of the PDMS itself. A stretchability of over 120% and average tensile strength of 3.78 MPa are observed, which demonstrates that desirable properties of both PDMS and polyethylene are incorporated into this material. After the material was created, we also investigated the possibility of printing conductive graphene layers onto the material through aerosol jet printing. The devices created through this process hold potential for use in many different areas of flexible electronics.

Solvent-in-Salt Liquid Crystalline Electrolytes for next- generation rechargeable batteries

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Faculty Advisor: Dr. Jennifer Schaefer
Grad Student or Postdoctoral Mentor: Jiacheng Liu

Organic liquid electrolytes are a key component in commercial lithium ion batteries as they permit conduction of lithium ions between the cathode and anode. Electrolytes that have high ionic conductivity are ideal as they allow the lithium-ion battery to charge/discharge efficiently. However, these electrolytes currently raise safety concerns as they are easily flammable and unstable towards high voltage and temperature. We introduce a new set of Solvent in Salt electrolyte that improves ionic conductivity and solvent stability, by utilizing Li+ containing liquid crystals as the salt. Additionally, liquid crystal molecules possess ordered liquid crystal phase which permits faster ion transport. By combining the two merits, we observed that the ion conductivity of the above system showed improved conductivity and stability.

Dynamic Peptide-based Nanomaterials for Enzyme Targeted Drug Delivery

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Drug delivery systems are devices and nanotechnologies which allow medications to be delivered more accurately to sites of disease, increasing drug efficacy while decreasing adverse effects on healthy cells. Peptide-drug conjugates are an exciting tool for drug delivery due to their innate biological composition, highly defined chemical structure, and ability to form tunable, self-assembled nanostructures which add to drug delivery function.

In this project, anti-inflammatory corticosteroid Dexamethasone (DEX) was conjugated via a hydrazone linker to various amphiphilic peptide sequences, ranging from 5 to 7 amino acid residues. The design of these drug amphiphiles (DA) was intended to promote the formation of long nanofibers, providing drug release over time due to the slow hydrolysis of DEX from the hydrazone bond. Solutions of DAs were found to form hydrogels in physiological buffer, suggesting the system could serve as a site-injectable delivery material for sustained release of anti-inflammatory. This NDNano project focused on the synthesis and characterization of the DA molecules, hydrogelation kinetics, and drug release. Future work in the project will include modifications to the peptide sequence which incorporate enzyme sensitivity as a means of identifying sites of chronic inflammation.

Fabrication of Gold Nanoplates Using Substrate-immobolized Seeds Lined with Planar Defects via a Directed-Shock wave

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Numerous applications of Au nanostructures, such as sensors and photovoltaics, require that they be immobilized on a substrate surface. Specifically, planar structures such as hexagonal Au nanoplates generate a plasmonic resonance that is tunable from visible to infrared frequencies, giving it potential applications that are not readily realizable using other plasmonic structures. However, the synthesis of substrate-immobilized hexagonal Au nanoplates remains a challenge due to the severe restrictions placed on the seeds used to promote growth and in adapting colloidal syntheses to the substrate surface. Here, we present a novel method for the solution-based synthesis of substrate-immobilized hexagonal Au nanoplates on sapphire using only the block copolymer Brij 700 and a Au3+ source, i.e., HAuCl4. The growth mode observed is kinetically driven and has been optimized with respect to the copolymer and Au salt concentrations, pH, temperature, and growth time. The initial fabrication of Au seeds is achieved through the solid-state dewetting of ultrathin Au films on sapphire substrates in combination with a sacrificial Sb layer. The unavoidably high crystallinity of Au seeds achieved via solid-state dewetting schemes, however, constrains the yield of structures containing the planar defects needed to promote nanoplate growth. Here, we prototyped a simple device designed to induce planar defects in single crystal Au structures by means of a manually generated shockwave through an aqueous environment. Preliminary spectroscopic data shows that the shock wave altered the Au morphology.

Microbial contamination of Ayurvedic medications collected in Nepal

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Microbial contamination of herbal medicinal products, specifically Ayurvedic medications, presents a potential threat to human health. It is currently estimated that up to two thirds of developing countries depend on herbal medicine as a primary source of drug therapy. Traditionally, developing countries have made up the majority for the use of herbal medicinal products, but acceptance of these preparations in the West is becoming increasingly prevalent. The purpose of this study was to assess the microbiological quality of Ayurvedic medications distributed in Nepal. A total of 50 Ayurvedic samples collected in Nepal were subjected to microbial isolation and identification tests following standard procedures in the laboratory at Saint Mary's College. Isolates were identified based on diagnostic staining, cultures and biochemical tests. Five control samples produced and distributed in the United States were included as negative controls. Microbial growth was obtained from 88% (39) of the total samples tested, and included 61 Gram-positive and 23 Gram-negative isolates. The Gram-positive isolates consisted of Corynebacterium spp. (23), Bacillus spp. (15), Brevibacillus spp. (13), Mycobacterium spp. (8), and Staphylococcus epidermidis (2). The Gram negative isolates included Enterobacter spp. (12), Hafnia alvei (3), Citrobacter freundii (3), and Moraxella catarrhalis (2), Serratia spp. (2), and Proteus mirabilis (1). No Gram-negative bacteria were obtained from the controls. However, eight Gram-positive isolates were obtained and are currently being identified. The results of this study indicate a higher level of microbial contamination in the Ayurvedic medications collected in Nepal compared to the controls.

Biosorption of Rare Earth Elements through Cell Surface Display of Lanthanide Binding Proteins

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Rare earth elements (REEs) are crucial in low-carbon and green energy technologies due to their unique physical and chemical properties. Currently, the extraction of REEs heavily relies on energy- and chemical-intensive metallurgical techniques, which are expensive, environmentally harmful, and inefficient in selectively separating different kinds of REEs. Therefore, there is a critical need to develop cost-effective and sustainable methods to extract and recover REEs. Compared with traditional methods for extraction and separation of REEs, biosorption is considered as an ecofriendly and inexpensive approach for REE recovery. As a step towards to this goal, in this project, a novel biosorbent was developed using cell surface display technique which genetically engineered bacterial cells with expression of a lanthanide-binding protein, called Lanmodulin (LanM), on their surface. The LanM-displayed bacterial cells exhibited improved adsorption efficiency to different kinds of REE ions, ranging from light and heavy REEs, in comparison to the cells without LanM proteins. The findings of this project suggest that there is an opportunity to harness the engineered biosorbent with cell surface display of LanM proteins to separate and recover technologically important REEs in an environmentally benign manner.

Preparation of semi-Interpenetrating Network (s-IPN) Membranes Based on Matrimid® Polyimide and Celazole® Polybenzimidazole (PBI) for Gas Separation Applications

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Traditional forms of industrial gas separation, such as distillation, are energy and cost intensive. Polymeric gas separation membranes present a promising alternative strategy due to good processability, higher energy efficiency, operational simplicity, and the ability to be coupled with other gas processing steps. Limitations of membranes for gas separations include the permeability-selectivity trade-off, plasticization, and physical aging. Plasticization is the dilation of fractional free volume (FFV) that occurs as condensable gas, such as CO2, dissolves in the membrane resulting in the loss of size-sieving capability; whereas, physical aging is induced by densification of free volume over time, which results in lowered permeability. The plasticization and physical aging of membranes can be effectively reduced via chemical crosslinking. Crosslinking builds tightly bonded integral network structures that helps maintain the microporosity by limiting segment movement. Previously, crosslinking studies largely surveyed random crosslinking, which leads to very complicated networks with poor structure tunability and unpredictable membrane properties. As such, to further clarify the ambiguous structure-property relationship, model network structures with well-controlled crosslink density and well-defined crosslink inhomogeneity are highly desired.

This project focuses on the development of semi-interpenetrating network (s-IPN) membranes from two commercial polymers, i.e., Matrimid® polyimide and Celazole® PBI for improved separation performance especially high temperature separation applications. Specifically, this new s-IPN design integrates crosslinked Matrimid® model networks and the superior selectivity of PBI as the penetrating linear chains that are locked in the Matrimid® networks to provide selective gas transportation. In addition, this study has the goal to refine and optimize thermal protocols to form robust s-IPN membranes with maximized performance. By combining these goals, we hope to learn more about the fundamental structure-property relationships to direct high-performance membrane design. This poster will cover the design of the s-IPN membranes, the synthesis of telechelic Matrimid® oligomers of controlled molecular weight, the preparation of Matrimid® model network membranes, the preparation of Matrimid®-PBI s-IPN membranes, and characterization of the final membranes.

Poster #50

Solving semidefinite programs using Bertini and Matlab

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Semidefinite programs are a class of nonlinear convex optimization problems that arise in a variety of applications. These optimization problems actually occur in primal-dual pairs and traditional solvers assume that these problems have the same solution, that is a zero duality gap. Therefore, when the duality gap is positive, traditional solvers typically fail as demonstrated by G. Pataki's test suite. The goal of our research was to develop a numerical algebraic geometric approach for solving all problems regardless of the duality gap. Our solver combines feasibility testing, facial reduction, and homotopy continuation. We implemented our approach utilizing Matlab and Bertini, which successfully solved all of the problems from Pataki's test suite.

Tuning a Hydrogen Bonding Network to Control the Phase, Dynamic and Electrochemical Behavior of Redox-active Deep Eutectic Solvents

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Deep Eutectic Solvents (DES) are recognized as a new class of Ionic Liquids (ILs), particularly known for their simplicity of preparation and having common relatively inexpensive components. DES have potential application areas such as removal of glycerol from biodiesel and processing of metal oxides. In the current work, DES will be used as electrolytes in flow battery systems. The DES studied here are known as type III and are highly adaptable generally consisting of choline chloride and a hydrogen bond donor (HBD). The physical properties of the mentioned systems are highly dependent on the nature of the pure HBD. In this work molecular dynamics (MD) simulations were used to compute physical properties such as density, expansion coefficient, viscosity and self-diffusion coefficient of pure HBD liquids in the temperature ranges of [300K,450K]. These HBDs will be mixed with Choline Chloride to form DESs and the structure-property relationship will be explored.

Iterative design and fabrication of a hexapedal robot

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This project focused on the development of a hexapedal walking robot with the introduction of a six bar, leg linkage design with 1 degree of freedom. Having gone through multiple stages of the design process, the first being an iterative process for the design of the robot as a whole; that being: the leg linkage, the chassis, as well as considering the motors needed, the control board, and the power source. The constraints for this design were a total mass of 300g, a center of mass around half the height of the robot, and compact packaging of motors and a control board. After laying out the design of the robot as a whole, focus was placed on synchronizing the movement of all six leg linkages and removing collisions and interferences in CAD software. Next an iterative prototyping phase took place where the CAD design was 3D printed in order to test the leg linkages effectiveness in following the foot path with no issues. After multiple changes to the design and tweaks to additive manufacturing process variables, we tested a single leg link with a simple rail like system in order to test the synchronization of the system. An effective leg linkage protype was successfully printed using manufactured joint connections and printed links.

Coordinated Robots Through Wireless Communication

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Modern robotics is an expanding field that has become increasingly popular in a lot of areas, including industry, medicine, and agriculture. There is now an increased interest in coordinating larger groups of robots to parallelize common problems and accomplish more complex tasks. The challenge lies in bridging the gap between individual dynamics and their collective behaviors. In this project, we aim to develop a provably correct framework for designing coordination commands for individual agents such that a global goal can be achieved.

The main task of this REU project is to implement an algorithm that deploys a large group of agents into a desired configuration in a decentralized manner. We model the robots' configuration as a probability density function (pdf) and compute the velocity field for the agents based on the difference of the current pdf and desired pdf for which the final convergence can be formally proved. Kernel density estimation is used to estimate the current pdf of the agents. We further parallelize the computation in a way that each agent computes its own local estimation of the current pdf based on its neighbors. This makes it practical when robots have limited sensing, communication and computation capabilities. In order to test this, we simulated Turtlebots using 2D and 3D simulation software to have them converge to distributions and shapes like circles, squares, and triangles. In addition, we find that a small number of real Turtlebots are able to converge to a desired distribution. These results demonstrate that using density feedback control with local estimation to compute velocities can be efficient, accurate, and decentralizable, traits that make it suitable to be introduced into industry.

Exploring Substituent Effects on Friedel-Crafts Hydroxyalkylation via Hammett plot projection

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Reactions involving para-substituted benzene-carbonyl molecules have been recorded in previous works exploring the impact of electron withdrawing/donating groups on kinetics of organic reactions as quantified by the Hammett Equation. This phenomenon is noted to exist primarily in Electrophilic Aromatic Substitution (EAS) reactions that involve aromatic rings attacking electrophilic groups. The type of EAS reaction that we studied here is known as acid-catalyzed Friedel-Crafts hydroxyalkylation, a reaction mechanism that holds its significance with the synthesis of small molecules and polymers. Recently Notre Dame's Gao research lab was able to design a reaction involving para- substituted benzaldehyde groups reacting with 1,4-dimethoxybenzene and made a cursory discovery that the electron effects of the substituents were influencing the reaction rate. This study has created a Hammett plot projection of the reaction of para-substituted benzaldehyde compounds in the reaction with excess 1,4-dimethoxybenzene in order to create a model pseudo first-order reaction that can be analyzed to find the kinetics of the reaction using the same compounds relating back to the previously mentioned polymerization reaction. The substituents evaluated in this study include: Nitro, halogen and cyano electron-withdrawing groups along with methyl and methoxy electron-donating groups. To calculate the initial rate the reaction is monitored using Gas Chromatography to analyze the conversion of the benzaldehyde derivatives in solution, against dodecane as a standard. In this study we have also quantified the effects of temperature on the reaction rate to calculate the activation energy using Arrhenius Equation. By creating a logarithmic relation between the benzaldehyde reaction and the various substituents we have, we successfully create a Hammett plot correlating the electron effects of the substituents to the reaction rate of the polymerization.

Tracking in Indiana's Schools

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Sociologists have been concerned with the presence of racial and ethnic inequalities since the emergence of the field itself (Coleman 1966). American policymakers have adjusted the education system to address its inequalities, with one controversial policy being the tracking system. Tracking is a practice in which students are divided across classrooms and placed into different courses based on a combination of prior performance and student/parental choice (Carbonaro et al 2016). Research has shown that despite these detracking efforts, racial and ethnic inequalities persist in school practices (Brewer et al 1995; Mickelson 2015). Consequently, researchers have delved deeper into possible factors that contribute to the racial gap in schools in addition to race. Gender, family background, and school racial and socioeconomic composition are also important factors to consider in the exacerbation of educational inequality (Carbonaro et al 2016; Covay Minor 2010). This intersection of social positions creates a larger picture of the sources of inequalities in schools and their effects on students.

The goal of tracking is to make learning more efficient and suited to the student's level of ability, but the variation in placement criteria increases the heterogeneity of tracks, leading to overlapping ability distributions (Hallinan 1994). Track placements are not always entirely meritocratic either, and can also reproduce inequalities; for instance, Carbonaro et al (2016) find that students from families with higher levels of educational attainment are more likely to have an academically rigorous curriculum in high school. This project aims to answer two questions: who, by race, places into advanced 8th-grade math courses, and what is the effect of track placements on these student's scores? We analyze data collected from the Indiana Department of Education, which contained course taking records as well as demographic information on each school and student. Using multinomial logistic regression, findings suggest racial differences in the probability of a student placing into either Algebra I or a lower-level course (basic math), controlling for student demographic variables and school context. Findings also suggest differences in placement by gender and free or reduced-price lunch (FRL) status. Specifically, non-FRL Black girls are more likely to take Algebra I compared to Latinas and White girls. Also, all boys, regardless of race/ethnicity and FRL status, are more likely than girls to take basic math. These findings demonstrate the importance of examining the intersection of gender, race, and socioeconomic status when researching education. Recognizing that inequalities cannot be traced to one source, but rather there are many nuances to its impact on students of different backgrounds will ensure more informed educational policies.

Cucurbituril Functionalized Absorptive Membranes for The Detection of Fentanyl in Water

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The overall goal of this project is to design absorptive membranes with high permeability and high binding affinity for fentanyl, a dangerous opioid in water. This project aims to create a way to detect fentanyl in water because there is currently no way to detect pharmaceuticals in water; this limitation can expose people to health complications. Cucurbit[n]uril-based (CB[n]-based) molecules, where n is referring to the number of glycoluril units, are macrocycles that can form host-guest complexes with a variety of chemical species. CB[n]s are essential to this approach because they have high binding constants, which can be modified by manipulating the cavity size. CB [7] is being used for this project because it has a cavity size that will allow it to attract and bind fentanyl. Absorptive membranes were prepared from a composite base material consisting of polystyrene-b-polyacrylic acid and polysulfone. The membranes are made by a casting process. First, the casting solution that consists of polysulfone and polystyrene-b-poly acrylic acid dissolved in 2-pyrrolidone is prepared. An even layer of casting solution is dispensed on a glass slide, then is thinned out using a doctor blade. During this process, the membrane is exposed to humid air for 90 seconds and is then put into a bath of deionized water to sit until further use. Following preparation, the membranes are alkyne functionalized using an EDC coupling reaction, which allows them to covalently-bind with the azide functionalized CB [7] molecule. Fourier Transform Infrared Spectroscopy (FTIR) was done on a portion of the membrane to test the success of the reaction. FTIR indicates that the reaction is successful because there is an appearance of a shoulder peak in the 1600-1700 cm-1 range. The functionalized membranes are then bound to CB [7] using a copper-catalyzed azide-alkyne cycloaddition reaction (CuAAC). FTIR indicated that the reaction was successful, but a way to quantify that success is being investigated. In the future, the membranes will be tested to see if they detect and bind to fentanyl in water.

Dialogue Structure Patterns Predictive of Success in a Communicative Search Task

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Language can be thought of as a joint action between speaker and hearer that requires multiple levels of coordination in order for communication to be successful. In a communicative exchange between speaker and hearer, a response from the hearer showing that the speaker's message has been understood and that the communicative goal has been understood and accepted is typically the evidence that shows that these levels of coordination have been achieved (and that the joint action has thus become part of the common ground between speaker and hearer). We seek to contribute to the literature that explores how this process (called "grounding") takes place in contexts where there is no face to face contact between speaker and hearer and language is by default the only form of communication. In order to gain a wealth of data on the factors that contribute to or detract from the ease of grounding, we proposed an experiment in which a pair of participants-- one designated as the "searcher" and the other designated as the "director"-- complete a complex search task with the director using a map to guide the searcher while communicating remotely via telephone. The dialogue of these participant pairs were recorded, transcribed, and annotated according to the complex dialogue structure coding scheme outlined in Carletta et. al (1997), which uses the categories initiation, response, and preparation as starting points. The coding of these dialogues will allow us to identify communication patterns that lead to more successful communication between the two participants, as evidenced by their success in the search task. Initial data suggests that the extent to which the participants are able to choose answers matching their partner on a survey is correlated to success in the search task.

Poster #58

Prototype Implementation of Frequency domain diffuse optical spectroscopy using a multi-phase approach.

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Frequency-Domain Diffuse optical spectroscopy is a model-based noninvasive imaging and sensing technique that can be used to measure chromophores concentrations such as hemoglobin, water and lipid. It can be used to image in brain and breast tumors by recovering tissue's optical properties such as scattering and absorption coefficients using intensity-modulated light. A single source-detector pair can be used to recover absorption and scattering coefficients from a homogeneous tissues. However, for a heterogeneous tissue such as brain, skin or breast tissues, multiple source-detector pairs with different source-detector separations are necessary to recover all the unknown optical properties. As a result, the measurement system becomes complicated to design and analyze. A new approach using the interference of two photon density waves uses two intensity modulated sources to create different illumination patterns within the tissue is proposed. Instead of requiring multiple sources and detectors, this method only requires two sources with a varying relative phase between them and a single detector. For my poster, I am presenting the hardware prototype implementation of this method. The design includes two laser diodes with a wavelength of 658nm as sources, a single detector and a homogeneous tissue-mimicking phantom. RF components such as a phase shifter and attenuators were used to generate a relative phase shift between the two sources and therefore create different interference patterns. A Vector network analyzer was used to modulate the lasers. The designed prototype verifies the simulation results reported in previous work experimentally.

Surveying for E. coli contamination of Drinking Water Sources in Nepal

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Sewage contamination in ground drinking water sources is a developing issue. According to the World Health Organization, it is estimated that 2 billion people worldwide use drinking water contaminated with fecal matter. To enable people to test the quality of their water, tests that are inexpensive and simple to use need to be developed. Three simple tests that use E. coli as an indicator species for the presence of fecal contamination were used to test drinking water sources in Nepal: the Micrology Labs Coliscan EasyGel, the Micrology Labs Coliscan EasyCard, and the Saint Mary's College MicroBio PAD. Eighty-eight drinking water sources, collected using a convenience sampling technique, were tested from four different regions: Central (the Kathmandu Valley), Northern (Pokhara), South (Butwal to Bardia National Park), and Southwest (Bardia to the Western Border with India). In general, the tests showed higher levels of E.coli in the Kathmandu Valley (50%) and Pokhara region (100%), two densely populated cities that had mainly taps as groundwater sources, in comparison to the South (17%) and South West (19%) regions, two more rural regions that use mainly wells. Problems with the colorimetric sugar substrate, not observed in previous years, confounded the MicroBio PAD results. Comparison to a 2018 summer survey conducted in Nepal provided insights into changes that could make widespread random sampling more practical in the future.

Poster #60

A 3D Map is More Effective When Giving Directions Than a 2D Map

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The current study investigated coordination through language in a collaborative task. Pairs of participants communicated via hands free telephone. One participant, the director, had a floor plan map of a search environment consisting of hallways, classrooms, and offices. The map showed the locations of different colored boxes which were hidden in cupboards, drawers, on chairs, and under furniture. The director directed the other participant (searcher) to find the boxes and perform various tasks with them within a 20-minute time limit. Crucially, the directors' map was either 2D or 3D. We predicted better coordination with the 3D maps because they were a more reliable source of common ground. Consistent with the prediction, the average number of boxes whose task was completed was significantly higher in the 3D map condition than in the 2D condition.

Composition Effect in Bimetallic (FeNi)x-Phosphides for Cinnamaldehyde Hydrogenation

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Transition metal phosphide catalysts are promising hydrogenation catalysts. One way to improve the catalytic performance of metal phosphides is through addition of a second metal to form a bimetallic phosphide. As an example, a synergistic effect can be observed in FeNiP where a small addition of Fe, forming Fe0.03Ni1.97P2.00/SiO2, increased the heteroatom removal (i.e., S) selectivity by 40% compared to Ni2P1.60/SiO2 catalyst during hydroprocessing (Oyama and co-workers, J. Catal. 2012). FeNi phosphide specifically forms naturally as terrestrial and meteoric materials in different Fe:Ni:P ratios (Britvin and co-workers, Sci. Rep. 2015). In this study, we synthesized various (FeNi)xP catalysts (x=1, 2, and 3) to mimic the naturally occurring materials and compared their catalytic performance. Powder x-ray diffraction (XRD) was used to confirm the crystal structure of the materials. The bulk ratio of the element was quantified using inductively coupled plasma (ICP) – optical emission spectroscopy (OES). The catalysts were tested in a batch reactor at 125°C and 600 psig H2 for the hydrogenation of cinnamaldehyde, which is an α,β-unsaturated aldehyde that has two major hydrogenation pathways. The first pathway is hydrogenation of the C=C bond to form hydrocinnamaldehyde (HCAL); the second pathway occurs if the C=O bond is hydrogenated producing cinnamyl alcohol (COL). The latter requires interaction between the heteroatom (i.e., O) and the catalyst surface. Based on our initial assessment of the (FeNi)3P, the product selectivity was affected by the Fe and Ni ratio, but not significantly. The selectivity to HCAL measured at similar conversion in FexNi3-xP was found to be 99%, 89%, 83%, and 99% for x = 1.00, 1.33, 1.88, and 2.26 respectively. The preliminary result showed that as the bulk ratio becomes more homogeneous, the HCAL selectivity decreased while the COL selectivity increased for FexNi3-xP. This poster also explores the catalytic consequence of decreasing the total metal to P ratio and evaluates the optimum Fe to Ni ratio for cinnamaldehyde hydrogenation.

Synthesis Toward a Trigonal Pyramidal Sulfur Radical Supported by a Triarylborane Framework

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Sulfur has the ability to catenate forming a structure which is easily protonated and reduced. The energy involved in this conversion can be harvested to use in battery applications. Hypervalent sulfur can form radicals of unique electronic configuration. Often the radicals are not stable at ambient conditions, however radicals stabilized by a tridentate ligand have been reported as stable. We targeted a trigonal pyramidal sulfur radical, which is a currently unknown geometry. By changing the geometry, the electronics of the radical are altered. First an unprotected tert-butyl phenol was used to make a triaryl boron species, but the phenol was too reactive with n-BuLi when generating the boron species. When using a methoxy-methyl (MOM) protecting group, triaryl boron species was formed.

This synthesis uses a robust, but easier to remove protecting group like trimethyl silyl, and forms the boron-carbon bonds first. TMS protected phenols with a meta methyl group and para bromine are treated with a Grignard reagent and boron trifluoride etherate or boron trichloride to prepare the desired triarylborane.

Lost in Translation: Love, Sex, and Death in the Autobiography of Nikolai Berdyaev

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Nikolai Berdyaev is one of the most famous and controversial Russian philosophers of the 20th century and his writings about Christianity, Marxism, and metaphysics made a huge impact in the West. However, very little is available in English about his personal life and no new English translations of several of his major books have been made since the 1950s. This project focuses on Berdyaev final work: Samopoznanie (known in English as "Self-knowledge" or "Dream and Reality"), Berdyaev's autobiography in which he reveals the influence of his personal life on his philosophy. The translation used for this project is that of Katharine Lampert, originally published by Geoffrey Bles, Ltd in 1950 and reprinted by Semantron Press in 2009. An extensive online search suggests that this is the only available published English translation of Samopoznanie.

The passages chosen for this translation project focus on Berdyaev's personal life and his views on love, sex, and death--subjects that are often neglected in studies of Berdyaev. An entry from the diary of Berdyaev's wife, Lydia Berdyaev, is also included. My project reveals that the 1950 translation omits and edits passages that are of central importance to understanding Berdyaev's thoughts on love, sex, and death and also omits passages describing Berdyaev's personal relationships. These omissions and edits alter the English-speaking reader's understanding of Berdyaev's final words on the central themes of his philosophy and how his personal relationships and experiences affected his views, particularly those relating to love, sex, and death. An accurate translation of Berdyaev's autobiography, Samopoznanie, is required before further research can be done on Berdyaev's thought; this project is the first step in that direction.

Poster #64

Selma: Sisters and Saints

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The purpose of this study was to discover the nature of the involvement of Catholic laymen and clergy within the Selma campaign of the Civil Rights Movement, focusing on some of its most prominent figures, strategies, and the reasons for their involvement. Through this research it can be shown that without the help and support of the Catholic Church, both in grassroots movements and major campaigns, the attainment of civil rights and the passing of major legislation benefitting African Americans would have looked much different and had less diversity of religious figures involved. Using research from original materials in the University of Notre Dame's archives from Catholics who were involved in the Selma voting rights campaign and the march to Montgomery, these documents and materials give a larger perspective of the people involved and sheds light on those who have been overlooked in past studies. Most notably involved in the Selma campaign was Sister Mary Benet, which this research focuses on. She herself was from the University of Notre Dame and answered the call of clergy already in Selma to march and work alongside those in the South facing severe persecution. She serves as an excellent representative of Catholic participation alongside Viola Liuzzo, a Roman Catholic mother who gave her life for the cause. Sister Benet's testimonies and experiences that are recorded in the archives are invaluable to this research project and the subject of Catholic involvement as a whole. This study will illuminate further the involvement of Catholics, and particularly Catholic women, in the Civil Rights Movement and act as a guide for further information involving Catholic involvement during the movement.

Advanced Wireless Communications for Drone Swarms

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There is a growing demand for drone swarms, given that they have a wide variety of applications, including search and rescue, surveillance, military operations, and scientific data collection. This increased interest in drone swarms has pushed technical challenges such as collision avoidance and drone communications over wireless links to the forefront of drone-related research. Currently, the platform for drone communication is to have drones receive commands from and send their data to a ground control station, thus requiring one unique telemetry dongle per one drone. Therefore, the number of drones is limited by the number of server USB ports.

However, this project seeks to change the way drones communicate by having them communicate to each other, thereby making drone swarm communications more efficient. My work focuses on implementing a distributed detect-and-avoid protocol called Position Intent Broadcast System, or PIBS, that was created in collaboration with Interdigital. In order to do this, I have worked on getting PIBS, which is run on a Raspberry Pi, to pull GPS directly from a SITL (Software in the Loop) drone.

RadioHound: A low cost spectrum sensor

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Spectrum sensing is the process of periodically monitoring a specific frequency band, aiming to identify presence or absence of primary users. The RadioHound spectrum sensor is able to tune into a wide range of frequencies that are used by radios, WiFi, television, and cellular devices. For the sensors to output information pertaining to network activity, wireless network packets must be decoded. Our team has created a MATLAB code that will interpret WiFi network packets, decode them, and provide the output in a PCAP file. The issue with our written code is that it cannot run natively on the RadioHound device because of its dependence on Matlab. Our goal is to be able to tune to a 20 MHz bandwidth signal with the RadioHound device, and demodulate any WiFi signal contained therein. To accomplish this, I am translating the Matlab code to Python, which can run natively on the RadioHound device. Once the Python code is completed, we will be able to identify and demodulate WiFi data readily.

Poster #67

Parallelization of NLP Applications for Genocide Prediction

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The Kellogg Institute for International Studies hopes to one day predict mass killings and genocide events by means of looking for specific triggering events within large amounts of news articles. With the help of the Center for Research Computing, through the power of computation and the knowledge from the social sciences, a software pipeline named SONNET is being developed, with Natural Language Processing (NLP) techniques, to help predict when a state sponsored mass killing or genocide event will occur based off the finding of smaller triggering events that have had significant influence of decision making for a country. The computing power needed to pass thousands and perhaps millions of articles is too great for an ordinary computer to handle. High Performance Computing (HPC) and parallelization are needed to help facilitate this need. With HPC the number of articles that can be passed through the SONNET software can be drastically increased without the repercussions of a limited computing architecture. Having SONNET running on parallel allows for more news articles to be processed with multiple triggering events being searched for within one country. The aim, and hope, of the project is to predict mass killings and genocides before such events occur for any country in the world.

Ionothermal Synthesis of Actinide-Based Metal Organic Frameworks and Clusters

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Nuclear chemistry applications for nuclear waste management demand a deep understanding of the behavior and chemistry of the actinides elements. In this research, uranium (VI) compounds (uranyl nitrate and uranyl acetate) were used as starting materials to form clusters, chains, and metal organic frameworks (MOFs) with commercially available organic ligands such as bipyridine, 4,4'-dicarboxyphenyl ether, and trimesic acid. Several ionic liquids were also employed for the ionothermal synthesis of actinides-based materials having a special interest in 1-ethyl-3-methylimidazolium chloride, 1-ethyl-3-methylimidazolium ethyl sulfate, and 1-ethyl-3-methylimidazolium tosylate. Ionic liquids are novel compounds with the ability of acting as both the solvent and templating agent when used in hydrothermal conditions. Different templates, such as 1,4-diazabicyclo [2.2.2] octane and Pluronic F127 were tested by the process. Likewise, different ratios and thermodynamic conditions were examined in order to optimized the synthesis methods. The resulting clusters and MOFs obtained were characterized by X-ray diffraction techniques (single crystal, powder, and small angle) and spectroscopy techniques (Raman, NMR, and mass spectroscopy). Future work includes the transition from uranium chemistry to neptunium chemistry due to the similarities between their properties.

Experimental and Computational Insights on Ethylene Oligomerization by Oxide-Supported Group 4 Metal Hydrides

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The goal of our research is to effectively convert the short-chain hydrocarbons found in shale formations into longer, more useful hydrocarbon chains. Precisely, we aim to oligomerize ethene (C_2H_4) into longer hydrocarbons like butene (C_4H_8), hexene (C_6H_{12}) and upto fuel range molecules. We are developing group 4 transition metals [M(IV) = Ti, Zr, Hf] supported on oxide supports like silica-alumina as oligomerization catalysts. To understand the reaction chemistry and the catalyst we have utilized both computational and experimental tools. Computations are performed in WebMO to find the ground state energies of metal hydride (MH_4, $MH(OH)_3$), ethene, and butene. Combined with vibrational frequency computations of these species we calculated the change in entropy, enthalpy and Gibbs free energy for oligomerization of ethene to butene. The overall reaction is exothermic with the change in gibbs free energy at 300K and 1 atm being negative. The computed M-H bond vibration lies within experimental range of 1750-1600 ± 50 cm^{-1} for Ti, Zr and Hf. Experimentally, we synthesize the catalyst by reacting tetrabenzylzirconium with partially dehydroxylated silica-alumina in benzene, followed by filtration, drying and hydrogen gas pre-treatment. To characterize the catalyst, we performed FTIR experiments on the catalyst. At first, we did hydrogen pre-treatment, followed by nitrogen purge both at approximately 150°C for about 1.5 hours, took the background scans in 30-150°C range, then saturated the sample with ethene at 30°C for 20 minutes. The background scans were obtained upon heating the sample as we expected to observe the hydrides and new bonds being formed. In the second experiment we did performed similar sample treatment steps, and the saturation gas was CO_2. We made toluene calibration curve using the incipient wet impregnation method and mass-spectrometry to quantify the toluene amount during hydrogen pretreatment of the catalysts. Conclusively, experimental and computational insights are vital for catalyst characterization, determining optimal reaction conditions and understanding the role of catalyst in ethylene oligomerization.

What Predicts Math Attitudes? Examining Associations with Demographic Characteristics and Personality Traits as Predictors

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Prior research has established that certain demographic factors are associated with students' attitudes toward mathematics, including race/ethnicity, biological sex, and socioeconomic status (Johns & Martens, 2005; Namkung & Peng 2019; Osborne 2001). Past research has also identified a close association between neuroticism (i.e. the extent to which a person is predisposed to experiencing negative emotion) and math attitudes, while, perhaps surprisingly, the strength of the association between conscientiousness (i.e. the extent to which a person tends to be thorough, hard-working, and efficient) and math attitudes has been questioned (Chew & Dillon 2013). In order to further understand the associations of these traits and attitudes with mathematics, we surveyed a sample of 134 AP Statistics students (mean age = 16.92, SD = 0.92, 56% female), administering the Big Five Inventory (BFI-2; Soto & John, 2016), a hierarchical model of personality that includes measures of conscientiousness and neuroticism, as well as a modified version of the Attitudes Toward Math inventory (ATMI; Lim & Chapman, 2013). We then conducted hierarchical, multi-regression analyses with blockwise entry of variables to examine the relation of race, sex, socioeconomic status (parents' level of education was used as a proxy), as well as neuroticism and conscientiousness to math attitudes. We hypothesized that after accounting for the demographic variables in block 1, neuroticism (entered in block 2) would account for significant variation in math attitudes. We further hypothesized that conscientiousness (entered in block 3) would account for significant variation in math attitudes.

The first block of the model incorporated just demographic variables – race, sex, and socioeconomic status. The second block added neuroticism as a variable, and the third added conscientiousness. Adjusted R2 increased with each progressive stage of variable entry (see Table 1). The effect of neuroticism on math attitudes was found to be statistically significant at both block 2 and 3 ($p < .001$), as was the effect of conscientiousness in block 3 ($p < .05$). These findings suggest that even when controlling for variables such as race/ethnicity, biological sex, and socioeconomic status, neuroticism still accounts for a significant amount of variation in math attitudes, as does conscientiousness even above and beyond the other variables. Further research using samples of students of different ages is needed in order to more fully parse the link between demographic factors, personality traits, and attitudes toward math.

Table 1
Multiple regression with math attitudes as an outcome measure (N = 134)

Variable	*Standard Estimate (β)*	*Std. Error*	*t*	*p*	R^2_{Ad} (ΔR^2_{Ad})
Block 1					.07
Intercept	7.16	1.6	4.48	0	
Sex (Female=0)	0.36	0.13	2.72	0.01	
Parental Education	0.18	0.14	1.29	0.2	
Race/Ethnicity					
Asian or Asian American	-1.31	0.53	-2.5	0.01	
African American	-1.49	0.57	-2.61	0.01	
Hispanic or Latino	-1.01	0.61	-1.66	0.1	
Native Hawaiian	-1.27	0.52	-2.43	0.02	
Block 2					.15 (.08)
Intercept	7.09	1.52	4.66	0	
Sex (Female=0)	0.18	0.14	1.28	0.2	
Parental Education	0.18	0.13	1.34	0.18	
Race/Ethnicity					
Asian or Asian American	-1.32	0.5	-2.63	0.01	
African American	-1.37	0.55	-2.5	0.01	
Hispanic or Latino	-1.01	0.58	-1.74	0.08	
Native Hawaiian	-1.19	0.5	-2.38	0.02	
Neuroticism	-0.23	0.07	-3.45	0	
Block 3					.17 (.02)
Intercept	6.99	1.51	4.64	0	
Sex (Female=0)	0.25	0.14	1.77	0.08	
Parental Education	0.21	0.13	1.56	0.12	
Race/Ethnicity					
Asian or Asian American	-1.32	0.5	-2.66	0.01	
African American	-1.34	0.54	-2.47	0.01	
Hispanic or Latino	-0.98	0.57	-1.71	0.09	
Native Hawaiian	-1.19	0.49	-2.41	0.02	
Neuroticism	-0.17	0.07	-2.47	0.01	
Conscientiousness	0.13	0.07	1.89	0.06	

Persistence of Work Orientation in Adolescents with ADHD: A Regression Analysis

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It is theorized that deficits in work orientation are an underlying feature of attention-deficit/hyperactivity disorder (ADHD). However, there is heterogeneity in the population and, while typical symptoms of ADHD may contribute to lack of work orientation, it is unclear what factors are likely to influence work orientation beyond ADHD symptoms. The goal of the current study was to examine relations between adolescent adjustment, dimensions of parenting, and adolescent work orientation. One-hundred seven mother-adolescent dyads participated in this study. Adolescents were previously diagnosed with ADHD. Mothers provided ratings of adolescent inattentive and hyperactive/ impulsive symptoms and adolescent internalizing and externalizing behaviors. Adolescents completed IQ assessment and provided ratings of their mothers' parenting behavior and their own work orientation. Hierarchical regression analysis examined the relative contribution of ADHD symptoms, internalizing and externalizing behaviors, and mothers' parenting to the prediction of adolescent work orientation. Mothers' positive parenting and involvement accounted for unique variance in work orientation over and above adolescent ADHD symptoms and internalizing and externalizing behaviors. These relations persisted after demographic variables were controlled.

Developing a Protocol for the Post-Assembly Functionalization of Chemically-Tailored Copolymer Membranes

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Membrane technology offers an efficient alternative to traditional energy-intensive, thermally driven chemical separations. With a global trend shifting towards energy efficiency and environmentally friendly commercial processes, membrane technology has been adapted for a wide variety of applications, including those in the water purification, pharmaceutical and biofuel industries. Typical commercially relied upon membranes; however, suffer from a few key downfalls. Most commercial membranes rely solely on size selective filtration, which in turn results in membranes with a low permeability that are only fit for very specific separations. Membranes derived from the self-assembly of copolymers offer an attractive alternative to traditional membranes, as they exhibit a unique surface chemistry that can easily be tailored to a wide variety of applications without sacrificing the permeability of the membrane. This work focuses specifically on casting copolymer membranes in the hollow fiber geometry that can be tailored to remove specific ionic solutes from solution. In this study, a poly (trifluoroethanol methacrylate -r-oligo (ethylene glycol) methyl ether methacrylate-r-glycidyl methacrylate) (P(TFEMA-r-OEGMA-r-GMA) copolymer was cast onto the surface of a commercially available hollow fibre membrane. The epoxide rings of the GMA moiety that line the surface of the copolymer membrane allow for a positively charged amine group to be introduced to the surface of the membrane. This now functionalized membrane exhibits a positive charge that can be used to repel dissolved cationic solutes, while still allowing much larger, neutrally charged molecules to pass through the membrane. The functionalization of these membranes was achieved by soaking the copolymer membranes in a solution containing either hexamethylenediamine or imidazole. The membranes functionalized using hexamethylenediamine have a permeability of 15 LMH/Bar and show up to 89% rejection of a 1mM Calcium Chloride feed solution. The membranes functionalized using imidazole are currently under study and quantitative results will be available at the time of the symposium. The performance of the functionalized membranes at varying pH and in the presence of chlorine and a number of other ionic solutes was evaluated.

Modular Assembly of Nanosystems Using Light Gradients

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The use of light gradient forces to manipulate and organize nanometer-scale matter is a radically new strategy for manufacturing nanosystems. Light gradient forces are developed by focusing a laser using a high numerical aperture objective lens on a small (nanometer-diameter) particle. Although the force is weak (< 100 pN), nanometer-scale objects have a miniscule mass so that light gradients can be effective for manipulation with nanometer-scale precision over a wide field. Ostensibly, using light gradient forces produced by a tightly focused, one-dimensional (1D) standing wave optical trap (SWOT), time-multiplexed across a two-dimensional (2D) lattice in the focal plane, a voxel consisting of pre-fabricated, monodispersed nanoparticles (NPs) could be assembled into a 3D-structure on a hydrogel scaffold. Thousands of NPs could be manipulated concurrently into a complex heterogeneous voxel this way, and then the process can be repeated to stitch together voxels, registered to one another, to form nanosystems of any size, shape and constituency.

We have been exploring the prospects for using light gradients to assemble a heterogeneous collection of NPs into three-dimensional (3D) photonic metamaterials (PM). PMs are difficult to manufacture because they demand nanometer-scale precision, yet they offer extraordinary physical properties for steering light, such as a negative index of refraction, that are useful for applications such as a superlens that works beyond the diffraction limit. A PM relies on sub-wavelength inclusions that resonantly couple to the electric and magnetic fields of light. A NP that is much smaller than the incident light behaves as an electric dipole and the scattering from it can be controlled by the size. Recently it has become apparent that PMs can be formed from purely dielectric NPs by leveraging Mie scattering resonances to produce negative magnetic permeabilities and electric permittivities. The first Mie scattering resonance, which occurs near d nNP/lambda =(m+1)/2, where nNP is the refractive index, d is the diameter of the NP, and lambda denotes the free-space wavelength, when m = 1, is a magnetic dipole mode; the second (m = 2) is an electric dipole resonance. So, to work in the visible, the diameter of the NP must be d < 500 nm, depending on the index; typically, lambda/d >10.

In this report, we describe our efforts using time-multiplexed Gaussian beam, SWOT to assemble NPs ranging in size from 100 nm to 500 nm in radius into regular 1D, 2D and 3D arrays. NPs were first shepherded into a voxel using a combination of multiple, independent computer-controlled optical traps in a microfluidic device and then encapsulated in a hydrogel scaffold formed by photo-polymerizing 400 Da polyethylene

glycol diacrylate (PEGDA). Subsequently, fluorescence confocal microscopy was used to interrogate the heterogeneous lattices consisting of nominally (red fluorescent) 100 nm- and (green fluorescent) 175 nm- and (red fluorescent) 500-nm-radius NPs. The size and positions of the NPs were inferred from the fluorescence after iterative de-convolution, which was used to recover a true representation of an image blurred by diffraction and aberrations or compromised by noise.

Magneto-silica nanoparticles (MagSiNs) for combinatorial chemotherapeutics and gene delivery against metastatic cancers

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Cancer research has been at the forefront of cutting edge therapeutics discovery in recent decades. With the development of new therapeutic agents for treating metastatic cancers, cancer research has decreased cancer morbidity rates. However, systemic cancer treatments such as chemotherapy have proven to remain very dangerous and toxic on the body, because they kill indiscriminately rapidly dividing cancer cells as well as normal cells. Chemotherapeutics have led to poor quality of patient life during treatment and longer patient recovery times post-treatment. Hence, there is a need for a chemotherapeutics delivery system that will selectively target only cancer cells. Recent research has discovered the difference in membrane permeability between normal and cancer cells, finding that cancer cells have a much more permeable membrane than normal, healthy cells. We intend to use this knowledge of cell permeability in this project to target cancer cells by fine-tuning a magnetic field induced force exerted by the magnetic nanocarriers to selectively permeate cancer cells and not the membranes of the stiffer, healthy cells. This project, therefore, seeks to combine the use of magneto-silica nanoparticles (MagSiNs) with a fluorescent payload to mimic selective chemotherapeutics delivery to metastatic cancer cells. Stable liposomes were synthesized with a fluorescent cell-impermeant payload. We 'CLICK'ed MagSiNs tagged with a Rhodamine Isothiocyanate (RITC) fluorophore to the surface of the liposomes to create a label-free magnetic nanocarrier system. In vitro studies were performed to look at the difference in the efficiency of payload delivery in different cancer cells with and without a magnetic force applied at the cell membrane.

Modeling Migration on a Global Scale

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Human migration is becoming more and more popular, which can largely affect the GDP of one country, and at the same time, the individuals including migrants and original citizens. We updated and validated the global scale migration model by evaluating the economic opportunities using Python.

In our model, we need to determine whether the expected earnings in destination minus the cost of migration outweigh the earnings in origin. These costs are composed of explicit monetary costs of travel and visas, and the implicit costs such as political barriers, the difficulty in learning a new language, and also the migration history between two countries so as to figure out the relationship between these two. We replaced the passport index, one of the factors of political barrier, with visa index data based on historical visa issuances and the monetary costs of obtaining an immigration or permanent residence visa of each country. Certain countries have relatively high salary to people with low skill level, which can largely affect the number of immigrants within those people.

Our concentration is on population change from 2015 to 2017 based on UN migration stock, and then compare it with the result derived from the model to see whether we made a solid prediction. Changing weights for different variables helped us to observe more consequences and figure out some specific important factors.

Future studies of comparing the real world population change and the predicted result after integrating the net migration derived from each continuous skill level are needed.

Sentiment Analysis on Global News

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Journalism and reporting should aim to be unbiased and fair. The Journalist's Creed, a declaration of the principles, values, and standards of a journalist, states that a journalist should "believe that clear thinking and clear statement, accuracy and fairness are fundamental to good journalism." However, in recent years there has been growing concern that personal, corporate, and government biases and opinions have had an effect on the fairness and integrity of modern journalism. Many mainstream media outlets are well known to have certain political inclinations and instances of "fake news" have become significantly more common. While many studies have been conducted on this phenomenon, most have focused on solely U.S. news sources. Studying international media and how foreign news sources report is important for a variety of reasons, including national security, cultural stability, and social/economic policy. Because of these concerns and the lack of studies performed on the topic of international media bias, our study investigates the state of global journalism. Through the use of modern natural language processing techniques, we performed sentiment analysis on 10,981 articles published by ten globally distributed sources covering eleven globally impactful events, spanning a period of eleven years. In order to alleviate our concern that any one sentiment analysis tool and text processing approach will introduce bias in our results, we tested four tools, including three open source libraries and one from Microsoft which has been commercialized for many years. We also tested three text processing approaches, i.e. sentence-based approach, paragraph-based approach and article-based approach, in our research. After obtaining results, we observed that, every news publisher holds a different view towards each event, instead of unquestioningly treating all events as negative or positive. In addition, for most events, overall sentiment polarity was, in general, consistent across all publishers, but absolute sentiment scores still differed among publishers for some events.

Modeling migration on a global scale

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Human migration affects global economies, regional stability and the lives of many people but preexisting migration models of some regions do not adequately capture contemporary intensities and patterns of global migration flows. We update the global scale migration model based on neoclassical economic migration theory and modified Python code on Jupyter Notebook which is the base modeling platform.

Our goals focus on optimizing the variables of cost and comparing the predictions against real world migration data. This will enhance the reliability of the model and improve social scientist' access to patterns of global migration visually and computationally.

We use visa index based on the latest data on visa issuances of 127 countries and the monetary cost of obtaining a permanent residence visa to study how Political Barrier affect agents' decisions to migrate. The actual migration data used for validation is from UN migration stock and we also use it to evaluate the effect of each factor on the result of the model.

The results show that the predictions of most countries are with one standard deviation but large GDP countries such as China, the USA , Germany and Japan, we are overpredicting the migrant stock.

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